Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 – 10:29 AM EDT

PDB ID	:	7JRI
Title	:	High-resolution Crystal Structures of Transient Intermediates in the Phytochrome Photocycle, 33 ms structure
Authors	:	Schmidt, M.; Stojkovic, E.
Deposited on	:	2020-08-12
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

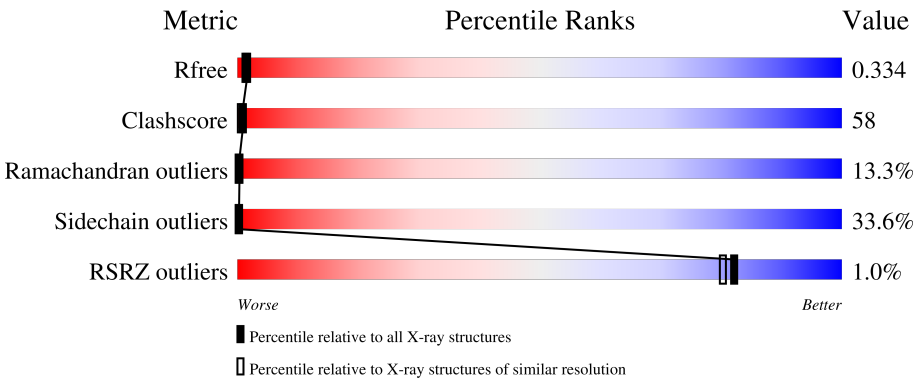
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

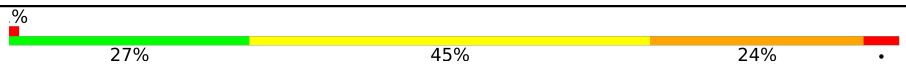
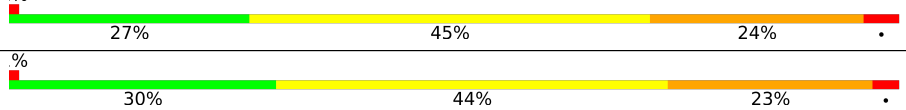
The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	482	
1	B	482	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3Q8	A	500[A]	-	-	X	-
2	3Q8	A	500[B]	-	-	X	-
2	3Q8	B	602[A]	-	-	X	-
2	3Q8	B	602[B]	-	-	X	-
3	BEN	B	601	-	-	-	X

2 Entry composition (i)

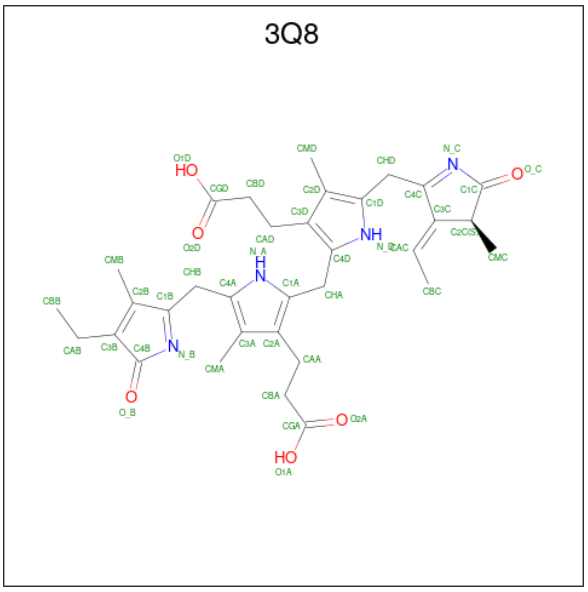
There are 4 unique types of molecules in this entry. The entry contains 7653 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photoreceptor-histidine kinase BphP.

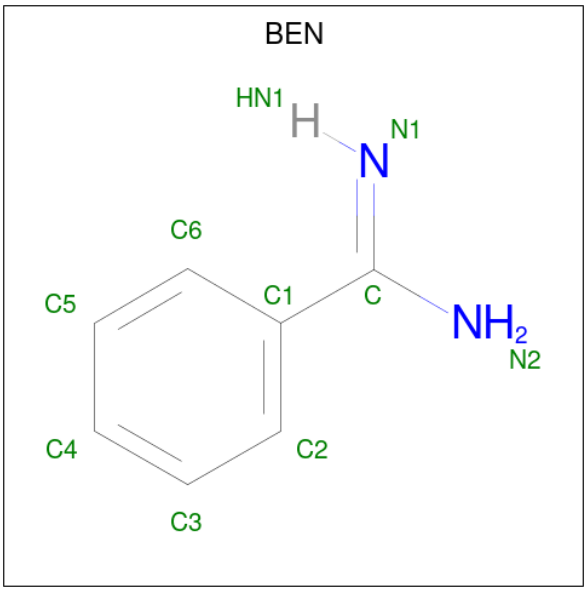
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	482	3696	2342	673	670	11	0	4	0
1	B	482	3677	2330	668	668	11	0	2	0

- Molecule 2 is 3-[2-[[5-[[(3E,4S)-3-ethylidene-4-methyl-5-oxidanylidene-pyrrol-2-yl]methyl]-3-(3-hydroxy-3-oxopropyl)-4-methyl-1H-pyrrol-2-yl]methyl]-5-[(4-ethyl-3-methyl-5-oxidanylidene-pyrrol-2-yl)methyl]-4-methyl-1H-pyrrol-3-yl]propanoic acid (three-letter code: 3Q8) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	86	66	8	12	0	1
2	B	1	86	66	8	12	0	1

- Molecule 3 is BENZAMIDINE (three-letter code: BEN) (formula: $C_7H_8N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N 9 7 2	0	0

- Molecule 4 is water.

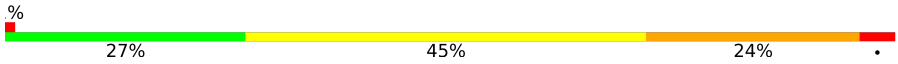
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	56	Total O 56 56	0	0
4	B	43	Total O 43 43	0	0

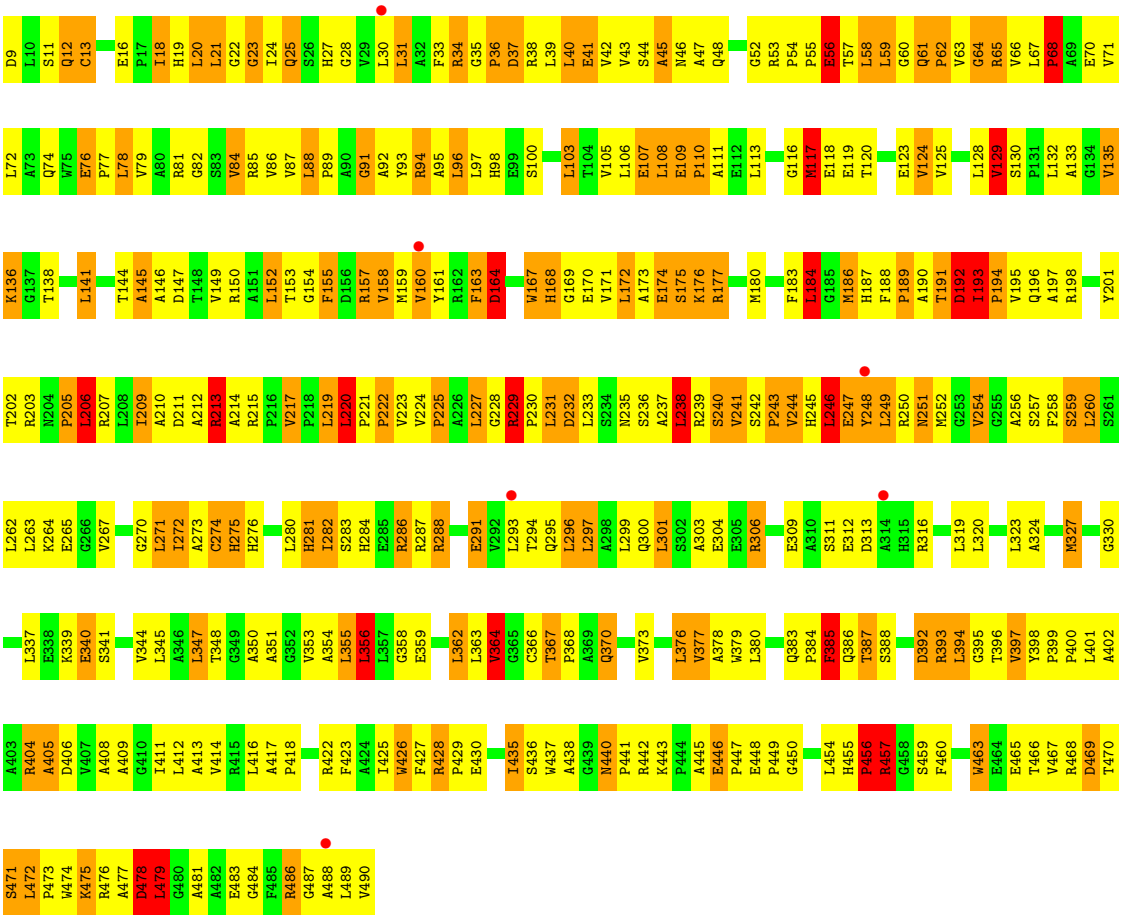
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Photoreceptor-histidine kinase BphP

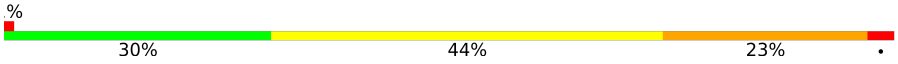
Chain A:

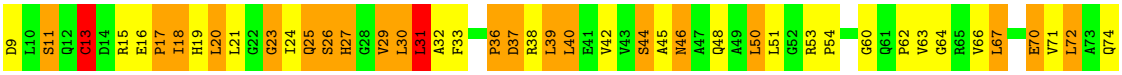


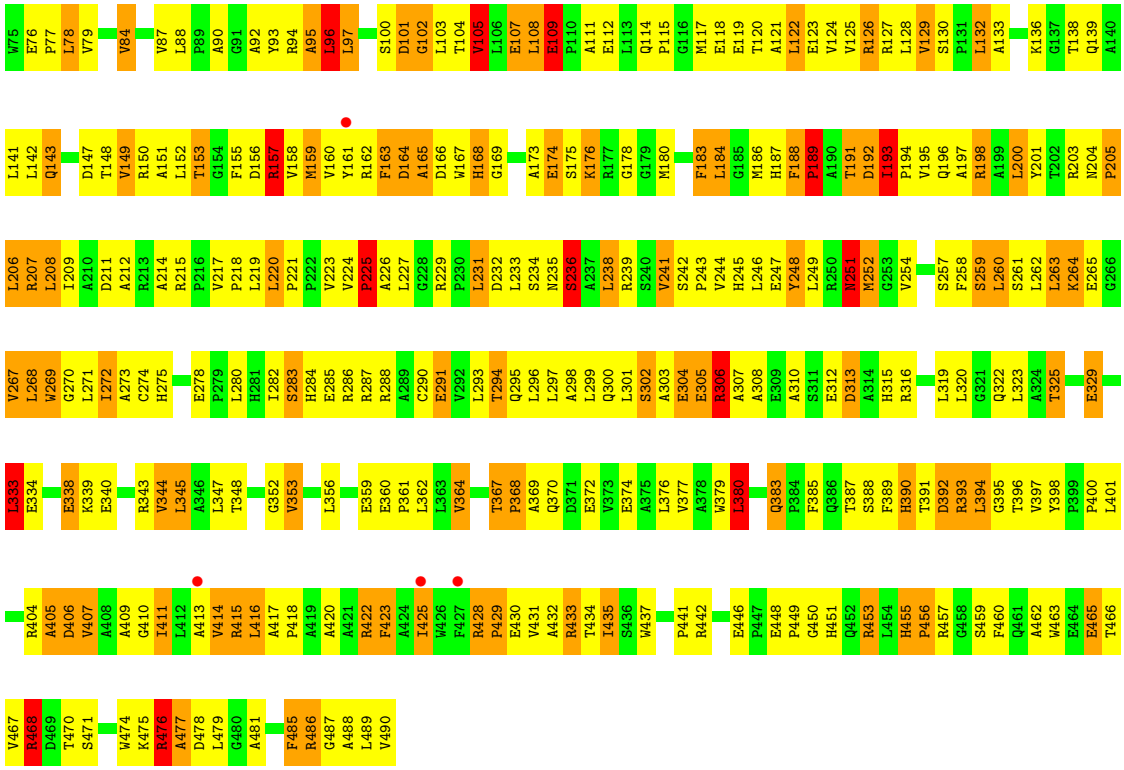


• Molecule 1: Photoreceptor-histidine kinase BphP

Chain B:






W75 E76 P77 L78 V79 V84 V87 L88 P89 A90 G91 A92 Y93 R94 A95 L96 L97 S100 D101 G102 L103 T104 V105 L106 E107 L108 E109 P110 A111 E112 L113 Q114 P115 G116 M117 E118 E119 T120 A121 L122 E123 V124 V125 R126 R127 L128 V129 S130 P131 L132 A133 K136 G137 T138 Q139 A140
L141 L142 Q143 D147 T148 V149 R150 A151 L152 T153 G154 F155 D156 R157 V158 M159 V160 Y161 R162 F163 D164 A165 D166 W167 H168 G169 A173 E174 S175 K176 R177 G178 G179 M180 F183 L184 G185 M186 H187 F188 P189 A190 T191 D192 I193 P194 V195 Q196 A197 R198 A199 L200 Y201 T202 R203 N204 P205
L206 R207 L208 I209 A210 D211 A212 R213 A214 R215 P216 V217 P218 L219 L220 P221 P222 V223 V224 P225 A226 L227 G228 R229 P230 L231 D232 L233 S234 N235 S236 A237 L238 R239 S240 V241 S242 P243 V244 H245 L246 E247 Y248 L249 R250 N251 M252 G253 V254 S257 F258 S259 L260 S261 L262 L263 K264 E265 G266
V267 L268 W269 G270 L271 I272 A273 C274 H275 E278 P279 L280 H281 I282 S283 H284 E285 R286 R287 R288 A289 C290 E291 V292 L293 T294 Q295 L296 L297 A298 L299 Q300 L301 S302 A303 E304 E305 R306 A307 A308 E309 A310 S311 E312 D313 A314 H315 R316 L319 L320 G321 Q322 L323 A324 T325 E329
L333 E334 E338 K339 E340 R343 V344 L345 A346 L347 T348 G352 V353 L356 E359 E360 P361 L362 L363 V364 T367 P368 A369 Q370 D371 E372 V373 E374 A375 L376 V377 A378 W379 L380 Q383 P384 F385 Q386 T387 S388 F389 H390 T391 D392 R393 L394 G395 T396 V397 Y398 P399 P400 L401
R404 A405 D406 V407 A408 A409 G410 T411 L412 A413 V414 R415 L416 A417 P418 A419 A420 A421 R422 F423 A424 I425 W426 F427 R428 P429 E430 V431 A432 R433 T434 T435 S436 W437 P441 R442 E446 P447 E448 P449 G450 H451 Q452 R453 L454 H455 P456 R457 G458 S459 F460 Q461 A462 W463 E464 E465 T466
V467 R468 D469 T470 S471 W474 K475 R476 A477 D478 L479 G480 A481 F485 R486 G487 A488 L489 V490

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.69Å 83.40Å 86.87Å 90.00° 107.63° 90.00°	Depositor
Resolution (Å)	24.33 – 2.40 24.33 – 2.40	Depositor EDS
% Data completeness (in resolution range)	85.5 (24.33-2.40) 85.6 (24.33-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.02 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.292 , 0.333 0.293 , 0.334	Depositor DCC
R_{free} test set	1792 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7653	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 3Q8, BEN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.84	4/3782 (0.1%)	1.11	4/5157 (0.1%)
1	B	1.06	5/3757 (0.1%)	1.09	8/5121 (0.2%)
All	All	0.96	9/7539 (0.1%)	1.10	12/10278 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	6
All	All	0	15

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	13[A]	CYS	CB-SG	-30.90	1.29	1.82
1	B	13[B]	CYS	CB-SG	-30.90	1.29	1.82
1	A	13[A]	CYS	CB-SG	-15.08	1.56	1.82
1	A	13[B]	CYS	CB-SG	-15.08	1.56	1.82
1	A	107	GLU	CD-OE2	-8.28	1.16	1.25
1	A	107	GLU	CD-OE1	-8.08	1.16	1.25
1	B	109	GLU	CD-OE2	-5.32	1.19	1.25
1	B	304	GLU	CD-OE1	-5.23	1.19	1.25
1	B	109	GLU	CD-OE1	-5.11	1.20	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	13[A]	CYS	N-CA-CB	-8.53	95.25	110.60
1	B	13[B]	CYS	N-CA-CB	-8.53	95.25	110.60
1	A	222	PRO	N-CA-CB	-6.86	95.05	102.60
1	B	306	ARG	CG-CD-NE	5.88	124.14	111.80
1	B	465	GLU	CB-CA-C	5.74	121.88	110.40
1	B	306	ARG	C-N-CA	5.60	135.70	121.70
1	B	305	GLU	CB-CA-C	5.56	121.52	110.40
1	A	68	PRO	N-CA-CB	-5.36	96.71	102.60
1	B	415	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	456	PRO	N-CA-CB	-5.16	96.93	102.60
1	A	68	PRO	N-CA-C	5.10	125.35	112.10
1	B	453	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ALA	Peptide
1	A	135	VAL	Peptide
1	A	186	MET	Peptide
1	A	220	LEU	Peptide
1	A	330	GLY	Peptide
1	A	404	ARG	Peptide
1	A	416	LEU	Peptide
1	A	478	ASP	Peptide
1	A	64	GLY	Peptide
1	B	109	GLU	Peptide
1	B	17	PRO	Peptide
1	B	208	LEU	Peptide
1	B	23	GLY	Peptide
1	B	251	ASN	Peptide
1	B	88	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3696	0	3726	451	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3677	0	3707	385	2
2	A	86	0	68	49	0
2	B	86	0	68	48	0
3	B	9	0	8	0	0
4	A	56	0	0	16	0
4	B	43	0	0	15	1
All	All	7653	0	7577	873	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 58.

