Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 11:19 PM EDT

PDB ID	:	6BAP
Title	:	Stigmatella aurantiaca bacterial phytochrome PAS-GAF-PHY, T289H mutant
Authors	:	Schmidt, M.; Stojkovic, E.
Deposited on	:	2017-10-14
Resolution	:	2.65 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:

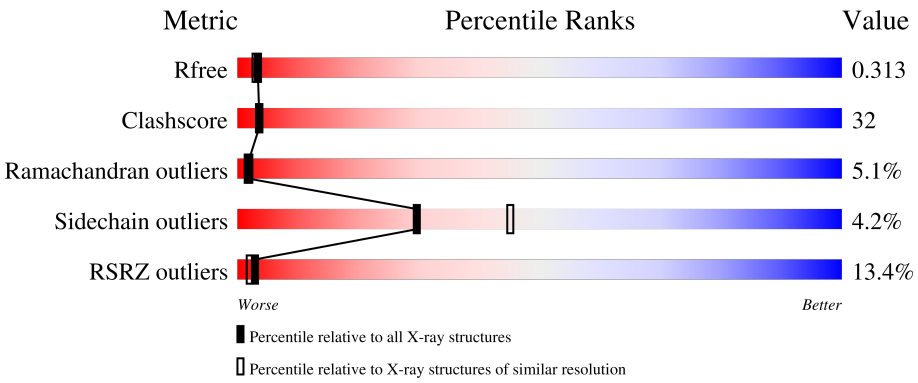
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	515	3% 63% 30% • • •
1	B	515	3% 57% 36% 5% • •
1	C	515	32% 38% 46% 11% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12158 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.

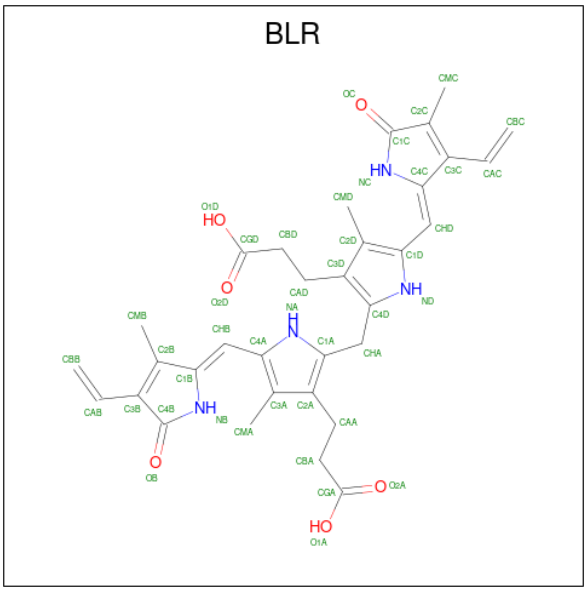
- Molecule 1 is a protein called Photoreceptor-histidine kinase BphP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	505	3982	2513	726	730	13	0	0	0
1	B	505	3982	2513	726	730	13	0	0	0
1	C	500	3941	2488	720	720	13	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	HIS	THR	engineered mutation	UNP Q097N3
B	289	HIS	THR	engineered mutation	UNP Q097N3
C	289	HIS	THR	engineered mutation	UNP Q097N3

- Molecule 2 is 3-[5-[(Z)-(4-ethenyl-3-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-2-[[5-[(Z)-(3-ethenyl-4-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-3-(3-hydroxy-3-oxopropyl)-4-methyl-1H-pyrrol-2-yl]methyl]-4-methyl-1H-pyrrol-3-yl]propanoic acid (three-letter code: BLR) (formula: $C_{33}H_{36}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	43	33	4	6	0	0
2	B	1	43	33	4	6	0	0
2	C	1	43	33	4	6	0	0

- Molecule 3 is water.