All (873) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ARG:NH1	4:A:601:HOH:O	1.58	1.25
2:A:500[B]:3Q8:C3A	2:A:500[B]:3Q8:H1	1.68	1.22
2:A:500[A]:3Q8:O2A	2:A:500[A]:3Q8:C3A	1.89	1.21
1:B:245:HIS:NE2	2:B:602[B]:3Q8:H15	1.59	1.18
2:A:500[B]:3Q8:H1	2:A:500[B]:3Q8:C4A	1.72	1.17
2:B:602[A]:3Q8:H18	2:B:602[A]:3Q8:H12	1.22	1.15
1:A:87:VAL:HA	1:A:92:ALA:HB1	1.25	1.11
1:B:385:PHE:O	1:B:415:ARG:NH1	1.85	1.10
1:A:299:LEU:HD11	1:B:300:GLN:HE21	0.99	1.10
1:B:16:GLU:O	1:B:196:GLN:NE2	1.84	1.09
1:A:238:LEU:HD22	1:A:238:LEU:O	1.49	1.09
2:A:500[B]:3Q8:C3A	2:A:500[B]:3Q8:CMB	2.31	1.07
1:A:232:ASP:O	4:A:602:HOH:O	1.74	1.03
2:A:500[A]:3Q8:H26	2:A:500[A]:3Q8:CHA	1.88	1.03
1:B:304:GLU:OE2	4:B:702:HOH:O	1.76	1.03
1:B:448:GLU:OE1	1:B:455:HIS:CE1	2.11	1.02
2:A:500[A]:3Q8:O2A	2:A:500[A]:3Q8:C2A	2.08	1.02
1:B:197:ALA:O	1:B:201:TYR:CE2	2.13	1.01
2:A:500[B]:3Q8:H26	2:A:500[B]:3Q8:CHA	1.89	1.01
2:B:602[A]:3Q8:CMB	2:B:602[A]:3Q8:H13	1.90	1.00
1:B:197:ALA:O	1:B:201:TYR:CD2	2.15	1.00
2:A:500[B]:3Q8:CMB	2:A:500[B]:3Q8:H14	1.92	0.99
1:A:95:ALA:HB2	1:A:108:LEU:HD22	1.45	0.98
2:A:500[B]:3Q8:H14	2:A:500[B]:3Q8:H2	1.44	0.97
1:B:246:LEU:C	1:B:247:GLU:N	2.18	0.97
1:A:378:ALA:O	4:A:603:HOH:O	1.83	0.96
1:B:16:GLU:O	1:B:196:GLN:CD	2.04	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:602[B]:3Q8:H34	2:B:602[B]:3Q8:CBC	1.95	0.96
2:B:602[A]:3Q8:H13	2:B:602[A]:3Q8:C2B	1.95	0.96
1:A:299:LEU:CD1	1:B:300:GLN:HE21	1.78	0.96
1:A:152:LEU:O	1:A:286:ARG:NH1	1.99	0.95
2:A:500[A]:3Q8:H25	2:A:500[A]:3Q8:H15	1.46	0.94
1:A:248[A]:TYR:HB2	1:A:456:PRO:HG2	1.47	0.94
1:B:248[A]:TYR:CG	1:B:248[A]:TYR:O	2.21	0.94
1:A:248[A]:TYR:HB2	1:A:456:PRO:CG	1.98	0.93
1:A:299:LEU:HD11	1:B:300:GLN:NE2	1.83	0.93
2:B:602[A]:3Q8:H13	2:B:602[A]:3Q8:H3	1.49	0.93
1:A:353:VAL:HG12	1:A:426:TRP:CD1	2.04	0.93
2:A:500[B]:3Q8:CMB	2:A:500[B]:3Q8:CMA	2.48	0.92
1:A:45:ALA:O	1:A:47:ALA:N	2.03	0.90
1:B:248[A]:TYR:OH	2:B:602[A]:3Q8:H9	1.70	0.90
1:B:46:ASN:HB3	1:B:217:VAL:HG21	1.53	0.89
1:B:16:GLU:O	1:B:196:GLN:OE1	1.91	0.89
1:A:299:LEU:HD21	1:B:300:GLN:NE2	1.87	0.88
1:A:186:MET:CG	1:A:438:ALA:HB2	2.04	0.88
2:A:500[B]:3Q8:H2	2:A:500[B]:3Q8:CMA	2.03	0.87
1:A:88:LEU:HB2	1:A:89:PRO:CD	2.05	0.87
1:A:18:ILE:HD13	1:A:18:ILE:O	1.75	0.86
1:B:198:ARG:HB2	1:B:268:LEU:HD22	1.54	0.86
1:A:244:VAL:HA	1:A:247:GLU:HB2	1.57	0.86
1:A:248[B]:TYR:HB3	1:A:456:PRO:CG	2.06	0.85
1:B:446:GLU:HB3	1:B:455:HIS:HB2	1.57	0.85
1:B:394:LEU:HB2	1:B:409:ALA:HA	1.58	0.85
1:A:355:LEU:O	1:A:356:LEU:HB2	1.77	0.84
1:B:235:ASN:O	1:B:236:SER:O	1.95	0.84
1:B:385:PHE:HB2	1:B:388:SER:O	1.76	0.84
2:A:500[B]:3Q8:H14	2:A:500[B]:3Q8:C2B	2.06	0.84
1:A:248[B]:TYR:CG	1:A:248[B]:TYR:O	2.32	0.83
1:A:205:PRO:O	1:A:207:ARG:NH1	2.13	0.82
1:B:167:TRP:HB3	1:B:198:ARG:HH12	1.44	0.82
1:B:466:THR:HG22	1:B:466:THR:O	1.80	0.82
2:B:602[A]:3Q8:H12	2:B:602[A]:3Q8:CBA	2.09	0.82
1:A:259:SER:OG	2:A:500[B]:3Q8:O2A	1.98	0.82
1:A:188:PHE:HB2	1:A:189:PRO:HD2	1.62	0.81
1:A:87:VAL:HA	1:A:92:ALA:CB	2.09	0.81
1:A:399:PRO:O	1:A:402:ALA:HB3	1.80	0.81
1:B:245:HIS:NE2	2:B:602[B]:3Q8:CAA	2.44	0.81
2:A:500[A]:3Q8:N_C	2:A:500[A]:3Q8:N_D	2.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LEU:HD22	1:A:394:LEU:O	1.79	0.81
1:A:244:VAL:O	1:A:244:VAL:HG22	1.81	0.80
1:B:92:ALA:O	1:B:111:ALA:HB3	1.82	0.80
1:A:248[A]:TYR:OH	2:A:500[A]:3Q8:H2	1.82	0.80
1:A:288:ARG:NH2	1:B:123:GLU:OE1	2.13	0.80
1:B:270:GLY:O	1:B:271:LEU:HD12	1.81	0.80
2:B:602[A]:3Q8:H18	2:B:602[A]:3Q8:CMA	2.07	0.80
1:A:64:GLY:CA	1:A:72:LEU:HD21	2.12	0.80
1:A:88:LEU:HB2	1:A:89:PRO:HD2	1.62	0.79
1:B:297:LEU:O	1:B:301:LEU:HG	1.81	0.79
1:A:64:GLY:HA2	1:A:72:LEU:HD21	1.64	0.79
1:B:302:SER:O	1:B:306:ARG:HB2	1.82	0.79
1:A:96:LEU:HD22	1:A:284:HIS:CD2	2.18	0.79
1:A:301:LEU:HD12	1:A:301:LEU:O	1.82	0.79
1:A:186:MET:HG2	1:A:438:ALA:HB2	1.66	0.78
1:A:188:PHE:HB2	1:A:189:PRO:CD	2.12	0.78
1:B:78:LEU:HG	1:B:97:LEU:HD22	1.65	0.78
1:A:306:ARG:O	4:A:604:HOH:O	2.00	0.78
1:B:153:THR:HB	1:B:282:ILE:HG12	1.66	0.78
1:B:157:ARG:HD2	1:B:159:MET:HE3	1.64	0.77
1:B:431:VAL:O	1:B:431:VAL:HG23	1.85	0.77
1:A:16:GLU:OE2	1:A:243:PRO:HD2	1.85	0.77
1:B:198:ARG:HB2	1:B:268:LEU:CD2	2.15	0.76
1:B:117:MET:SD	1:B:286:ARG:HG2	2.26	0.76
1:B:239:ARG:NE	4:B:704:HOH:O	2.19	0.76
1:A:147:ASP:OD1	1:A:175:SER:OG	2.02	0.75
1:B:39:LEU:HA	1:B:62:PRO:HA	1.68	0.75
1:B:385:PHE:CB	1:B:388:SER:O	2.34	0.75
1:A:248[A]:TYR:CD1	1:A:248[A]:TYR:O	2.40	0.75
1:A:354:ALA:HB3	1:A:425:ILE:CG2	2.16	0.75
1:A:58:LEU:H	1:A:58:LEU:HD23	1.50	0.75
1:A:117:MET:SD	1:A:286:ARG:HD3	2.26	0.75
1:A:24:ILE:O	1:A:24:ILE:HD12	1.87	0.75
2:B:602[B]:3Q8:CBC	2:B:602[B]:3Q8:CMC	2.65	0.75
1:B:193:ILE:HG12	2:B:602[B]:3Q8:H11	1.51	0.74
1:A:36:PRO:O	1:A:38:ARG:N	2.21	0.74
1:B:18:ILE:HA	1:B:21:LEU:HD11	1.70	0.74
1:B:385:PHE:CD1	1:B:389:PHE:HB2	2.21	0.74
2:A:500[A]:3Q8:CHA	2:A:500[A]:3Q8:CBD	2.66	0.74
1:A:31:LEU:HD11	1:A:106:LEU:HB3	1.70	0.73
1:A:228:GLY:O	1:A:229:ARG:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275[B]:HIS:HD2	1:A:275[B]:HIS:O	1.70	0.73
1:B:260:LEU:HD12	1:B:294:THR:HG23	1.69	0.73
1:A:337:LEU:O	1:A:341:SER:HB3	1.88	0.73
1:B:260:LEU:HD12	1:B:294:THR:CG2	2.19	0.73
1:A:157:ARG:O	1:A:274:CYS:HA	1.89	0.73
1:A:245:HIS:NE2	2:A:500[B]:3Q8:H17	2.04	0.73
2:A:500[B]:3Q8:CHA	2:A:500[B]:3Q8:CBD	2.67	0.73
1:A:168:HIS:ND1	1:A:168:HIS:O	2.22	0.72
1:A:248[B]:TYR:CB	1:A:456:PRO:HG2	2.18	0.72
1:B:392:ASP:OD2	1:B:393:ARG:NH1	2.21	0.72
1:B:380:LEU:O	1:B:383:GLN:N	2.23	0.72
1:B:74:GLN:OE1	1:B:74:GLN:HA	1.90	0.72
1:B:329:GLU:HG3	1:B:329:GLU:O	1.90	0.72
1:B:263:LEU:HA	1:B:267:VAL:O	1.90	0.72
1:A:161:TYR:HE1	1:A:169:GLY:HA3	1.55	0.72
1:A:248[B]:TYR:HB3	1:A:456:PRO:HG3	1.70	0.72
1:B:200:LEU:O	1:B:200:LEU:HD22	1.89	0.72
1:B:248[A]:TYR:OH	2:B:602[A]:3Q8:CHB	2.37	0.72
1:B:489:LEU:C	1:B:490:VAL:N	2.43	0.72
1:B:152:LEU:HD23	1:B:290:CYS:SG	2.30	0.71
1:A:24:ILE:HD11	1:A:217:VAL:HG22	1.72	0.71
1:A:275[B]:HIS:O	1:A:275[B]:HIS:CD2	2.43	0.71
1:B:96:LEU:HD12	1:B:107:GLU:O	1.89	0.71
1:A:247:GLU:OE1	1:A:456:PRO:HD3	1.90	0.71
1:B:260:LEU:O	1:B:294:THR:HG21	1.90	0.71
1:B:479:LEU:HD23	1:B:479:LEU:O	1.89	0.71
1:B:275:HIS:CE1	2:B:602[B]:3Q8:H7	2.26	0.71
1:A:354:ALA:HB3	1:A:425:ILE:HG22	1.71	0.71
1:A:354:ALA:N	1:A:425:ILE:O	2.25	0.70
1:B:391:THR:O	1:B:410:GLY:HA2	1.91	0.70
2:B:602[A]:3Q8:C2B	2:B:602[A]:3Q8:CMA	2.68	0.70
1:A:319:LEU:HD11	1:A:347:LEU:HG	1.73	0.70
1:A:353:VAL:HG23	1:A:364:VAL:HG23	1.74	0.70
1:A:31:LEU:CD1	1:A:106:LEU:HB3	2.22	0.70
1:A:247:GLU:OE1	1:A:456:PRO:CD	2.40	0.70
1:B:241:VAL:O	4:B:703:HOH:O	2.08	0.70
1:B:62:PRO:O	1:B:66:VAL:HG23	1.92	0.70
1:B:84:VAL:H	1:B:95:ALA:HB3	1.56	0.70
1:A:95:ALA:HB1	1:A:106:LEU:HD12	1.74	0.69
1:B:36:PRO:O	1:B:38:ARG:N	2.25	0.69
1:B:42:VAL:HG21	1:B:231:LEU:HD12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:GLU:OE1	1:A:468:ARG:NH2	2.25	0.69
2:B:602[A]:3Q8:CMB	2:B:602[A]:3Q8:CMA	2.69	0.69
2:A:500[B]:3Q8:C4A	2:A:500[B]:3Q8:CMB	2.54	0.69
1:B:109:GLU:OE1	1:B:287:ARG:NH1	2.26	0.69
1:B:420:ALA:HB1	1:B:422:ARG:HG2	1.73	0.69
1:A:244:VAL:CA	1:A:247:GLU:HB2	2.23	0.69
1:A:248[A]:TYR:O	1:A:248[A]:TYR:CG	2.46	0.69
1:A:237:ALA:O	1:A:239:ARG:N	2.23	0.69
1:A:299:LEU:CD2	1:B:300:GLN:NE2	2.56	0.68
1:B:46:ASN:OD1	1:B:46:ASN:O	2.11	0.68
1:A:489:LEU:O	1:A:490:VAL:N	2.26	0.68
1:A:210:ALA:O	1:A:256:ALA:HA	1.93	0.68
1:B:67:LEU:HB3	1:B:71:VAL:HG11	1.76	0.68
1:B:159:MET:O	1:B:272:ILE:HA	1.93	0.68
1:B:241:VAL:HG12	1:B:242:SER:H	1.58	0.67
2:B:602[A]:3Q8:C4A	2:B:602[A]:3Q8:H1	2.24	0.67
1:B:78:LEU:HD13	1:B:84:VAL:HG12	1.76	0.67
1:A:95:ALA:HB2	1:A:108:LEU:CD2	2.23	0.67
1:A:248[B]:TYR:CB	1:A:456:PRO:CG	2.71	0.67
1:A:107:GLU:OE2	1:A:238:LEU:CD1	2.43	0.67
1:A:367:THR:HG22	1:A:368:PRO:O	1.94	0.66
1:B:258:PHE:CZ	1:B:260:LEU:HD23	2.30	0.66
1:A:395:GLY:HA2	1:A:402:ALA:HB2	1.78	0.66
1:A:33:PHE:CE1	1:A:63:VAL:HA	2.30	0.66
1:A:244:VAL:HA	1:A:247:GLU:CB	2.24	0.66
1:A:428:ARG:NE	1:A:474:TRP:CH2	2.64	0.66
2:A:500[B]:3Q8:O2A	2:A:500[B]:3Q8:H12	1.94	0.66
1:B:40:LEU:CD1	1:B:66:VAL:HG11	2.26	0.66
1:B:248[B]:TYR:O	1:B:248[B]:TYR:CG	2.48	0.66
1:B:205:PRO:HB2	1:B:206:LEU:HD23	1.77	0.66
1:A:212:ALA:O	1:A:213:ARG:HB2	1.93	0.66
1:A:224:VAL:HG21	1:A:231:LEU:HA	1.76	0.66
2:A:500[A]:3Q8:O2A	2:A:500[A]:3Q8:CMA	2.43	0.66
1:B:164:ASP:O	1:B:166:ASP:N	2.29	0.66
1:A:380:LEU:HD22	1:A:385:PHE:HE2	1.59	0.66
1:B:138:THR:N	4:B:705:HOH:O	2.27	0.65
1:B:94:ARG:NH1	1:B:285:GLU:OE1	2.25	0.65
1:B:193:ILE:HG12	2:B:602[B]:3Q8:N_A	2.11	0.65
1:A:174:GLU:OE1	4:A:605:HOH:O	2.12	0.65
1:B:201:TYR:CZ	1:B:207:ARG:NH1	2.64	0.65
1:A:155:PHE:HE2	1:A:258:PHE:HB2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HG21	1:A:454:LEU:O	1.96	0.65
1:A:299:LEU:CD1	1:B:300:GLN:NE2	2.53	0.65
1:B:242:SER:OG	1:B:243:PRO:HD2	1.97	0.65
1:A:209:ILE:HD13	4:A:634:HOH:O	1.95	0.65
1:A:446:GLU:OE1	4:A:606:HOH:O	2.14	0.65
1:A:354:ALA:HA	1:A:362:LEU:O	1.96	0.65
1:B:273:ALA:HB2	2:B:602[A]:3Q8:H4	1.78	0.65
1:A:153:THR:HG21	1:A:258:PHE:CD2	2.32	0.65
1:A:440:ASN:ND2	1:A:442:ARG:H	1.95	0.64
1:A:237:ALA:CB	1:A:287:ARG:NH2	2.60	0.64
1:A:55:PRO:O	1:A:57:THR:N	2.30	0.64
1:A:259:SER:HA	1:A:272:ILE:O	1.98	0.64
1:B:193:ILE:HD11	2:B:602[B]:3Q8:H10	1.79	0.64
1:A:35:GLY:O	1:A:38:ARG:NH2	2.31	0.64
1:A:291:GLU:O	1:A:294:THR:OG1	2.15	0.64
1:A:476:ARG:O	1:A:479:LEU:HB3	1.98	0.64
1:B:257:SER:HB2	4:B:711:HOH:O	1.97	0.63
2:A:500[A]:3Q8:H15	2:A:500[A]:3Q8:CBD	2.25	0.63
1:B:259:SER:OG	2:B:602[B]:3Q8:O1A	2.16	0.63
1:B:476:ARG:O	1:B:476:ARG:HG3	1.97	0.63
1:A:116:GLY:O	1:A:119:GLU:N	2.32	0.63
1:B:248[B]:TYR:HA	1:B:251:ASN:HD21	1.63	0.63
1:B:417:ALA:HB3	1:B:420:ALA:HB3	1.81	0.63
1:A:133:ALA:CB	1:A:300:GLN:HE22	2.11	0.63
1:A:248[A]:TYR:OH	2:A:500[A]:3Q8:CMB	2.45	0.63
1:B:437:TRP:HB2	1:B:463:TRP:O	1.99	0.63
1:A:129:VAL:CG1	1:B:295:GLN:OE1	2.46	0.63
1:A:231:LEU:O	1:A:232:ASP:HB2	1.97	0.63
1:B:48:GLN:HB2	1:B:54:PRO:HA	1.81	0.63
1:B:248[A]:TYR:HB2	1:B:456:PRO:HG3	1.81	0.62
1:A:238:LEU:O	1:A:238:LEU:CD2	2.35	0.62
1:B:167:TRP:HB3	1:B:198:ARG:NH1	2.13	0.62
2:B:602[B]:3Q8:H17	2:B:602[B]:3Q8:H12	1.81	0.62
1:A:25:GLN:HG2	1:A:27:HIS:CE1	2.33	0.62
1:A:273:ALA:CB	2:A:500[B]:3Q8:H5	2.30	0.62
1:B:174:GLU:OE2	1:B:183:PHE:O	2.18	0.62
1:A:168:HIS:ND1	1:A:168:HIS:C	2.51	0.62
1:A:243:PRO:O	1:A:245:HIS:N	2.31	0.62
1:B:117:MET:CE	1:B:117:MET:HA	2.30	0.62
1:A:45:ALA:C	1:A:47:ALA:H	1.97	0.62
1:B:221:PRO:O	1:B:223:VAL:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248[B]:TYR:O	1:B:248[B]:TYR:CD1	2.53	0.62
1:B:431:VAL:O	1:B:431:VAL:CG2	2.48	0.62
1:B:143:GLN:HE21	1:B:143:GLN:HA	1.63	0.61
1:B:161:TYR:CD2	2:B:602[A]:3Q8:H2	2.35	0.61
1:B:164:ASP:O	1:B:167:TRP:N	2.33	0.61
2:B:602[A]:3Q8:H30	2:B:602[A]:3Q8:H26	1.82	0.61
1:A:430:GLU:OE1	1:A:468:ARG:CZ	2.48	0.61
1:B:252:MET:HE3	2:B:602[B]:3Q8:H5	1.81	0.61
1:B:356:LEU:HD12	1:B:423:PHE:CD1	2.36	0.61
1:A:78:LEU:HA	1:A:82:GLY:H	1.65	0.61
1:A:116:GLY:O	1:A:118:GLU:N	2.33	0.61
1:B:248[A]:TYR:HA	1:B:251:ASN:HD21	1.64	0.61
1:B:247:GLU:OE1	1:B:455:HIS:CG	2.53	0.61
2:B:602[B]:3Q8:O2A	2:B:602[B]:3Q8:C2A	2.47	0.61
1:B:333:LEU:HD12	1:B:334:GLU:OE2	2.00	0.61
1:B:124:VAL:HG11	1:B:152:LEU:HD22	1.83	0.61
1:A:281:HIS:ND1	1:A:281:HIS:C	2.54	0.60
1:A:95:ALA:CB	1:A:106:LEU:HD12	2.31	0.60
1:B:76:GLU:HB3	1:B:77:PRO:HD3	1.82	0.60
1:B:183:PHE:CZ	1:B:252:MET:HE2	2.36	0.60
1:B:248[A]:TYR:O	1:B:248[A]:TYR:CD1	2.54	0.60
1:B:356:LEU:O	1:B:422:ARG:HB3	2.02	0.60
1:A:146:ALA:CA	1:A:158:VAL:HG11	2.32	0.60
1:A:345:LEU:O	1:A:350:ALA:O	2.19	0.60
1:A:399:PRO:HA	1:A:402:ALA:CB	2.31	0.60
1:B:183:PHE:CZ	1:B:252:MET:CE	2.84	0.60
1:A:264:LYS:HE2	1:A:301:LEU:HD11	1.83	0.60
1:A:345:LEU:HD13	1:A:351:ALA:O	2.01	0.60
1:B:333:LEU:HD12	1:B:334:GLU:OE1	2.02	0.60
1:A:299:LEU:HD21	1:B:300:GLN:CD	2.22	0.60
1:B:13[B]:CYS:O	2:B:602[B]:3Q8:H37	2.02	0.60
1:B:394:LEU:HB2	1:B:409:ALA:CA	2.31	0.60
1:A:64:GLY:HA3	1:A:72:LEU:HD21	1.82	0.60
1:A:78:LEU:HB3	1:A:84:VAL:CG2	2.32	0.60
1:B:24:ILE:O	1:B:217:VAL:HG12	2.01	0.60
1:B:374:GLU:O	1:B:377:VAL:HG22	2.02	0.60
1:B:33:PHE:O	1:B:103:LEU:HA	2.02	0.59
1:B:248[A]:TYR:HB2	1:B:456:PRO:CB	2.32	0.59
1:B:248[B]:TYR:HD2	1:B:456:PRO:HB2	1.67	0.59
1:A:158:VAL:HG12	1:A:175:SER:HB3	1.83	0.59
1:A:192:ASP:O	1:A:194:PRO:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LEU:HB3	1:A:426:TRP:CE3	2.37	0.59
1:B:147:ASP:O	1:B:150:ARG:HB3	2.03	0.59
1:A:84:VAL:O	1:A:94:ARG:HB2	2.03	0.59
1:A:109:GLU:HG3	1:A:110:PRO:HD2	1.85	0.59
1:B:261:SER:OG	1:B:268:LEU:HD11	2.02	0.59
1:A:24:ILE:HD11	1:A:217:VAL:O	2.03	0.59
1:B:40:LEU:HD13	1:B:66:VAL:HG11	1.85	0.59
1:A:283:SER:OG	1:A:284:HIS:N	2.36	0.59
1:A:488:ALA:HA	1:B:488:ALA:HA	1.85	0.59
2:A:500[B]:3Q8:CMA	2:A:500[B]:3Q8:C2B	2.79	0.58
1:B:30:LEU:O	1:B:31:LEU:C	2.42	0.58
1:A:363:LEU:CD2	1:A:373:VAL:HG21	2.33	0.58
1:A:193:ILE:HG22	2:A:500[A]:3Q8:H10	1.85	0.58
1:A:471:SER:OG	1:A:472:LEU:O	2.21	0.58
1:A:58:LEU:HD12	1:A:66:VAL:HA	1.84	0.58
1:A:353:VAL:HG23	1:A:364:VAL:CG2	2.34	0.58
1:B:283:SER:H	1:B:286:ARG:HD3	1.69	0.58
1:B:428:ARG:HG3	1:B:428:ARG:HH11	1.68	0.58
1:A:398:TYR:O	1:A:398:TYR:CD2	2.57	0.58
1:A:437:TRP:O	1:A:463:TRP:N	2.36	0.58
1:A:146:ALA:HA	1:A:158:VAL:HG11	1.84	0.58
1:A:155:PHE:HD1	1:A:276:HIS:CD2	2.22	0.58
1:A:58:LEU:HD23	1:A:58:LEU:N	2.19	0.58
1:A:385:PHE:O	1:A:385:PHE:CD1	2.57	0.58
1:B:92:ALA:O	1:B:111:ALA:CB	2.51	0.58
1:B:428:ARG:HD3	4:B:734:HOH:O	2.04	0.57
1:A:19:HIS:ND1	1:A:20:LEU:HG	2.19	0.57
1:B:25:GLN:HE22	1:B:238:LEU:C	2.07	0.57
1:B:160:VAL:HG22	1:B:173:ALA:HB3	1.85	0.57
1:B:201:TYR:OH	2:B:602[B]:3Q8:H26	2.04	0.57
1:A:155:PHE:CD1	1:A:276:HIS:HB2	2.39	0.57
1:A:161:TYR:CE1	1:A:169:GLY:HA3	2.38	0.57
1:B:477:ALA:O	1:B:481:ALA:N	2.35	0.57
1:A:186:MET:HG3	1:A:438:ALA:HB2	1.84	0.57
1:A:260:LEU:O	1:A:271:LEU:CB	2.53	0.57
1:A:239:ARG:HG3	1:A:240:SER:O	2.05	0.57
1:A:366:CYS:SG	1:A:366:CYS:O	2.63	0.57
1:A:385:PHE:HB2	1:A:388:SER:O	2.04	0.57
2:A:500[A]:3Q8:C3A	2:A:500[A]:3Q8:CGA	2.80	0.57
1:A:237:ALA:HB1	1:A:287:ARG:NH2	2.19	0.57
1:A:245:HIS:C	1:A:247:GLU:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:PHE:O	1:B:189:PRO:O	2.23	0.57
1:B:242:SER:OG	1:B:243:PRO:CD	2.53	0.57
1:A:192:ASP:O	1:A:194:PRO:HG3	2.05	0.57
1:A:399:PRO:O	1:A:402:ALA:CB	2.51	0.57
2:A:500[A]:3Q8:H14	2:A:500[A]:3Q8:N_B	2.20	0.57
1:A:96:LEU:CD2	1:A:284:HIS:CD2	2.88	0.56
1:A:193:ILE:HG22	2:A:500[B]:3Q8:H10	1.87	0.56
1:B:405:ALA:C	1:B:407:VAL:H	2.08	0.56
1:B:470:THR:HG22	1:B:471:SER:N	2.20	0.56
1:A:36:PRO:O	1:A:37:ASP:C	2.43	0.56
1:A:469:ASP:OD1	1:A:469:ASP:O	2.22	0.56
1:B:38:ARG:HG3	1:B:63:VAL:CG1	2.35	0.56
1:B:125:VAL:O	1:B:128:LEU:N	2.38	0.56
1:A:95:ALA:HB3	1:A:106:LEU:HD11	1.87	0.56
1:B:313:ASP:C	1:B:313:ASP:OD1	2.43	0.56
1:A:244:VAL:O	1:A:244:VAL:CG2	2.50	0.56
1:B:24:ILE:HD11	1:B:44:SER:OG	2.05	0.56
1:B:258:PHE:HB3	1:B:274:CYS:HB2	1.88	0.56
2:B:602[A]:3Q8:H3	2:B:602[A]:3Q8:CMA	2.31	0.56
1:A:30:LEU:HD23	1:A:30:LEU:O	2.06	0.56
1:B:307:ALA:O	1:B:310:ALA:N	2.38	0.56
1:A:135:VAL:O	1:A:136:LYS:HG2	2.05	0.56
1:A:275[A]:HIS:N	1:A:275[A]:HIS:CD2	2.74	0.56
1:B:25:GLN:NE2	1:B:238:LEU:O	2.38	0.56
1:B:404:ARG:O	1:B:404:ARG:CG	2.54	0.56
1:A:16:GLU:CD	1:A:242:SER:HB2	2.24	0.56
1:B:264:LYS:HG2	1:B:265:GLU:N	2.20	0.56
2:B:602[A]:3Q8:H1	2:B:602[A]:3Q8:C3A	2.35	0.56
1:A:129:VAL:HG12	1:B:295:GLN:OE1	2.06	0.56
1:B:193:ILE:CD1	2:B:602[B]:3Q8:H10	2.36	0.56
1:B:25:GLN:NE2	1:B:238:LEU:C	2.60	0.55
1:B:405:ALA:O	1:B:407:VAL:N	2.34	0.55
1:B:437:TRP:CE3	1:B:441:PRO:HG3	2.41	0.55
1:B:117:MET:HB2	1:B:118:GLU:OE2	2.05	0.55
1:A:191:THR:O	1:A:194:PRO:HA	2.07	0.55
1:A:392:ASP:O	1:A:409:ALA:O	2.24	0.55
1:A:398:TYR:C	1:A:400:PRO:HD2	2.26	0.55
1:A:244:VAL:C	1:A:247:GLU:HB2	2.26	0.55
1:B:117:MET:HA	1:B:117:MET:HE3	1.88	0.55
1:B:167:TRP:CB	1:B:198:ARG:HH12	2.19	0.55
2:B:602[A]:3Q8:CMB	2:B:602[A]:3Q8:C3A	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ALA:CB	1:A:106:LEU:CD1	2.84	0.55
1:A:345:LEU:HD12	1:A:345:LEU:C	2.25	0.55
1:A:87:VAL:CA	1:A:92:ALA:HB1	2.18	0.55
1:A:197:ALA:O	1:A:201:TYR:CG	2.60	0.55
1:A:245:HIS:C	1:A:247:GLU:N	2.59	0.55
1:A:275[B]:HIS:CD2	1:A:275[B]:HIS:C	2.79	0.55
1:B:353:VAL:HA	1:B:425:ILE:O	2.06	0.55
1:A:33:PHE:HE1	1:A:63:VAL:HA	1.71	0.55
1:A:125:VAL:HG22	1:A:293:LEU:HD11	1.88	0.55
1:A:189:PRO:HD3	1:A:437:TRP:HZ3	1.71	0.55
1:A:245:HIS:CE1	2:A:500[B]:3Q8:C1A	2.89	0.55
1:B:24:ILE:HD13	1:B:30:LEU:HD23	1.87	0.55
1:B:333:LEU:HD12	1:B:334:GLU:CD	2.27	0.55
1:A:150:ARG:HH21	1:A:176:LYS:C	2.09	0.55
1:A:174:GLU:HG3	1:A:175:SER:N	2.22	0.55
1:B:258:PHE:CE2	1:B:260:LEU:HD21	2.42	0.54
1:B:334:GLU:O	1:B:338:GLU:OE2	2.25	0.54
1:A:124:VAL:HG21	1:A:152:LEU:CD2	2.37	0.54
1:A:404:ARG:C	1:A:406:ASP:H	2.11	0.54
1:A:430:GLU:HB2	1:A:469:ASP:HA	1.89	0.54
1:A:448:GLU:O	1:A:449:PRO:C	2.42	0.54
1:A:244:VAL:HA	1:A:247:GLU:CG	2.37	0.54
1:A:192:ASP:HA	2:A:500[A]:3Q8:C1C	2.38	0.54
2:B:602[B]:3Q8:H34	2:B:602[B]:3Q8:H39	1.86	0.54
1:A:324:ALA:HA	1:A:327:MET:HB2	1.90	0.54
1:A:380:LEU:HD23	1:A:383:GLN:HE22	1.72	0.54
1:A:399:PRO:HA	1:A:402:ALA:HB2	1.90	0.54
1:B:159:MET:SD	1:B:273:ALA:HB3	2.47	0.54
1:B:197:ALA:HB1	1:B:201:TYR:CZ	2.43	0.54
1:B:159:MET:HE2	2:B:602[B]:3Q8:H8	1.90	0.54
1:B:163:PHE:N	1:B:163:PHE:CD1	2.75	0.54
1:A:478:ASP:O	1:A:479:LEU:C	2.46	0.54
1:A:191:THR:O	1:A:192:ASP:O	2.25	0.54
1:A:484:GLY:O	1:A:487:GLY:N	2.41	0.54
1:B:163:PHE:CZ	1:B:193:ILE:HD12	2.43	0.54
1:B:201:TYR:OH	2:B:602[A]:3Q8:O2D	2.26	0.54
1:A:24:ILE:CD1	1:A:217:VAL:HG13	2.39	0.53
1:A:435:ILE:O	1:A:435:ILE:HG22	2.07	0.53
1:A:34:ARG:HB3	1:A:41:GLU:HB2	1.89	0.53
1:A:123:GLU:OE1	1:B:288:ARG:NH2	2.41	0.53
1:A:304:GLU:HA	1:A:304:GLU:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:VAL:HA	1:A:347:LEU:HD12	1.90	0.53
1:A:441:PRO:HD2	1:A:463:TRP:CZ3	2.43	0.53
1:B:17:PRO:HB2	1:B:20:LEU:CD2	2.38	0.53
1:A:283:SER:HB3	1:A:286:ARG:HB2	1.91	0.53
1:A:398:TYR:HE2	1:A:401:LEU:HB3	1.72	0.53
1:B:361:PRO:HD2	1:B:370:GLN:HE21	1.72	0.53
1:B:470:THR:HG22	1:B:471:SER:H	1.73	0.53
1:A:155:PHE:CE1	1:A:276:HIS:HB2	2.43	0.53
1:A:275[A]:HIS:CD2	1:A:275[A]:HIS:H	2.25	0.53
1:A:440:ASN:HD22	1:A:441:PRO:N	2.06	0.53
1:B:19:HIS:CE1	1:B:20:LEU:HD22	2.44	0.53
1:A:18:ILE:HD11	2:A:500[A]:3Q8:O2D	2.09	0.53
1:A:412:LEU:HB3	1:A:426:TRP:HE3	1.73	0.53
1:B:45:ALA:HB2	1:B:218:PRO:HG2	1.91	0.53
1:B:248[A]:TYR:HB2	1:B:456:PRO:CG	2.39	0.53
1:A:78:LEU:O	1:A:82:GLY:HA2	2.09	0.53
1:A:133:ALA:HB3	1:A:300:GLN:HE22	1.72	0.53
1:A:413:ALA:O	1:A:414:VAL:HG13	2.08	0.53
1:B:45:ALA:CB	1:B:218:PRO:HG2	2.39	0.53
1:B:194:PRO:HD2	1:B:197:ALA:HB3	1.91	0.53
1:B:367:THR:OG1	1:B:368:PRO:HD2	2.09	0.53
1:B:117:MET:O	1:B:121:ALA:CB	2.56	0.53
1:A:157:ARG:HH21	1:A:275[B]:HIS:CE1	2.27	0.53
1:A:170:GLU:HG3	1:A:187:HIS:CE1	2.44	0.53
1:A:248[B]:TYR:HB2	1:A:456:PRO:HG2	1.87	0.53
1:A:174:GLU:HG3	1:A:175:SER:H	1.75	0.52
1:A:294:THR:O	1:A:297:LEU:HD23	2.09	0.52
1:A:183:PHE:HB3	1:A:186:MET:HB3	1.92	0.52
1:B:153:THR:CB	1:B:282:ILE:HG12	2.37	0.52
1:B:264:LYS:HG3	1:B:302:SER:OG	2.09	0.52
1:B:479:LEU:O	1:B:479:LEU:CD2	2.56	0.52
1:A:37:ASP:O	1:A:39:LEU:HB2	2.09	0.52
1:A:192:ASP:O	1:A:194:PRO:CG	2.57	0.52
1:A:229:ARG:NH1	1:A:231:LEU:O	2.42	0.52
1:B:437:TRP:CZ3	1:B:441:PRO:HB3	2.45	0.52
1:A:161:TYR:O	1:A:270:GLY:HA3	2.10	0.52
1:A:248[A]:TYR:CE2	1:A:460:PHE:HE2	2.28	0.52
1:B:109:GLU:HB3	1:B:238:LEU:HD21	1.92	0.52
1:B:353:VAL:HG13	1:B:353:VAL:O	2.09	0.52
2:A:500[B]:3Q8:H15	2:A:500[B]:3Q8:H25	1.91	0.52
2:A:500[B]:3Q8:N_C	2:A:500[B]:3Q8:N_D	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ASP:O	1:B:194:PRO:HD3	2.09	0.52
1:A:109:GLU:CG	1:A:110:PRO:HD2	2.39	0.52
1:A:21:LEU:HD22	4:A:633:HOH:O	2.09	0.52
1:A:282:ILE:HG22	1:A:286:ARG:HG2	1.92	0.52
1:A:488:ALA:HB1	1:B:487:GLY:O	2.10	0.52
1:B:232:ASP:OD1	1:B:234:SER:HB2	2.10	0.52
1:B:291:GLU:HA	1:B:294:THR:OG1	2.09	0.52
1:A:209:ILE:CG1	1:A:257:SER:HB3	2.39	0.52
1:A:440:ASN:HD21	1:A:442:ARG:HG3	1.75	0.52
1:A:213:ARG:HD2	1:A:250:ARG:HH11	1.74	0.51
1:A:483:GLU:HA	1:A:483:GLU:OE2	2.09	0.51
1:B:33:PHE:HA	1:B:39:LEU:O	2.10	0.51
1:B:258:PHE:CE2	1:B:260:LEU:CD2	2.92	0.51
1:B:379:TRP:CZ3	1:B:398:TYR:HB2	2.46	0.51
1:B:437:TRP:CD2	1:B:441:PRO:HG3	2.46	0.51
1:A:107:GLU:OE2	1:A:238:LEU:HD13	2.09	0.51
1:A:150:ARG:NH2	1:A:176:LYS:C	2.63	0.51
1:A:236:SER:OG	1:A:237:ALA:N	2.43	0.51
1:A:467:VAL:HG23	1:A:467:VAL:O	2.10	0.51
1:B:248[A]:TYR:HB2	1:B:456:PRO:HB3	1.91	0.51
1:B:312:GLU:OE2	1:B:312:GLU:C	2.49	0.51
1:A:96:LEU:HD23	1:A:284:HIS:CG	2.45	0.51
1:A:155:PHE:HA	1:A:276:HIS:CD2	2.46	0.51
1:A:344:VAL:O	1:A:347:LEU:HB2	2.10	0.51
1:A:363:LEU:HD22	1:A:373:VAL:HG21	1.91	0.51
1:B:39:LEU:HD11	1:B:60:GLY:O	2.10	0.51
1:A:95:ALA:HB3	1:A:106:LEU:CD1	2.41	0.51
1:B:24:ILE:HG21	1:B:30:LEU:HD23	1.93	0.51
1:A:98:HIS:HE1	1:A:107:GLU:OE1	1.93	0.51
1:B:316:ARG:O	1:B:319:LEU:HB2	2.11	0.51
1:B:38:ARG:HG3	1:B:63:VAL:HG12	1.92	0.51
1:B:124:VAL:HG13	1:B:148:THR:HB	1.92	0.51
1:B:260:LEU:CD1	1:B:294:THR:HG23	2.38	0.51
1:B:414:VAL:HG12	1:B:486:ARG:HB2	1.92	0.51
1:A:168:HIS:HA	1:A:190:ALA:HB2	1.91	0.51
1:A:435:ILE:CG2	1:A:437:TRP:CD1	2.94	0.51
1:B:153:THR:HA	1:B:286:ARG:HH21	1.76	0.51
1:A:103:LEU:C	1:A:103:LEU:HD12	2.31	0.51
1:B:235:ASN:C	1:B:236:SER:O	2.50	0.51
1:A:201:TYR:OH	2:A:500[A]:3Q8:H25	2.09	0.50
1:A:209:ILE:HB	1:A:257:SER:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ILE:O	1:A:272:ILE:HD13	2.11	0.50
1:A:355:LEU:O	1:A:356:LEU:CB	2.56	0.50
1:A:396:THR:OG1	1:A:397:VAL:N	2.44	0.50
1:B:270:GLY:O	1:B:271:LEU:CD1	2.56	0.50
1:B:404:ARG:O	1:B:404:ARG:HG2	2.11	0.50
1:A:340:GLU:CA	1:A:340:GLU:OE1	2.59	0.50
1:A:404:ARG:C	1:A:406:ASP:N	2.65	0.50
1:B:293:LEU:N	1:B:293:LEU:HD23	2.24	0.50
1:A:273:ALA:HB1	2:A:500[B]:3Q8:H5	1.93	0.50
1:B:241:VAL:HG12	1:B:242:SER:N	2.25	0.50
2:B:602[B]:3Q8:H16	2:B:602[B]:3Q8:H23	1.93	0.50
1:B:67:LEU:HB3	1:B:71:VAL:CG1	2.40	0.50
1:B:398:TYR:C	1:B:400:PRO:HD2	2.31	0.50
1:B:428:ARG:HH11	1:B:428:ARG:CG	2.25	0.50
1:A:378:ALA:HA	4:A:603:HOH:O	2.11	0.50
1:B:102:GLY:N	4:B:710:HOH:O	2.45	0.50
1:B:206:LEU:HD22	1:B:291:GLU:HB2	1.94	0.50
1:A:124:VAL:HG21	1:A:152:LEU:HD22	1.94	0.50
1:A:319:LEU:CD1	1:A:347:LEU:HG	2.39	0.50
1:B:100:SER:HB2	1:B:105:VAL:HG21	1.94	0.50
1:B:129:VAL:HG22	1:B:296:LEU:HD21	1.94	0.50
1:A:117:MET:HG3	1:A:118:GLU:N	2.27	0.50
1:A:394:LEU:HG	1:A:411:ILE:HG23	1.93	0.50
1:A:395:GLY:CA	1:A:402:ALA:CB	2.90	0.50
1:B:112:GLU:OE1	1:B:286:ARG:HD2	2.12	0.50
2:B:602[A]:3Q8:H24	2:B:602[A]:3Q8:H15	1.93	0.50
1:A:56:GLU:N	1:A:56:GLU:OE2	2.44	0.49
1:A:96:LEU:CD2	1:A:284:HIS:CG	2.95	0.49
1:A:188:PHE:HD2	1:A:438:ALA:HB3	1.76	0.49
1:B:30:LEU:O	1:B:31:LEU:O	2.29	0.49
1:B:97:LEU:HD12	1:B:104:THR:HG22	1.94	0.49
1:B:264:LYS:HB3	1:B:298:ALA:O	2.12	0.49
1:A:203:ARG:CD	4:A:622:HOH:O	2.60	0.49
1:A:430:GLU:HA	1:A:470:THR:O	2.12	0.49
1:A:248[B]:TYR:O	1:A:248[B]:TYR:CD2	2.65	0.49
1:A:221:PRO:O	1:A:223:VAL:N	2.41	0.49
1:B:334:GLU:HG3	1:B:362:LEU:HD22	1.95	0.49
2:B:602[B]:3Q8:C1B	2:B:602[B]:3Q8:CMA	2.90	0.49
1:A:48:GLN:HG2	4:A:640:HOH:O	2.13	0.49
1:A:96:LEU:HD12	1:A:96:LEU:O	2.12	0.49
1:A:395:GLY:CA	1:A:402:ALA:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASP:O	1:A:429:PRO:HB3	2.12	0.49
1:B:260:LEU:HD12	1:B:294:THR:HG21	1.93	0.49
1:A:38:ARG:HG3	1:A:63:VAL:HB	1.94	0.49
1:A:110:PRO:HD2	1:A:281:HIS:HE2	1.76	0.49
1:B:101:ASP:N	1:B:101:ASP:OD1	2.42	0.49
1:B:163:PHE:N	1:B:163:PHE:HD1	2.11	0.49
1:B:168:HIS:CE1	1:B:187:HIS:HD1	2.30	0.49
1:B:239:ARG:CD	4:B:704:HOH:O	2.60	0.49
1:A:186:MET:HG2	1:A:438:ALA:CB	2.42	0.49
1:A:348:THR:HG21	1:A:412:LEU:HD23	1.94	0.49
1:B:267:VAL:C	1:B:268:LEU:O	2.50	0.49
1:B:125:VAL:HG13	1:B:126:ARG:H	1.77	0.49
1:B:160:VAL:HG22	1:B:173:ALA:CB	2.42	0.49
1:A:22:GLY:O	1:A:23:GLY:O	2.31	0.49
1:A:55:PRO:C	1:A:57:THR:H	2.17	0.49
1:A:320:LEU:HD23	1:A:320:LEU:O	2.13	0.49
1:B:416:LEU:O	1:B:416:LEU:HD13	2.13	0.49
1:A:301:LEU:HD12	1:A:301:LEU:C	2.32	0.48
1:B:84:VAL:HG13	1:B:84:VAL:O	2.13	0.48
1:A:260:LEU:O	1:A:271:LEU:HB2	2.13	0.48
1:B:87:VAL:HG23	1:B:92:ALA:HB2	1.93	0.48
1:A:31:LEU:HB3	1:A:43:VAL:HG23	1.94	0.48
1:B:42:VAL:CG2	1:B:231:LEU:HD12	2.43	0.48
1:A:245:HIS:CE1	2:A:500[B]:3Q8:CHA	2.96	0.48
1:A:303:ALA:HB2	1:B:303:ALA:HB2	1.94	0.48
1:B:147:ASP:OD1	1:B:175:SER:HB3	2.13	0.48
1:B:245:HIS:C	1:B:245:HIS:HD1	2.17	0.48
1:B:247:GLU:OE1	1:B:455:HIS:ND1	2.46	0.48
1:B:428:ARG:HG3	1:B:428:ARG:NH1	2.29	0.48
1:B:437:TRP:CE3	1:B:441:PRO:HB3	2.49	0.48
2:B:602[B]:3Q8:H8	2:B:602[B]:3Q8:O_B	2.13	0.48
1:B:263:LEU:HD12	1:B:263:LEU:O	2.13	0.48
1:A:18:ILE:O	1:A:18:ILE:CD1	2.57	0.48
1:A:394:LEU:HD13	1:A:394:LEU:C	2.34	0.48
1:B:344:VAL:HG11	1:B:353:VAL:HG11	1.96	0.48
1:B:448:GLU:O	1:B:450:GLY:N	2.46	0.48
1:A:24:ILE:HA	1:A:239:ARG:HA	1.96	0.48
1:A:144:THR:O	1:A:146:ALA:N	2.47	0.48
1:A:353:VAL:CG2	1:A:364:VAL:HG23	2.42	0.48
1:A:393:ARG:C	1:A:395:GLY:H	2.17	0.48
1:A:193:ILE:CG2	2:A:500[A]:3Q8:H10	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ILE:HD13	2:B:602[A]:3Q8:O1D	2.14	0.47
1:B:208:LEU:HD22	1:B:287:ARG:NE	2.29	0.47
1:B:11:SER:HB2	1:B:13[A]:CYS:HB2	1.96	0.47
1:B:157:ARG:HG2	1:B:275:HIS:HB2	1.96	0.47
1:B:267:VAL:HG13	1:B:268:LEU:O	2.14	0.47
1:B:420:ALA:HB1	1:B:422:ARG:CG	2.43	0.47
1:A:86:VAL:HG23	1:A:86:VAL:O	2.13	0.47
1:A:189:PRO:HD3	1:A:437:TRP:CZ3	2.48	0.47
1:A:248[A]:TYR:CE2	1:A:460:PHE:CE2	3.01	0.47
1:A:260:LEU:O	1:A:271:LEU:HB3	2.14	0.47
1:A:405:ALA:HA	1:A:430:GLU:HB2	1.95	0.47
1:A:430:GLU:CB	1:A:469:ASP:HA	2.44	0.47
1:A:430:GLU:OE2	1:A:469:ASP:HB3	2.14	0.47
1:B:78:LEU:CG	1:B:97:LEU:HD22	2.41	0.47
1:A:167:TRP:CD1	1:A:198:ARG:NE	2.82	0.47
1:A:211:ASP:O	1:A:214:ALA:HB3	2.15	0.47
1:B:63:VAL:HG13	1:B:64:GLY:N	2.29	0.47
1:B:161:TYR:CE2	1:B:188:PHE:CE1	3.03	0.47
1:B:23:GLY:HA2	1:B:233:LEU:HD22	1.94	0.47
1:B:143:GLN:HE21	1:B:143:GLN:CA	2.27	0.47
1:B:248[A]:TYR:O	1:B:248[A]:TYR:CD2	2.67	0.47
1:B:390:HIS:NE2	1:B:479:LEU:HD12	2.29	0.47