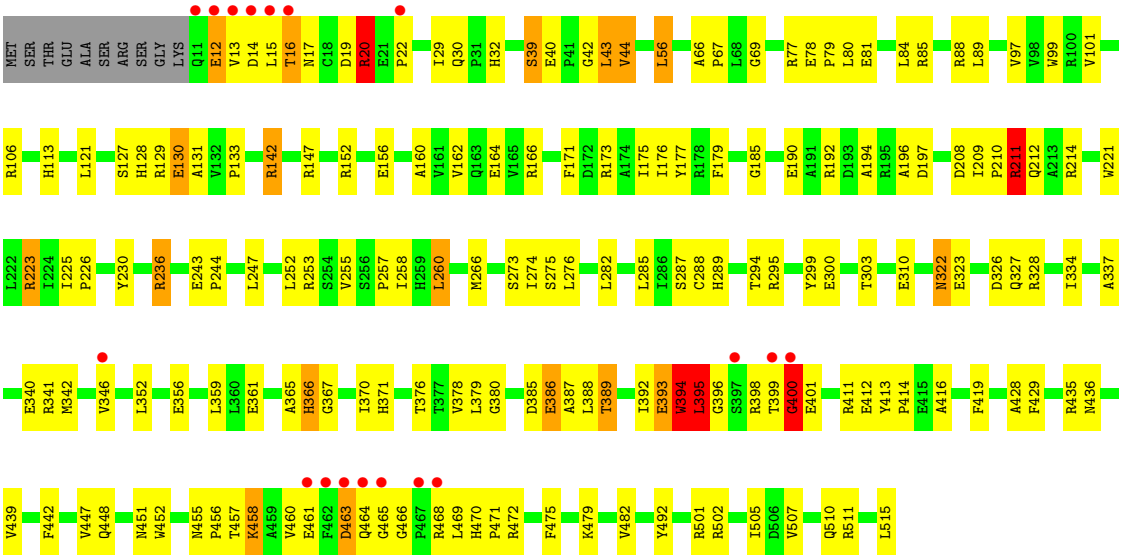
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	46	46	46	0	0
3	B	42	42	42	0	0
3	C	36	36	36	0	0

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.

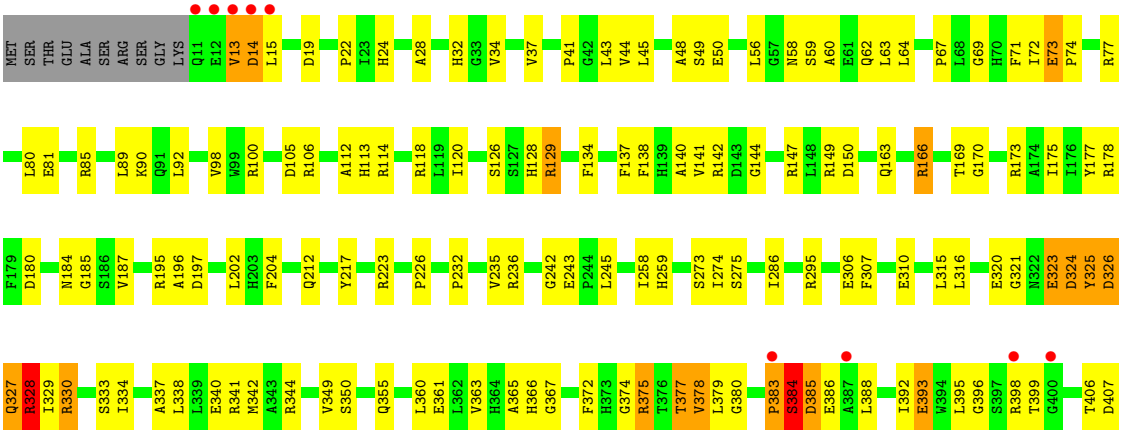
• Molecule 1: Photoreceptor-histidine kinase BphP

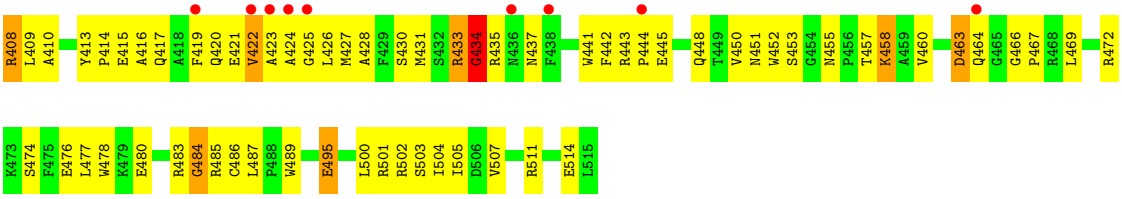
Chain A:



• Molecule 1: Photoreceptor-histidine kinase BphP

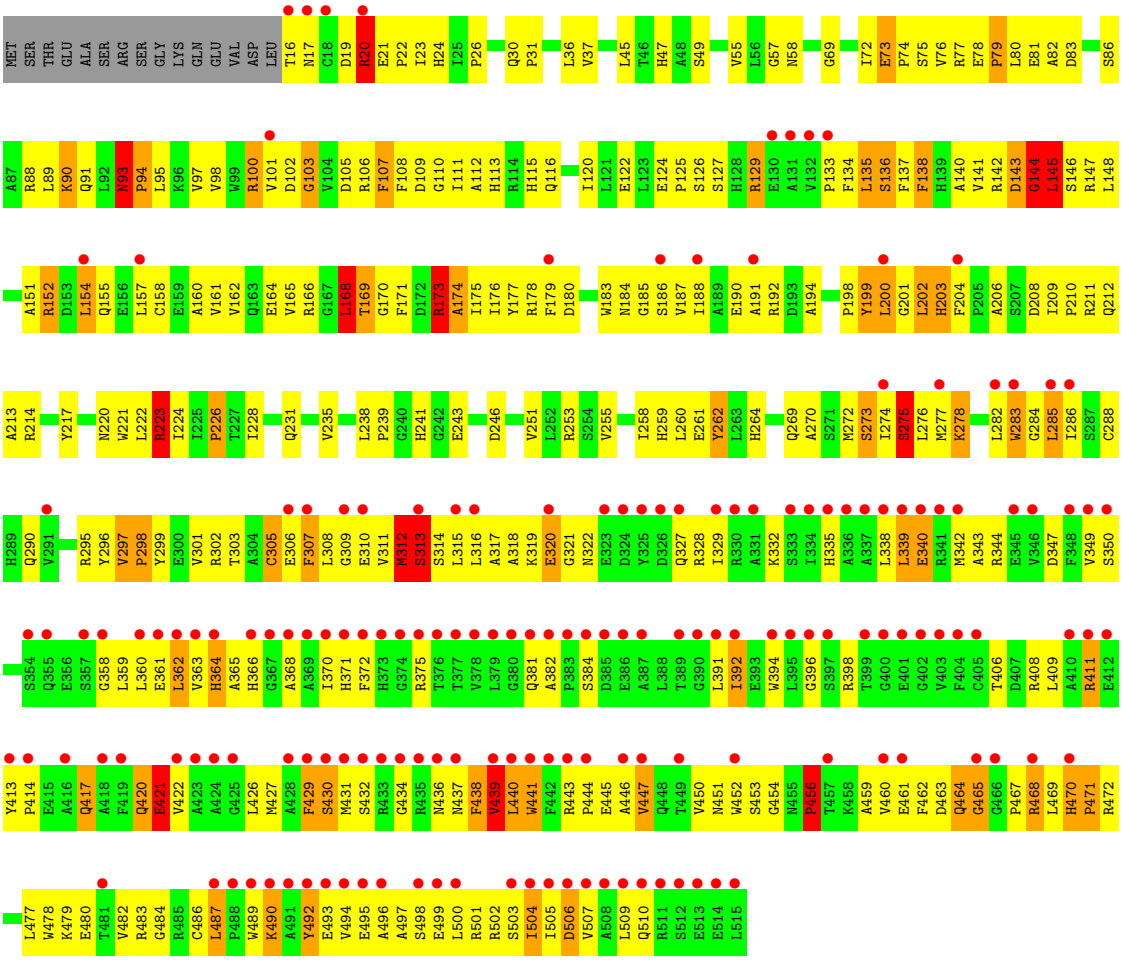
Chain B:





- Molecule 1: Photoreceptor-histidine kinase BphP

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	83.31Å 83.31Å 475.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.28 – 2.65 40.28 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.8 (40.28-2.65) 98.6 (40.28-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.241 , 0.315 0.241 , 0.313	Depositor DCC
R_{free} test set	3051 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	70.1	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.068 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12158	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: BLR

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	0.61	4/4075 (0.1%)	0.77	6/5529 (0.1%)
1	B	0.59	3/4075 (0.1%)	0.75	4/5529 (0.1%)
1	C	0.93	16/4034 (0.4%)	0.91	18/5473 (0.3%)
All	All	0.73	23/12184 (0.2%)	0.81	28/16531 (0.2%)