1:B:428:ARG:NH1	1:B:474:TRP:CZ3	2.83	0.47
1:A:155:PHE:HD1	1:A:276:HIS:HD2	1.62	0.47
1:A:296:LEU:O	1:A:296:LEU:HD12	2.14	0.47
1:B:36:PRO:O	1:B:37:ASP:C	2.53	0.47
1:A:243:PRO:C	1:A:245:HIS:H	2.14	0.47
1:A:337:LEU:O	1:A:341:SER:N	2.48	0.47
1:B:248[B]:TYR:HB2	1:B:456:PRO:CB	2.44	0.47
1:B:305:GLU:C	1:B:307:ALA:H	2.18	0.47
1:A:171:VAL:O	1:A:172:LEU:C	2.53	0.47
1:A:219:LEU:O	1:A:220:LEU:O	2.32	0.47
1:A:385:PHE:CD1	1:A:385:PHE:C	2.88	0.47
1:B:162:ARG:O	1:B:169:GLY:HA3	2.14	0.47
1:B:224:VAL:HG13	1:B:227:LEU:HD23	1.97	0.47
1:B:369:ALA:O	1:B:372:GLU:HG3	2.14	0.47
1:A:78:LEU:CB	1:A:84:VAL:CG2	2.92	0.47
1:B:248[B]:TYR:HB2	1:B:456:PRO:HG3	1.97	0.46
1:A:394:LEU:HG	1:A:411:ILE:CG2	2.46	0.46
1:B:353:VAL:O	1:B:353:VAL:CG1	2.63	0.46
1:B:156:ASP:HB3	1:B:180:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248[B]:TYR:CD1	1:B:248[B]:TYR:C	2.88	0.46
1:A:100:SER:CB	4:A:602:HOH:O	2.56	0.46
1:A:130:SER:O	1:A:132:LEU:N	2.47	0.46
1:B:221:PRO:HG2	1:B:223:VAL:O	2.15	0.46
1:B:353:VAL:O	1:B:364:VAL:CG1	2.63	0.46
1:A:251:ASN:O	1:A:460:PHE:CE1	2.68	0.46
1:A:401:LEU:HD13	1:A:401:LEU:O	2.15	0.46
1:B:211:ASP:O	1:B:214:ALA:N	2.46	0.46
1:B:315:HIS:O	1:B:319:LEU:HD23	2.15	0.46
1:A:39:LEU:O	1:A:40:LEU:O	2.34	0.46
1:A:145:ALA:O	1:A:149:VAL:HG22	2.15	0.46
1:A:306:ARG:HG2	1:B:307:ALA:HB2	1.97	0.46
1:B:148:THR:O	1:B:151:ALA:N	2.48	0.46
1:B:283:SER:OG	1:B:284:HIS:N	2.47	0.46
1:A:190:ALA:HB1	4:A:614:HOH:O	2.16	0.46
1:A:398:TYR:CZ	1:A:400:PRO:HG2	2.51	0.46
1:A:404:ARG:O	1:A:406:ASP:N	2.49	0.46
1:B:129:VAL:CG2	1:B:296:LEU:HD21	2.46	0.46
1:A:141:LEU:HD21	1:A:300:GLN:NE2	2.30	0.46
1:B:29:VAL:HG23	1:B:108:LEU:HG	1.98	0.46
1:A:168:HIS:HA	1:A:190:ALA:CB	2.45	0.46
1:A:224:VAL:CG2	1:A:231:LEU:HA	2.43	0.46
1:B:334:GLU:OE1	1:B:334:GLU:N	2.46	0.46
1:B:466:THR:O	1:B:468:ARG:HB3	2.15	0.46
1:A:243:PRO:O	1:A:246:LEU:HD13	2.15	0.45
1:A:248[A]:TYR:HB2	1:A:456:PRO:CB	2.46	0.45
1:B:348:THR:HG22	1:B:478:ASP:HA	1.98	0.45
1:B:466:THR:O	1:B:466:THR:CG2	2.53	0.45
1:A:18:ILE:HG13	1:A:242:SER:HB3	1.97	0.45
1:B:53:ARG:HG2	1:B:54:PRO:HD2	1.98	0.45
1:B:258:PHE:CZ	1:B:260:LEU:CD2	2.98	0.45
1:B:388:SER:HA	1:B:413:ALA:O	2.16	0.45
1:A:33:PHE:CZ	1:A:63:VAL:HG23	2.52	0.45
1:A:435:ILE:O	1:A:435:ILE:CG2	2.64	0.45
1:A:475:LYS:O	1:A:478:ASP:HB3	2.16	0.45
1:B:385:PHE:CG	1:B:389:PHE:HB2	2.51	0.45
1:A:370:GLN:HE21	1:A:370:GLN:HB3	1.58	0.45
1:B:248[B]:TYR:HB2	1:B:456:PRO:HB3	1.98	0.45
1:A:246:LEU:HA	1:A:249:LEU:HG	1.98	0.45
1:A:394:LEU:HD23	1:A:411:ILE:HD13	1.97	0.45
1:A:41:GLU:OE2	1:A:225:PRO:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:PRO:HD2	1:A:197:ALA:HB3	1.99	0.45
1:B:299:LEU:O	1:B:302:SER:HB2	2.16	0.45
1:A:377:VAL:HA	1:A:380:LEU:HB2	1.99	0.45
1:B:101:ASP:C	4:B:710:HOH:O	2.55	0.45
1:B:149:VAL:HG21	1:B:272:ILE:HD13	1.99	0.45
1:B:200:LEU:HD21	1:B:234:SER:OG	2.17	0.45
1:B:434:THR:CG2	4:B:738:HOH:O	2.63	0.45
1:B:476:ARG:O	1:B:477:ALA:HB2	2.16	0.45
1:A:58:LEU:HB2	1:A:66:VAL:HG22	1.98	0.45
1:A:233:LEU:HD23	1:A:239:ARG:HB2	1.99	0.45
1:A:281:HIS:CE1	1:A:282:ILE:O	2.69	0.45
1:A:435:ILE:HG22	1:A:465:GLU:HB3	1.98	0.45
1:B:201:TYR:OH	2:B:602[B]:3Q8:CBD	2.65	0.45
1:A:59:LEU:HD23	1:A:59:LEU:N	2.32	0.45
2:B:602[A]:3Q8:H26	2:B:602[A]:3Q8:CMD	2.46	0.45
1:A:386:GLN:HB2	1:A:387:THR:HG23	1.98	0.44
1:B:459:SER:OG	1:B:460:PHE:N	2.48	0.44
1:B:161:TYR:O	1:B:270:GLY:CA	2.66	0.44
1:B:239:ARG:HD3	4:B:704:HOH:O	2.18	0.44
1:A:58:LEU:CB	1:A:61:GLN:HG3	2.47	0.44
1:B:42:VAL:HA	1:B:220:LEU:O	2.18	0.44
1:B:67:LEU:N	1:B:67:LEU:HD23	2.33	0.44
1:B:273:ALA:CB	2:B:602[A]:3Q8:H4	2.46	0.44
1:B:476:ARG:O	1:B:476:ARG:CG	2.65	0.44
1:A:245:HIS:O	1:A:247:GLU:N	2.50	0.44
1:A:457:ARG:NH1	4:A:611:HOH:O	2.50	0.44
1:A:428:ARG:CZ	1:A:474:TRP:CZ3	3.00	0.44
2:A:500[A]:3Q8:O2A	2:A:500[A]:3Q8:C4A	2.59	0.44
1:A:146:ALA:O	1:A:158:VAL:HG11	2.17	0.44
1:B:161:TYR:HD2	2:B:602[A]:3Q8:H5	1.83	0.44
1:B:205:PRO:CB	1:B:206:LEU:HD23	2.46	0.44
1:A:149:VAL:HG23	1:A:158:VAL:HG21	1.99	0.44
1:B:23:GLY:HA2	1:B:233:LEU:CD2	2.48	0.44
1:B:25:GLN:CD	1:B:238:LEU:HB3	2.37	0.44
1:B:84:VAL:O	1:B:95:ALA:HB2	2.18	0.44
1:B:128:LEU:HG	1:B:128:LEU:O	2.17	0.44
1:A:163:PHE:CZ	1:A:270:GLY:HA2	2.53	0.44
1:B:18:ILE:HG22	1:B:239:ARG:HH12	1.83	0.44
1:B:129:VAL:O	1:B:133:ALA:HB2	2.18	0.44
1:A:44:SER:HA	1:A:219:LEU:HA	2.00	0.44
1:A:160:VAL:HB	1:A:173:ALA:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:TRP:O	1:A:190:ALA:CB	2.65	0.44
1:A:283:SER:O	1:A:287:ARG:HD3	2.18	0.44
1:A:296:LEU:HD12	1:A:296:LEU:C	2.39	0.44
1:A:387:THR:HG22	1:A:486:ARG:HH22	1.83	0.44
1:A:446:GLU:HA	1:A:447:PRO:HD3	1.86	0.44
2:A:500[B]:3Q8:H39	2:A:500[B]:3Q8:H34	1.99	0.44
1:A:437:TRP:N	1:A:463:TRP:O	2.49	0.43
1:A:91:GLY:O	1:A:93:TYR:CD1	2.72	0.43
1:A:316:ARG:HG2	1:A:481:ALA:HB2	2.00	0.43
1:A:440:ASN:HD22	1:A:441:PRO:CD	2.30	0.43
1:B:161:TYR:CE2	2:B:602[A]:3Q8:H2	2.52	0.43
1:A:251:ASN:N	1:A:251:ASN:OD1	2.52	0.43
1:A:468:ARG:O	1:A:469:ASP:OD1	2.36	0.43
1:B:48:GLN:CG	1:B:48:GLN:O	2.67	0.43
1:B:249:LEU:C	1:B:251:ASN:N	2.72	0.43
1:B:446:GLU:HB2	1:B:456:PRO:O	2.18	0.43
1:A:150:ARG:HH22	1:A:177:ARG:HA	1.83	0.43
1:B:125:VAL:O	1:B:127:ARG:N	2.51	0.43
1:B:150:ARG:HD2	1:B:175:SER:OG	2.18	0.43
1:B:414:VAL:CG1	1:B:486:ARG:HB2	2.49	0.43
2:B:602[A]:3Q8:CMA	2:B:602[A]:3Q8:C1B	2.97	0.43
1:A:76:GLU:N	1:A:77:PRO:HD2	2.32	0.43
1:A:393:ARG:O	1:A:395:GLY:N	2.52	0.43
1:A:477:ALA:O	1:A:478:ASP:CB	2.67	0.43
1:A:13[B]:CYS:HA	2:A:500[B]:3Q8:H37	2.01	0.43
1:A:158:VAL:HG13	1:A:159:MET:N	2.33	0.43
1:A:78:LEU:HB3	1:A:84:VAL:HG21	2.00	0.43
1:B:225:PRO:O	1:B:226:ALA:C	2.57	0.43
1:A:96:LEU:H	1:A:96:LEU:HG	1.58	0.43
1:A:316:ARG:O	1:A:319:LEU:HB3	2.19	0.43
1:A:395:GLY:HA2	1:A:402:ALA:CB	2.47	0.43
1:B:38:ARG:HG3	1:B:63:VAL:HG11	2.00	0.43
1:B:262:LEU:C	1:B:263:LEU:HG	2.39	0.43
1:B:272:ILE:HD12	1:B:294:THR:CG2	2.48	0.43
1:B:344:VAL:HG12	1:B:345:LEU:N	2.34	0.43
1:A:159:MET:O	1:A:160:VAL:HB	2.18	0.43
1:B:191:THR:O	1:B:192:ASP:O	2.37	0.43
1:B:198:ARG:CB	1:B:268:LEU:CD2	2.92	0.43
1:B:260:LEU:CD1	1:B:294:THR:CG2	2.93	0.43
1:B:262:LEU:HD13	1:B:269:TRP:CE3	2.54	0.43
1:A:55:PRO:C	1:A:57:THR:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:TRP:O	1:A:463:TRP:HB2	2.19	0.43
1:B:27:HIS:ND1	1:B:27:HIS:C	2.72	0.43
1:B:278:GLU:HA	1:B:278:GLU:OE1	2.19	0.43
1:B:345:LEU:HD11	1:B:352:GLY:CA	2.49	0.43
1:A:87:VAL:HG13	1:A:92:ALA:HB2	2.01	0.42
1:A:155:PHE:CD1	1:A:276:HIS:HD2	2.37	0.42
1:A:440:ASN:HD22	1:A:441:PRO:HD2	1.84	0.42
1:A:454:LEU:HD12	1:A:454:LEU:N	2.33	0.42
1:B:122:LEU:O	1:B:126:ARG:NH1	2.52	0.42
1:B:221:PRO:O	1:B:223:VAL:O	2.37	0.42
1:B:248[B]:TYR:OH	2:B:602[B]:3Q8:CMB	2.66	0.42
1:B:262:LEU:O	1:B:263:LEU:HB3	2.20	0.42
1:A:24:ILE:HD12	1:A:24:ILE:C	2.39	0.42
1:A:28:GLY:HA3	1:A:238:LEU:HG	2.01	0.42
1:A:163:PHE:C	1:A:164:ASP:O	2.57	0.42
1:A:259:SER:HG	2:A:500[B]:3Q8:CGA	2.13	0.42
1:A:363:LEU:O	1:A:364:VAL:HG13	2.19	0.42
1:A:486:ARG:HH21	1:B:325:THR:HG23	1.84	0.42
1:B:162:ARG:HG2	1:B:163:PHE:O	2.20	0.42
1:B:183:PHE:HZ	1:B:252:MET:HE2	1.83	0.42
1:B:220:LEU:HD13	1:B:220:LEU:HA	1.91	0.42
1:B:288:ARG:O	1:B:291:GLU:HB3	2.19	0.42
1:B:345:LEU:HD11	1:B:352:GLY:C	2.40	0.42
1:A:116:GLY:O	1:A:117:MET:C	2.58	0.42
1:A:428:ARG:HD2	1:A:474:TRP:CZ2	2.55	0.42
1:A:440:ASN:ND2	1:A:442:ARG:N	2.65	0.42
1:B:11:SER:HB2	1:B:13[A]:CYS:CB	2.49	0.42
1:A:163:PHE:O	1:A:164:ASP:O	2.38	0.42
1:A:393:ARG:HB3	1:A:396:THR:HG23	2.01	0.42
1:B:90:ALA:HB3	1:B:93:TYR:HE1	1.84	0.42
1:B:429:PRO:HD2	4:B:734:HOH:O	2.18	0.42
1:A:87:VAL:CA	1:A:92:ALA:CB	2.91	0.42
1:A:201:TYR:OH	2:A:500[B]:3Q8:H25	2.19	0.42
1:A:254:VAL:HB	1:A:275[B]:HIS:CD2	2.55	0.42
1:A:392:ASP:HB2	1:A:471:SER:HB3	2.01	0.42
1:B:392:ASP:OD1	1:B:392:ASP:N	2.53	0.42
1:B:407:VAL:HA	1:B:429:PRO:HB3	2.01	0.42
1:A:164:ASP:OD1	1:A:164:ASP:C	2.58	0.42
1:A:340:GLU:OE1	1:A:340:GLU:N	2.53	0.42
1:A:358:GLY:HA2	1:A:422:ARG:NE	2.35	0.42
1:A:401:LEU:O	1:A:401:LEU:CD1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:GLY:C	1:B:103:LEU:HG	2.40	0.42
1:B:265:GLU:HG2	4:B:714:HOH:O	2.19	0.42
1:A:87:VAL:HG22	1:A:92:ALA:CB	2.50	0.42
1:A:109:GLU:CG	1:A:110:PRO:CD	2.98	0.42
1:B:19:HIS:ND1	1:B:20:LEU:HD22	2.34	0.42
1:B:367:THR:CB	1:B:368:PRO:HD2	2.50	0.42
1:A:24:ILE:CD1	1:A:217:VAL:O	2.68	0.42
1:A:84:VAL:O	1:A:94:ARG:NH1	2.52	0.42
1:A:340:GLU:OE1	1:A:340:GLU:HA	2.19	0.42
1:B:50:LEU:HD22	1:B:50:LEU:HA	1.87	0.42
1:B:84:VAL:O	1:B:95:ALA:CB	2.68	0.42
1:A:30:LEU:HD12	1:A:107:GLU:HG2	2.01	0.42
1:B:272:ILE:O	1:B:272:ILE:HG22	2.19	0.42
1:A:11:SER:C	1:A:13[B]:CYS:H	2.22	0.42
1:B:489:LEU:O	1:B:490:VAL:C	2.58	0.42
1:A:11:SER:C	1:A:13[A]:CYS:H	2.22	0.41
1:A:206:LEU:H	1:A:206:LEU:HD12	1.85	0.41
1:A:224:VAL:HG12	1:A:227:LEU:HB2	2.02	0.41
2:A:500[B]:3Q8:H1	2:A:500[B]:3Q8:C2A	2.39	0.41
1:B:32:ALA:O	1:B:40:LEU:HA	2.20	0.41
1:B:272:ILE:HD12	1:B:294:THR:HG23	2.02	0.41
1:B:320:LEU:HD11	1:B:347:LEU:HD13	2.01	0.41
1:B:489:LEU:C	1:B:490:VAL:C	2.79	0.41
1:A:133:ALA:HB1	1:A:300:GLN:HE22	1.85	0.41
1:A:163:PHE:CE1	1:A:270:GLY:HA2	2.54	0.41
1:A:183:PHE:O	1:A:184:LEU:C	2.58	0.41
1:B:26:SER:O	1:B:26:SER:OG	2.33	0.41
1:B:155:PHE:CD2	1:B:274:CYS:HB3	2.55	0.41
1:B:263:LEU:O	1:B:263:LEU:CD1	2.68	0.41
1:B:470:THR:CG2	1:B:471:SER:H	2.32	0.41
1:A:20:LEU:C	1:A:230:PRO:HG2	2.41	0.41
1:A:147:ASP:OD1	1:A:175:SER:CB	2.68	0.41
1:A:353:VAL:CG1	1:A:426:TRP:CD1	2.89	0.41
1:A:362:LEU:HD13	1:A:362:LEU:HA	1.83	0.41
1:A:376:LEU:O	1:A:379:TRP:N	2.54	0.41
1:A:435:ILE:CG2	1:A:437:TRP:HD1	2.33	0.41
1:A:174:GLU:HG2	1:A:176:LYS:HD2	2.02	0.41
1:B:18:ILE:O	1:B:19:HIS:CG	2.73	0.41
1:B:18:ILE:HG21	1:B:239:ARG:HH22	1.85	0.41
1:B:435:ILE:HD11	1:B:437:TRP:HE1	1.86	0.41
1:A:54:PRO:O	1:A:58:LEU:CD2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ALA:CB	1:A:287:ARG:HH22	2.33	0.41
1:A:248[A]:TYR:CZ	2:A:500[A]:3Q8:H2	2.55	0.41
1:B:66:VAL:HG12	1:B:67:LEU:HD23	2.03	0.41
1:B:209:ILE:CD1	1:B:246:LEU:HD11	2.50	0.41
1:B:323:LEU:HD21	1:B:485:PHE:CE1	2.56	0.41
1:B:468:ARG:HA	4:B:716:HOH:O	2.21	0.41
1:A:284:HIS:CG	1:A:284:HIS:O	2.73	0.41
1:A:404:ARG:O	1:A:408:ALA:O	2.38	0.41
1:B:209:ILE:HD11	1:B:241:VAL:HG21	2.03	0.41
1:B:264:LYS:HG2	1:B:265:GLU:H	1.82	0.41
1:B:353:VAL:O	1:B:364:VAL:HG12	2.20	0.41
1:A:144:THR:C	1:A:146:ALA:N	2.72	0.41
1:A:153:THR:HG21	1:A:258:PHE:CE2	2.55	0.41
1:A:227:LEU:HD23	1:A:229:ARG:NH1	2.36	0.41
1:A:150:ARG:HH22	1:A:177:ARG:CA	2.34	0.41
1:B:31:LEU:HG	1:B:40:LEU:HD11	2.02	0.41
1:B:42:VAL:HG21	1:B:231:LEU:CD1	2.46	0.41
1:A:13[B]:CYS:HA	2:A:500[B]:3Q8:CAC	2.51	0.41
1:A:74:GLN:HB3	1:A:84:VAL:HG11	2.03	0.41
1:A:152:LEU:HD13	1:A:152:LEU:HA	1.94	0.41
1:B:160:VAL:O	1:B:160:VAL:HG23	2.21	0.41
1:B:194:PRO:O	1:B:198:ARG:HD3	2.21	0.41
1:B:283:SER:O	1:B:287:ARG:HG3	2.21	0.41
1:B:296:LEU:HD12	1:B:296:LEU:O	2.21	0.41
1:B:376:LEU:O	1:B:380:LEU:HD13	2.20	0.41
2:B:602[A]:3Q8:CGA	4:B:711:HOH:O	2.69	0.41
1:A:24:ILE:HD12	1:A:217:VAL:HG13	2.03	0.41
1:A:394:LEU:O	1:A:394:LEU:CD2	2.61	0.41
1:A:405:ALA:O	1:A:430:GLU:HB3	2.20	0.41
1:B:394:LEU:HD21	1:B:411:ILE:HD11	2.02	0.41
1:A:192:ASP:HA	2:A:500[A]:3Q8:O_C	2.20	0.40
1:A:378:ALA:CA	4:A:603:HOH:O	2.68	0.40
1:B:38:ARG:O	1:B:39:LEU:CB	2.69	0.40
1:B:367:THR:OG1	1:B:368:PRO:CD	2.69	0.40
1:B:379:TRP:CZ2	1:B:397:VAL:O	2.74	0.40
1:A:41:GLU:CD	4:A:627:HOH:O	2.60	0.40
1:A:241:VAL:HG12	2:A:500[A]:3Q8:CGD	2.51	0.40
1:A:262:LEU:CD1	1:A:294:THR:HG22	2.52	0.40
1:A:468:ARG:HE	1:A:468:ARG:HA	1.86	0.40
1:B:117:MET:O	1:B:121:ALA:N	2.36	0.40
1:B:148:THR:O	1:B:149:VAL:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:LYS:HE3	1:B:180:MET:HB2	2.03	0.40
1:B:224:VAL:O	1:B:225:PRO:C	2.59	0.40
1:A:44:SER:HA	1:A:219:LEU:HB3	2.03	0.40
1:A:58:LEU:HD12	1:A:66:VAL:HG22	2.04	0.40
1:A:71:VAL:HG13	1:A:86:VAL:HG11	2.03	0.40
1:A:188:PHE:HA	1:A:437:TRP:CZ3	2.56	0.40
1:A:206:LEU:HD22	1:A:287:ARG:HG3	2.03	0.40
1:A:363:LEU:HD11	1:A:370:GLN:HG2	2.04	0.40
1:A:448:GLU:O	1:A:450:GLY:N	2.54	0.40
1:B:18:ILE:CG2	1:B:239:ARG:HH22	2.35	0.40
1:B:122:LEU:HA	1:B:125:VAL:HG12	2.02	0.40
1:A:24:ILE:HG23	1:A:219:LEU:HD21	2.03	0.40
1:A:174:GLU:CG	1:A:176:LYS:HD2	2.52	0.40
1:A:284:HIS:HA	1:A:287:ARG:HG2	2.04	0.40
1:A:428:ARG:O	1:A:428:ARG:HG2	2.22	0.40
1:A:441:PRO:HD2	1:A:463:TRP:CE3	2.56	0.40
1:A:58:LEU:N	1:A:58:LEU:CD2	2.83	0.40
1:A:128:LEU:O	1:A:129:VAL:HG23	2.22	0.40
1:A:207:ARG:NH2	1:A:259:SER:O	2.55	0.40
1:A:414:VAL:O	1:A:423:PHE:HA	2.21	0.40
1:B:63:VAL:CG1	1:B:64:GLY:N	2.83	0.40
1:B:164:ASP:O	1:B:165:ALA:C	2.59	0.40
1:B:268:LEU:HD12	1:B:268:LEU:HA	1.84	0.40
1:B:470:THR:CG2	1:B:471:SER:N	2.83	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:HIS:ND1	4:B:702:HOH:O[2_444]	2.15	0.05
1:A:89:PRO:O	1:B:72:LEU:O[2_555]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	483/482 (100%)	313 (65%)	108 (22%)	62 (13%)	0	0
1	B	479/482 (99%)	306 (64%)	107 (22%)	66 (14%)	0	0
All	All	962/964 (100%)	619 (64%)	215 (22%)	128 (13%)	0	0

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	36	PRO
1	A	37	ASP
1	A	41	GLU
1	A	46	ASN
1	A	65	ARG
1	A	117	MET
1	A	175	SER
1	A	189	PRO
1	A	192	ASP
1	A	220	LEU
1	A	222	PRO
1	A	229	ARG
1	A	231	LEU
1	A	232	ASP
1	A	238	LEU
1	A	244	VAL
1	A	405	ALA
1	A	417	ALA
1	A	478	ASP
1	B	31	LEU
1	B	37	ASP
1	B	44	SER
1	B	70	GLU
1	B	126	ARG
1	B	157	ARG
1	B	165	ALA
1	B	178	GLY
1	B	189	PRO
1	B	192	ASP
1	B	236	SER
1	B	252	MET
1	B	263	LEU

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Mol	Chain	Res	Type
1	B	344	VAL
1	B	359	GLU
1	B	405	ALA
1	B	406	ASP
1	B	418	PRO
1	B	432	ALA
1	B	456	PRO
1	B	477	ALA
1	A	40	LEU
1	A	45	ALA
1	A	52	GLY
1	A	56	GLU
1	A	60	GLY
1	A	68	PRO
1	A	91	GLY
1	A	129	VAL
1	A	145	ALA
1	A	155	PHE
1	A	184	LEU
1	A	205	PRO
1	A	213	ARG
1	A	246	LEU
1	A	364	VAL
1	A	385	PHE
1	A	418	PRO
1	A	469	ASP
1	A	479	LEU
1	B	26	SER
1	B	39	LEU
1	B	51	LEU
1	B	79	VAL
1	B	84	VAL
1	B	95	ALA
1	B	129	VAL
1	B	184	LEU
1	B	193	ILE
1	B	268	LEU
1	B	364	VAL
1	B	429	PRO
1	B	433	ARG
1	B	449	PRO
1	B	467	VAL

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Mol	Chain	Res	Type
1	B	468	ARG
1	A	62	PRO
1	A	160	VAL
1	A	164	ASP
1	A	172	LEU
1	A	194	PRO
1	A	206	LEU
1	A	252	MET
1	A	355	LEU
1	A	356	LEU
1	A	387	THR
1	A	457	ARG
1	B	13[A]	CYS
1	B	13[B]	CYS
1	B	36	PRO
1	B	96	LEU
1	B	102	GLY
1	B	132	LEU
1	B	225	PRO
1	B	269	TRP
1	B	333	LEU
1	B	387	THR
1	B	395	GLY
1	B	407	VAL
1	A	23	GLY
1	A	61	GLN
1	A	110	PRO
1	A	174	GLU
1	A	445	ALA
1	B	174	GLU
1	B	241	VAL
1	B	329	GLU
1	B	380	LEU
1	B	414	VAL
1	B	462	ALA
1	B	476	ARG
1	A	193	ILE
1	A	459	SER
1	B	212	ALA
1	B	272	ILE
1	B	308	ALA
1	A	243	PRO

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Mol	Chain	Res	Type
1	A	473	PRO
1	B	115	PRO
1	B	302	SER
1	B	368	PRO
1	A	456	PRO
1	B	205	PRO
1	B	105	VAL
1	B	149	VAL
1	B	353	VAL
1	A	154	GLY
1	A	384	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	379/375 (101%)	242 (64%)	137 (36%)	0 0
1	B	376/375 (100%)	257 (68%)	119 (32%)	0 0
All	All	755/750 (101%)	499 (66%)	256 (34%)	0 0

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	12	GLN
1	A	18	ILE
1	A	20	LEU
1	A	21	LEU
1	A	25	GLN
1	A	31	LEU
1	A	34	ARG
1	A	42	VAL
1	A	53	ARG
1	A	56	GLU
1	A	58	LEU

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Mol	Chain	Res	Type
1	A	59	LEU
1	A	62	PRO
1	A	65	ARG
1	A	67	LEU
1	A	68	PRO
1	A	70	GLU
1	A	76	GLU
1	A	78	LEU
1	A	79	VAL
1	A	81	ARG
1	A	84	VAL
1	A	85	ARG
1	A	88	LEU
1	A	94	ARG
1	A	96	LEU
1	A	97	LEU
1	A	103	LEU
1	A	105	VAL
1	A	108	LEU
1	A	109	GLU
1	A	113	LEU
1	A	117	MET
1	A	120	THR
1	A	124	VAL
1	A	129	VAL
1	A	136	LYS
1	A	138	THR
1	A	141	LEU
1	A	152	LEU
1	A	157	ARG
1	A	158	VAL
1	A	163	PHE
1	A	164	ASP
1	A	167	TRP
1	A	168	HIS
1	A	176	LYS
1	A	177	ARG
1	A	180	MET
1	A	184	LEU
1	A	191	THR
1	A	192	ASP
1	A	193	ILE

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Mol	Chain	Res	Type
1	A	195	VAL
1	A	202	THR
1	A	206	LEU
1	A	209	ILE
1	A	213	ARG
1	A	215	ARG
1	A	217	VAL
1	A	219	LEU
1	A	220	LEU
1	A	225	PRO
1	A	227	LEU
1	A	229	ARG
1	A	235	ASN
1	A	238	LEU
1	A	240	SER
1	A	241	VAL
1	A	246	LEU
1	A	247	GLU
1	A	248[A]	TYR
1	A	248[B]	TYR
1	A	249	LEU
1	A	251	ASN
1	A	254	VAL
1	A	259	SER
1	A	260	LEU
1	A	263	LEU
1	A	265	GLU
1	A	267	VAL
1	A	271	LEU
1	A	272	ILE
1	A	274	CYS
1	A	275[A]	HIS
1	A	275[B]	HIS
1	A	280	LEU
1	A	281	HIS
1	A	282	ILE
1	A	286	ARG
1	A	288	ARG
1	A	291	GLU
1	A	295	GLN
1	A	296	LEU
1	A	297	LEU

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Mol	Chain	Res	Type
1	A	301	LEU
1	A	306	ARG
1	A	309	GLU
1	A	311	SER
1	A	312	GLU
1	A	313	ASP
1	A	323	LEU
1	A	327	MET
1	A	339	LYS
1	A	340	GLU
1	A	347	LEU
1	A	356	LEU
1	A	359	GLU
1	A	362	LEU
1	A	364	VAL
1	A	367	THR
1	A	370	GLN
1	A	376	LEU
1	A	377	VAL
1	A	385	PHE
1	A	392	ASP
1	A	393	ARG
1	A	394	LEU
1	A	397	VAL
1	A	426	TRP
1	A	427	PHE
1	A	428	ARG
1	A	435	ILE
1	A	436	SER
1	A	440	ASN
1	A	443	LYS
1	A	446	GLU
1	A	455	HIS
1	A	457	ARG
1	A	463	TRP
1	A	466	THR
1	A	471	SER
1	A	472	LEU
1	A	475	LYS
1	A	479	LEU
1	A	486	ARG
1	B	9	ASP

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Mol	Chain	Res	Type
1	B	11	SER
1	B	13[A]	CYS
1	B	13[B]	CYS
1	B	15	ARG
1	B	18	ILE
1	B	20	LEU
1	B	25	GLN
1	B	27	HIS
1	B	29	VAL
1	B	30	LEU
1	B	31	LEU
1	B	40	LEU
1	B	46	ASN
1	B	50	LEU
1	B	67	LEU
1	B	70	GLU
1	B	72	LEU
1	B	78	LEU
1	B	96	LEU
1	B	97	LEU
1	B	101	ASP
1	B	105	VAL
1	B	107	GLU
1	B	108	LEU
1	B	114	GLN
1	B	119	GLU
1	B	120	THR
1	B	122	LEU
1	B	130	SER
1	B	132	LEU
1	B	136	LYS
1	B	139	GLN
1	B	141	LEU
1	B	142	LEU
1	B	143	GLN
1	B	153	THR
1	B	157	ARG
1	B	158	VAL
1	B	159	MET
1	B	163	PHE
1	B	164	ASP
1	B	168	HIS

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Mol	Chain	Res	Type
1	B	176	LYS
1	B	183	PHE
1	B	184	LEU
1	B	186	MET
1	B	188	PHE
1	B	189	PRO
1	B	191	THR
1	B	193	ILE
1	B	195	VAL
1	B	198	ARG
1	B	200	LEU
1	B	203	ARG
1	B	204	ASN
1	B	206	LEU
1	B	207	ARG
1	B	215	ARG
1	B	219	LEU
1	B	220	LEU
1	B	225	PRO
1	B	229	ARG
1	B	231	LEU
1	B	236	SER
1	B	238	LEU
1	B	244	VAL
1	B	248[A]	TYR
1	B	248[B]	TYR
1	B	251	ASN
1	B	254	VAL
1	B	259	SER
1	B	260	LEU
1	B	264	LYS
1	B	267	VAL
1	B	280	LEU
1	B	283	SER
1	B	291	GLU
1	B	294	THR
1	B	306	ARG
1	B	313	ASP
1	B	322	GLN
1	B	325	THR
1	B	333	LEU
1	B	338	GLU

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Mol	Chain	Res	Type
1	B	339	LYS
1	B	340	GLU
1	B	343	ARG
1	B	345	LEU
1	B	360	GLU
1	B	367	THR
1	B	380	LEU
1	B	383	GLN
1	B	390	HIS
1	B	392	ASP
1	B	393	ARG
1	B	394	LEU
1	B	396	THR
1	B	401	LEU
1	B	406	ASP
1	B	411	ILE
1	B	416	LEU
1	B	422	ARG
1	B	423	PHE
1	B	425	ILE
1	B	428	ARG
1	B	430	GLU
1	B	433	ARG
1	B	435	ILE
1	B	442	ARG
1	B	453	ARG
1	B	455	HIS
1	B	457	ARG
1	B	465	GLU
1	B	468	ARG
1	B	475	LYS
1	B	476	ARG
1	B	485	PHE
1	B	486	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	139	GLN
1	A	143	GLN
1	A	204	ASN

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Mol	Chain	Res	Type
1	A	276	HIS
1	A	284	HIS
1	A	300	GLN
1	A	370	GLN
1	A	440	ASN
1	B	25	GLN
1	B	46	ASN
1	B	114	GLN
1	B	143	GLN
1	B	251	ASN
1	B	275	HIS
1	B	300	GLN
1	B	370	GLN
1	B	383	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	BEN	B	601	-	9,9,9	0.86	0	7,11,11	1.38	1 (14%)
2	3Q8	B	602[A]	1	39,46,46	6.97	18 (46%)	34,67,67	2.77	10 (29%)
2	3Q8	B	602[B]	1	39,46,46	6.71	18 (46%)	34,67,67	2.79	9 (26%)
2	3Q8	A	500[A]	1	39,46,46	6.83	17 (43%)	34,67,67	2.36	11 (32%)
2	3Q8	A	500[B]	1	39,46,46	6.85	15 (38%)	34,67,67	2.62	14 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BEN	B	601	-	-	3/4/4/4	0/1/1/1
2	3Q8	B	602[A]	1	-	20/22/58/58	0/4/4/4
2	3Q8	B	602[B]	1	-	12/22/58/58	0/4/4/4
2	3Q8	A	500[A]	1	-	13/22/58/58	0/4/4/4
2	3Q8	A	500[B]	1	-	14/22/58/58	0/4/4/4

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602[A]	3Q8	CHA-C4D	-26.66	1.31	1.51
2	A	500[A]	3Q8	CHA-C4D	-26.02	1.31	1.51
2	A	500[B]	3Q8	CHA-C4D	-25.42	1.32	1.51
2	B	602[B]	3Q8	CHA-C4D	-24.65	1.32	1.51
2	B	602[A]	3Q8	CHB-C1B	-18.61	1.30	1.50
2	A	500[B]	3Q8	CHB-C1B	-17.78	1.31	1.50
2	A	500[B]	3Q8	CHD-C4C	-17.57	1.31	1.50
2	A	500[A]	3Q8	CHB-C1B	-17.51	1.31	1.50
2	A	500[A]	3Q8	CHD-C4C	-17.15	1.31	1.50
2	B	602[B]	3Q8	CHB-C1B	-16.86	1.32	1.50
2	B	602[A]	3Q8	CHD-C4C	-15.61	1.33	1.50
2	B	602[B]	3Q8	CHD-C4C	-15.42	1.33	1.50
2	B	602[B]	3Q8	C4C-N-C	11.69	1.56	1.35
2	B	602[A]	3Q8	C4C-N-C	11.63	1.56	1.35
2	A	500[B]	3Q8	C1B-N-B	11.06	1.55	1.35
2	A	500[A]	3Q8	C1B-N-B	10.70	1.54	1.35
2	B	602[B]	3Q8	C1B-N-B	10.68	1.54	1.35
2	A	500[B]	3Q8	C4B-N-B	10.45	1.56	1.37
2	A	500[B]	3Q8	C4C-N-C	9.96	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500[A]	3Q8	C4C-N-C	9.91	1.53	1.35
2	B	602[A]	3Q8	C1B-N-B	9.62	1.52	1.35
2	B	602[A]	3Q8	C4B-N-B	9.31	1.54	1.37
2	B	602[A]	3Q8	C1C-N-C	9.17	1.56	1.36
2	B	602[B]	3Q8	C1C-N-C	9.10	1.55	1.36
2	B	602[B]	3Q8	C3D-C4D	9.05	1.52	1.39
2	A	500[A]	3Q8	C4B-N-B	9.05	1.53	1.37
2	B	602[A]	3Q8	C3D-C4D	8.76	1.52	1.39
2	B	602[B]	3Q8	C4B-N-B	8.70	1.53	1.37
2	A	500[A]	3Q8	C3D-C4D	8.49	1.51	1.39
2	A	500[B]	3Q8	C3D-C4D	8.47	1.51	1.39
2	A	500[A]	3Q8	C1C-N-C	7.50	1.52	1.36
2	A	500[B]	3Q8	C1C-N-C	7.48	1.52	1.36
2	B	602[A]	3Q8	C2D-C1D	4.84	1.49	1.42
2	A	500[A]	3Q8	C2D-C1D	4.71	1.49	1.42
2	B	602[B]	3Q8	CBB-CAB	-4.55	1.31	1.51
2	B	602[A]	3Q8	CBB-CAB	-4.44	1.31	1.51
2	A	500[B]	3Q8	CBB-CAB	-4.41	1.31	1.51
2	A	500[B]	3Q8	C2D-C1D	4.32	1.48	1.42
2	A	500[A]	3Q8	CBB-CAB	-4.29	1.32	1.51
2	B	602[B]	3Q8	CHA-C1A	4.27	1.54	1.51
2	B	602[B]	3Q8	C2D-C1D	4.00	1.48	1.42
2	A	500[A]	3Q8	C2C-C1C	-3.88	1.47	1.52
2	B	602[B]	3Q8	C3A-C4A	-3.83	1.36	1.42
2	A	500[A]	3Q8	O-B-C4B	-3.77	1.17	1.23
2	B	602[B]	3Q8	C3D-C2D	3.46	1.47	1.37
2	A	500[B]	3Q8	O-C-C1C	-3.34	1.17	1.23
2	B	602[B]	3Q8	O-B-C4B	-3.31	1.18	1.23
2	A	500[B]	3Q8	C2C-C1C	-3.24	1.47	1.52
2	B	602[A]	3Q8	C3D-C2D	3.13	1.47	1.37
2	B	602[A]	3Q8	O-B-C4B	-3.12	1.18	1.23
2	A	500[A]	3Q8	O-C-C1C	-3.04	1.18	1.23
2	B	602[A]	3Q8	C2C-C1C	-2.95	1.48	1.52
2	B	602[A]	3Q8	O-C-C1C	-2.94	1.18	1.23
2	B	602[B]	3Q8	O-C-C1C	-2.71	1.18	1.23
2	A	500[A]	3Q8	C3D-C2D	2.58	1.45	1.37
2	B	602[A]	3Q8	C3A-C4A	-2.47	1.38	1.42
2	A	500[B]	3Q8	C3B-C2B	2.43	1.41	1.36
2	B	602[B]	3Q8	C2A-C1A	-2.41	1.35	1.39
2	A	500[B]	3Q8	C3D-C2D	2.36	1.44	1.37
2	A	500[A]	3Q8	C3B-C2B	2.35	1.41	1.36
2	B	602[B]	3Q8	C2C-C1C	-2.28	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500[B]	3Q8	CHA-C1A	2.26	1.53	1.51
2	B	602[A]	3Q8	C2A-C1A	-2.23	1.35	1.39
2	B	602[A]	3Q8	C3B-C2B	2.17	1.41	1.36
2	B	602[B]	3Q8	C3B-C2B	2.16	1.41	1.36
2	A	500[A]	3Q8	CHA-C1A	2.16	1.53	1.51
2	A	500[A]	3Q8	C2B-C1B	2.09	1.50	1.43
2	B	602[A]	3Q8	CHA-C1A	2.07	1.53	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	602[B]	3Q8	CAA-C2A-C1A	-11.24	119.40	127.30
2	B	602[A]	3Q8	CAA-C2A-C1A	-9.81	120.40	127.30
2	A	500[A]	3Q8	CAD-C3D-C4D	-6.73	122.57	127.30
2	A	500[B]	3Q8	CAD-C3D-C4D	-6.42	122.78	127.30
2	A	500[B]	3Q8	CBD-CAD-C3D	-6.11	102.19	112.62
2	B	602[A]	3Q8	CAD-C3D-C4D	-5.81	123.22	127.30
2	B	602[B]	3Q8	C4B-C3B-C2B	5.66	112.73	107.40
2	A	500[A]	3Q8	CBD-CAD-C3D	-5.55	103.15	112.62
2	A	500[B]	3Q8	CHB-C1B-C2B	-5.53	119.19	129.53
2	B	602[B]	3Q8	C3C-C2C-C1C	5.32	108.57	103.16
2	A	500[A]	3Q8	C3C-C2C-C1C	5.24	108.49	103.16
2	A	500[B]	3Q8	C3C-C2C-C1C	5.01	108.26	103.16
2	B	602[A]	3Q8	CBC-CAC-C3C	-4.82	112.62	126.72
2	A	500[B]	3Q8	C4B-C3B-C2B	4.33	111.47	107.40
2	B	602[A]	3Q8	C3C-C2C-C1C	4.20	107.44	103.16
2	B	602[B]	3Q8	CAD-C3D-C4D	-4.08	124.43	127.30
2	A	500[A]	3Q8	C4B-C3B-C2B	4.02	111.18	107.40
2	A	500[A]	3Q8	CBA-CAA-C2A	-3.85	106.05	112.62
2	B	602[A]	3Q8	CHB-C1B-C2B	-3.83	122.37	129.53
3	B	601	BEN	C1-C-N2	3.65	123.54	118.05
2	B	602[A]	3Q8	O-C-C1C-N-C	3.57	130.19	125.05
2	B	602[A]	3Q8	C4B-C3B-C2B	3.54	110.73	107.40
2	B	602[A]	3Q8	CAD-CBD-CGD	-3.11	105.05	113.76
2	A	500[B]	3Q8	CBC-CAC-C3C	-3.07	117.73	126.72
2	B	602[B]	3Q8	CAD-CBD-CGD	-2.99	105.37	113.76
2	A	500[B]	3Q8	CAB-C3B-C2B	-2.94	122.50	127.53
2	B	602[B]	3Q8	O-C-C1C-N-C	2.93	129.26	125.05
2	B	602[B]	3Q8	CBC-CAC-C3C	-2.89	118.27	126.72
2	A	500[B]	3Q8	CAD-CBD-CGD	-2.72	106.13	113.76
2	B	602[A]	3Q8	CAA-CBA-CGA	-2.65	106.33	113.76
2	A	500[B]	3Q8	CAB-C3B-C4B	2.61	126.03	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500[B]	3Q8	CBB-CAB-C3B	2.58	119.54	112.43
2	A	500[A]	3Q8	CAA-C2A-C1A	-2.55	125.51	127.30
2	A	500[A]	3Q8	O-B-C4B-N-B	2.52	129.47	124.36
2	A	500[A]	3Q8	CAD-CBD-CGD	-2.37	107.12	113.76
2	B	602[B]	3Q8	CMA-C3A-C2A	2.35	129.38	124.94
2	A	500[B]	3Q8	CBA-CAA-C2A	-2.33	108.65	112.62
2	B	602[A]	3Q8	O1A-CGA-O2A	-2.29	117.60	123.30
2	A	500[B]	3Q8	C3B-C4B-N-B	-2.26	105.07	110.44
2	A	500[B]	3Q8	O1A-CGA-O2A	-2.17	117.89	123.30
2	A	500[A]	3Q8	CBC-CAC-C3C	-2.17	120.37	126.72
2	A	500[B]	3Q8	O1A-CGA-CBA	2.12	120.83	114.03
2	A	500[A]	3Q8	O1D-CGD-CBD	2.08	120.72	114.03
2	B	602[B]	3Q8	C3B-C4B-N-B	-2.08	105.51	110.44
2	A	500[A]	3Q8	CBB-CAB-C3B	2.01	117.99	112.43

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500[A]	3Q8	C4B-C3B-CAB-CBB
2	A	500[A]	3Q8	C4D-C3D-CAD-CBD
2	A	500[A]	3Q8	C2D-C3D-CAD-CBD
2	A	500[A]	3Q8	C4C-C3C-CAC-CBC
2	A	500[A]	3Q8	C2C-C3C-CAC-CBC
2	A	500[B]	3Q8	B-N-C1B-CHB-C4A
2	A	500[B]	3Q8	C3A-C4A-CHB-C1B
2	A	500[B]	3Q8	C4D-C3D-CAD-CBD
2	A	500[B]	3Q8	C2D-C3D-CAD-CBD
2	A	500[B]	3Q8	C4C-C3C-CAC-CBC
2	A	500[B]	3Q8	C2C-C3C-CAC-CBC
2	B	602[A]	3Q8	C4B-C3B-CAB-CBB
2	B	602[A]	3Q8	B-N-C1B-CHB-C4A
2	B	602[A]	3Q8	C3A-C4A-CHB-C1B
2	B	602[A]	3Q8	C3A-C2A-CAA-CBA
2	B	602[A]	3Q8	C1A-C2A-CAA-CBA
2	B	602[A]	3Q8	C4D-C3D-CAD-CBD
2	B	602[A]	3Q8	C2D-C3D-CAD-CBD
2	B	602[A]	3Q8	C3D-CAD-CBD-CGD
2	B	602[A]	3Q8	C-N-C4C-CHD-C1D
2	B	602[A]	3Q8	C3C-C4C-CHD-C1D
2	B	602[A]	3Q8	C4C-C3C-CAC-CBC
2	B	602[A]	3Q8	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	B	602[B]	3Q8	C3A-C4A-CHB-C1B
2	B	602[B]	3Q8	C3A-C2A-CAA-CBA
2	B	602[B]	3Q8	C1A-C2A-CAA-CBA
2	B	602[B]	3Q8	C3D-CAD-CBD-CGD
2	B	602[B]	3Q8	C4C-C3C-CAC-CBC
2	B	602[B]	3Q8	C2C-C3C-CAC-CBC
3	B	601	BEN	N2-C-C1-C2
3	B	601	BEN	N2-C-C1-C6
2	A	500[B]	3Q8	C2B-C3B-CAB-CBB
2	B	602[B]	3Q8	C2B-C3B-CAB-CBB
2	B	602[A]	3Q8	C2B-C3B-CAB-CBB
2	A	500[A]	3Q8	C2B-C3B-CAB-CBB
2	A	500[A]	3Q8	C2A-CAA-CBA-CGA
2	A	500[A]	3Q8	C3D-CAD-CBD-CGD
2	A	500[B]	3Q8	C3D-CAD-CBD-CGD
2	B	602[A]	3Q8	C2A-CAA-CBA-CGA
2	A	500[B]	3Q8	C4B-C3B-CAB-CBB
2	B	602[B]	3Q8	C4B-C3B-CAB-CBB
2	A	500[A]	3Q8	C2B-C1B-CHB-C4A
2	A	500[B]	3Q8	C2B-C1B-CHB-C4A
2	B	602[B]	3Q8	CAD-CBD-CGD-O2D
2	B	602[A]	3Q8	CAA-CBA-CGA-O2A
2	B	602[A]	3Q8	CAA-CBA-CGA-O1A
2	B	602[A]	3Q8	CAD-CBD-CGD-O2D
2	B	602[B]	3Q8	CAD-CBD-CGD-O1D
2	A	500[A]	3Q8	CAD-CBD-CGD-O1D
2	A	500[A]	3Q8	CAD-CBD-CGD-O2D
2	B	602[A]	3Q8	CAD-CBD-CGD-O1D
2	A	500[B]	3Q8	CAD-CBD-CGD-O1D
2	A	500[B]	3Q8	CAD-CBD-CGD-O2D
2	B	602[B]	3Q8	C2A-CAA-CBA-CGA
2	A	500[A]	3Q8	C2A-C1A-CHA-C4D
2	A	500[B]	3Q8	C2A-C1A-CHA-C4D
2	B	602[A]	3Q8	C2D-C1D-CHD-C4C
2	B	602[B]	3Q8	C2D-C1D-CHD-C4C
3	B	601	BEN	N1-C-C1-C2
2	A	500[A]	3Q8	C3C-C4C-CHD-C1D
2	A	500[B]	3Q8	C3C-C4C-CHD-C1D
2	B	602[A]	3Q8	C2B-C1B-CHB-C4A

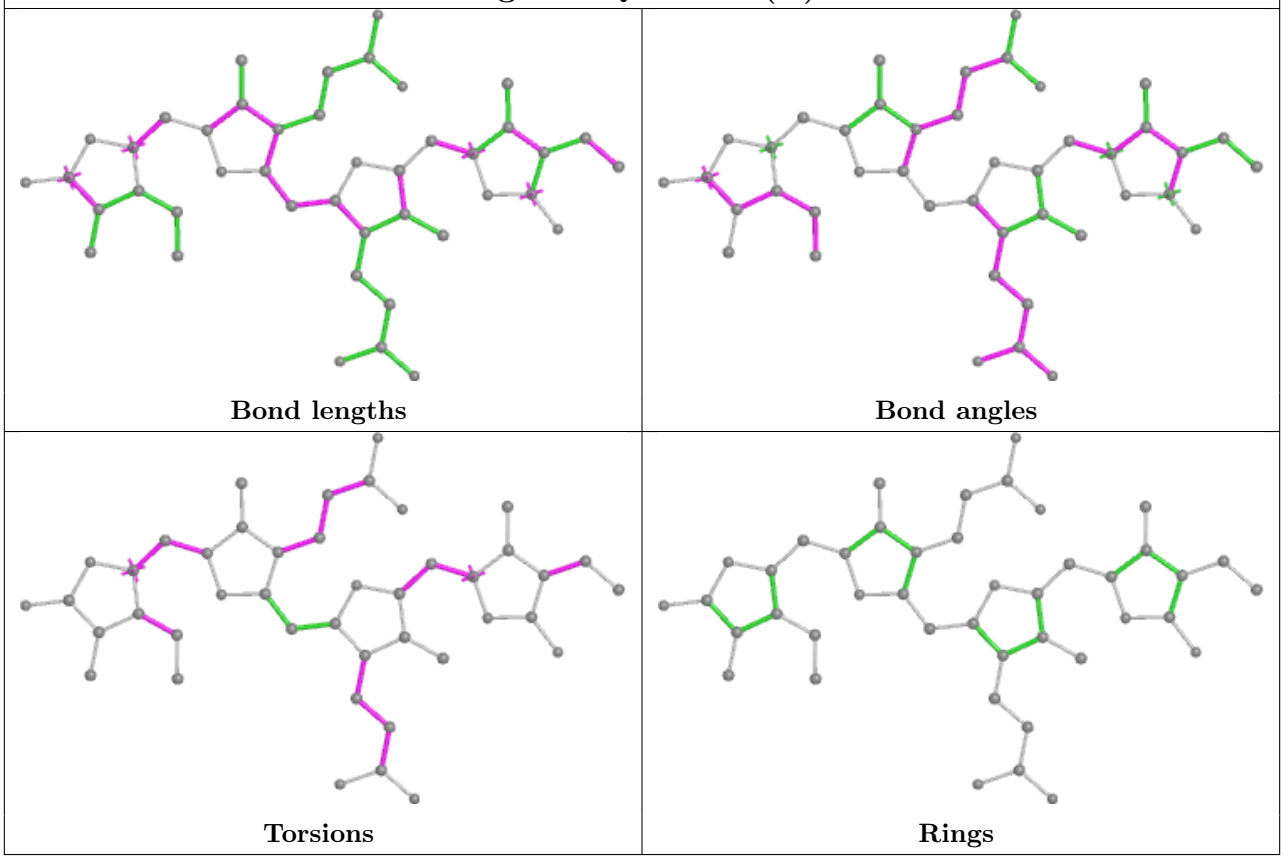
There are no ring outliers.

4 monomers are involved in 97 short contacts:

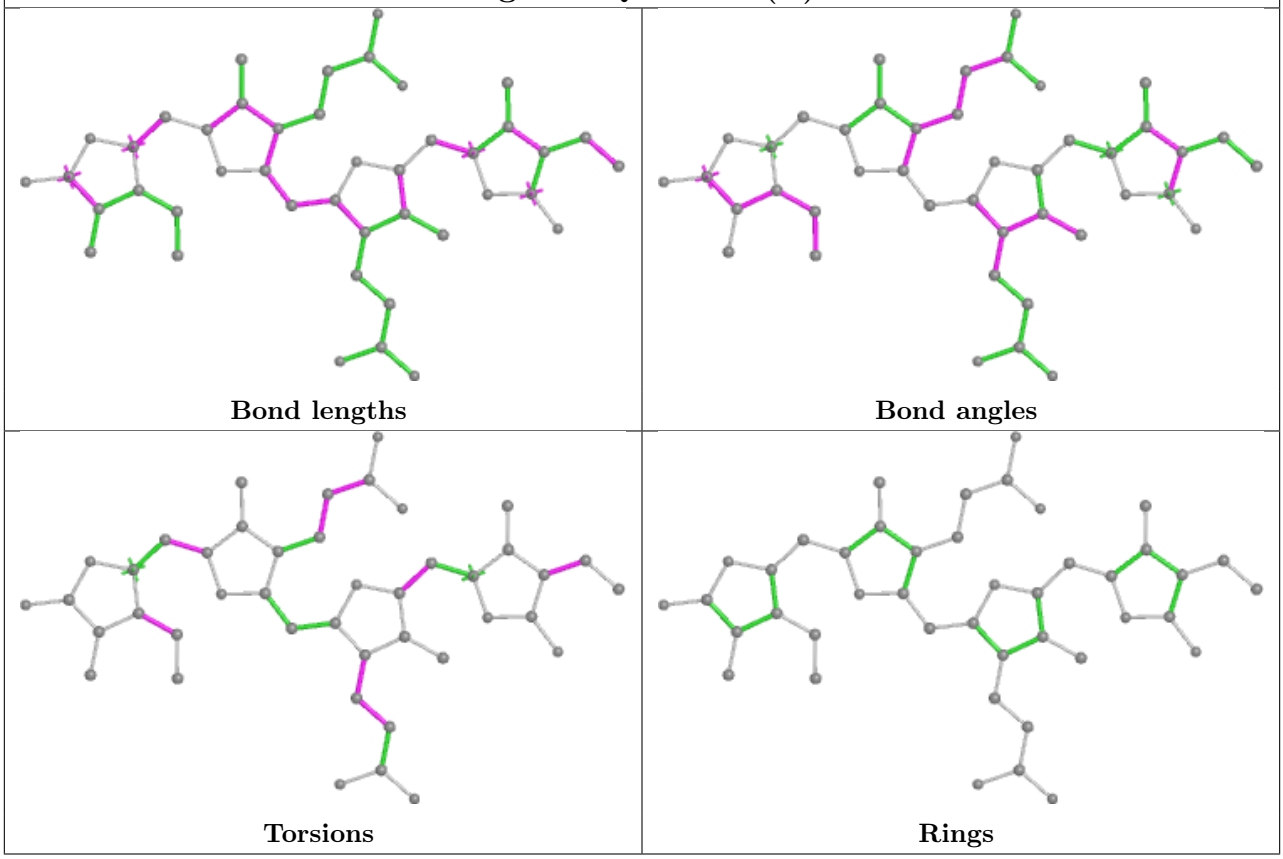
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602[A]	3Q8	26	0
2	B	602[B]	3Q8	22	0
2	A	500[A]	3Q8	21	0
2	A	500[B]	3Q8	28	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

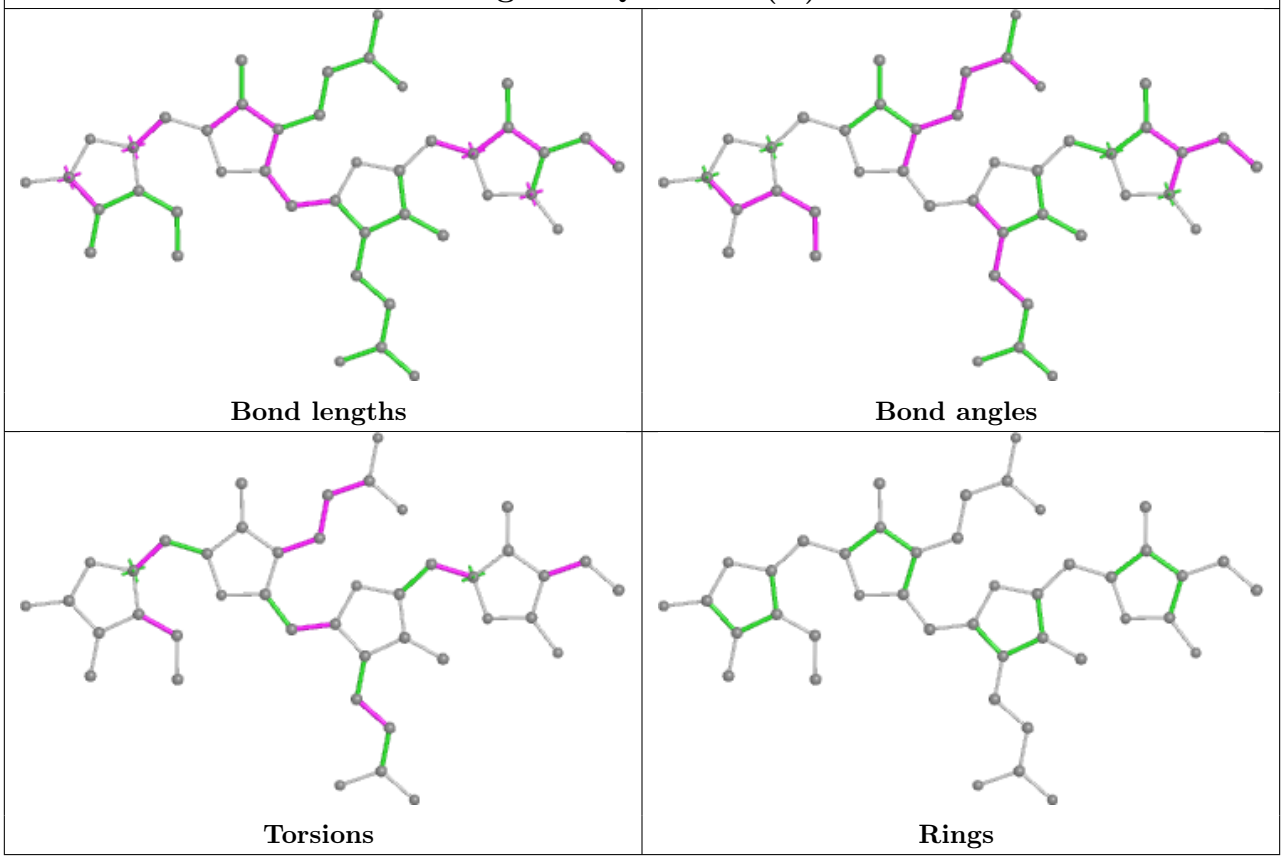
Ligand 3Q8 B 602 (A)



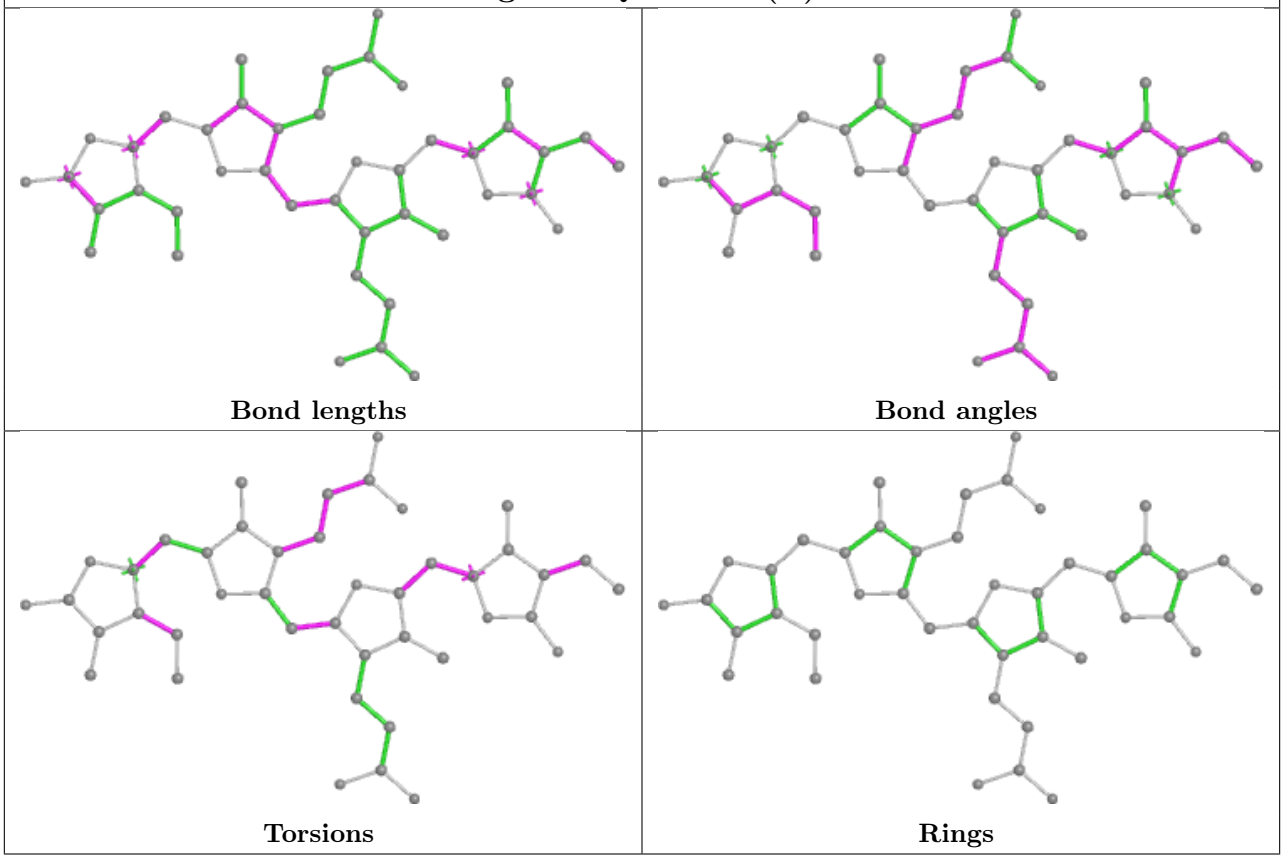
Ligand 3Q8 B 602 (B)



Ligand 3Q8 A 500 (A)



Ligand 3Q8 A 500 (B)



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	489:LEU	C	490:VAL	N	2.81
1	B	489:LEU	C	490:VAL	N	2.43
1	B	246:LEU	C	247:GLU	N	2.18

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	482/482 (100%)	-0.25	6 (1%)	79	77	3, 23, 43, 61	0
1	B	482/482 (100%)	-0.27	4 (0%)	86	84	3, 23, 42, 72	0
All	All	964/964 (100%)	-0.26	10 (1%)	82	80	3, 23, 43, 72	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	VAL	3.3
1	B	161	TYR	2.6
1	B	427	PHE	2.6
1	A	488	ALA	2.5
1	A	293	LEU	2.5
1	B	425	ILE	2.3
1	A	30	LEU	2.3
1	B	413	ALA	2.2
1	A	314	ALA	2.2
1	A	248[A]	TYR	2.2

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

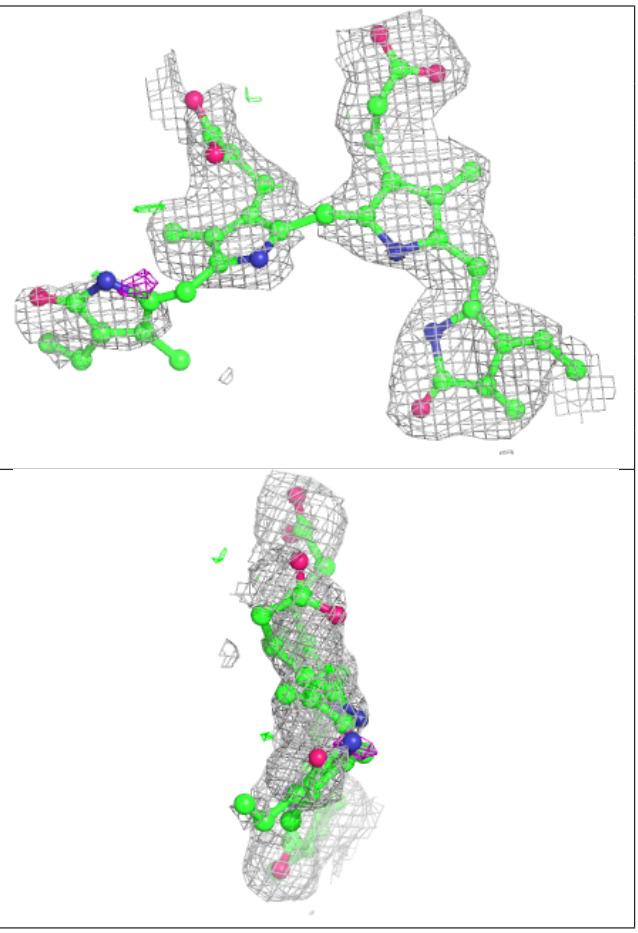
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BEN	B	601	9/9	0.37	0.59	117,118,124,125	0
2	3Q8	B	602[B]	43/43	0.86	0.26	20,22,30,30	43
2	3Q8	B	602[A]	43/43	0.86	0.26	18,19,29,30	43
2	3Q8	A	500[B]	43/43	0.88	0.23	13,18,21,23	43
2	3Q8	A	500[A]	43/43	0.88	0.23	16,20,23,24	43

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

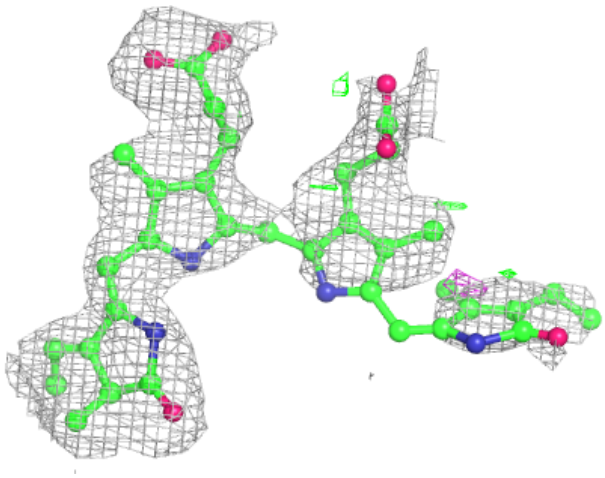
Electron density around 3Q8 B 602 (B):

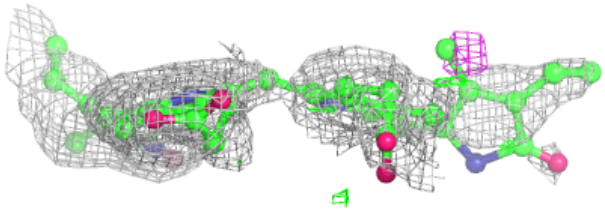
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

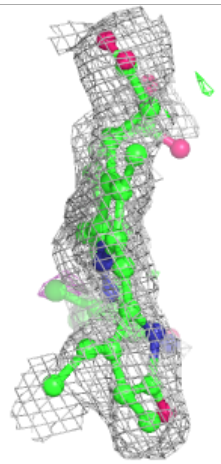


Electron density around 3Q8 B 602 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

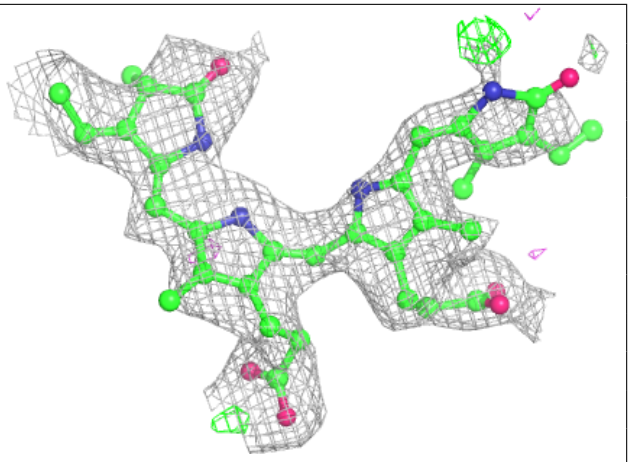


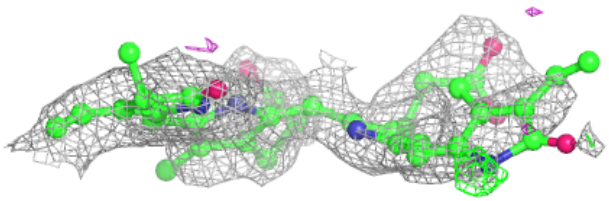


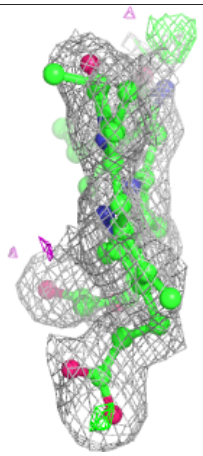


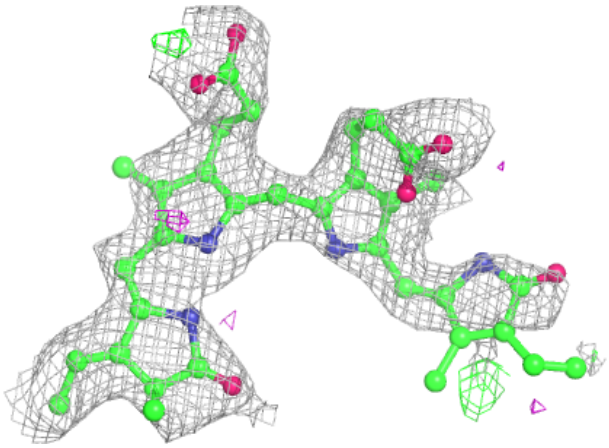
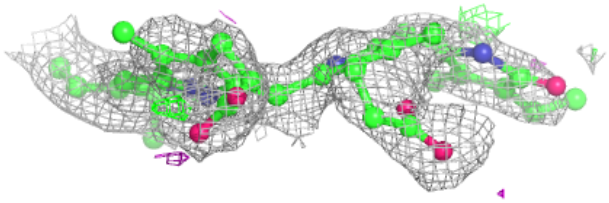
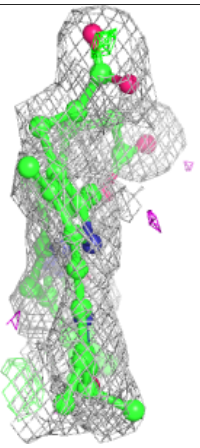
Electron density around 3Q8 A 500 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around 3Q8 A 500 (A): $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.