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	1
1	B	0	4
1	C	0	14
All	All	0	19

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	298	PRO	N-CD	-34.79	0.99	1.47
1	C	74	PRO	N-CD	-17.44	1.23	1.47
1	B	495	GLU	CD-OE1	-9.56	1.15	1.25
1	C	173	ARG	CZ-NH2	-8.98	1.21	1.33
1	C	100	ARG	CZ-NH1	-8.33	1.22	1.33
1	C	173	ARG	NE-CZ	-8.29	1.22	1.33
1	C	483	ARG	CZ-NH2	-7.92	1.22	1.33
1	B	495	GLU	CD-OE2	-7.89	1.17	1.25
1	C	100	ARG	NE-CZ	-7.85	1.22	1.33
1	C	483	ARG	NE-CZ	-7.76	1.23	1.33
1	C	100	ARG	CZ-NH2	-7.68	1.23	1.33
1	A	236	ARG	CZ-NH1	-7.02	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	483	ARG	CZ-NH1	-6.82	1.24	1.33
1	C	483	ARG	CD-NE	-6.80	1.34	1.46
1	A	236	ARG	NE-CZ	-6.55	1.24	1.33
1	B	458	LYS	CD-CE	-6.47	1.35	1.51
1	C	305	CYS	CB-SG	-6.27	1.71	1.82
1	A	393	GLU	CB-CG	6.21	1.64	1.52
1	C	421	GLU	CD-OE1	-5.85	1.19	1.25
1	C	487	LEU	C-N	5.71	1.45	1.34
1	C	297	VAL	CB-CG1	-5.66	1.41	1.52
1	C	100	ARG	CD-NE	-5.51	1.37	1.46
1	A	130	GLU	CD-OE1	-5.16	1.20	1.25

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	413	TYR	C-N-CD	-10.37	97.78	120.60
1	A	394	TRP	CA-CB-CG	10.16	133.01	113.70
1	C	145	LEU	CB-CG-CD1	-9.99	94.02	111.00
1	C	223	ARG	CG-CD-NE	-9.22	92.44	111.80
1	C	173	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	C	202	LEU	CB-CG-CD2	-7.38	98.45	111.00
1	A	43	LEU	CA-CB-CG	7.25	131.98	115.30
1	A	56	LEU	CA-CB-CG	7.19	131.84	115.30
1	C	20	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	A	395	LEU	CA-CB-CG	6.91	131.19	115.30
1	C	285	LEU	CA-CB-CG	6.87	131.10	115.30
1	C	440	LEU	CA-CB-CG	6.81	130.97	115.30
1	A	20	ARG	CG-CD-NE	6.67	125.80	111.80
1	C	223	ARG	CB-CA-C	-6.39	97.62	110.40
1	C	298	PRO	N-CA-CB	-6.18	95.80	102.60
1	C	413	TYR	C-N-CA	5.68	145.87	122.00
1	B	434	GLY	C-N-CA	5.66	135.84	121.70
1	A	211	ARG	CG-CD-NE	5.60	123.55	111.80
1	C	441	TRP	CA-CB-CG	-5.58	103.09	113.70
1	C	339	LEU	CA-CB-CG	5.56	128.08	115.30
1	C	168	LEU	CB-CG-CD1	-5.54	101.59	111.00
1	B	327	GLN	N-CA-C	5.37	125.51	111.00
1	C	456	PRO	CA-N-CD	-5.28	104.11	111.50
1	B	13	VAL	C-N-CA	5.17	134.63	121.70
1	B	328	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	477	LEU	CA-CB-CG	5.07	126.95	115.30
1	C	144	GLY	N-CA-C	-5.04	100.50	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	298	PRO	CB-CG-CD	-5.03	86.89	106.50

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	400	GLY	Peptide
1	B	325	TYR	Peptide
1	B	326	ASP	Peptide
1	B	393	GLU	Peptide
1	B	422	VAL	Peptide
1	C	135	LEU	Peptide
1	C	143	ASP	Peptide
1	C	144	GLY	Peptide
1	C	199	TYR	Peptide
1	C	222	LEU	Peptide
1	C	273	SER	Peptide
1	C	275	SER	Peptide
1	C	313	SER	Peptide
1	C	420	GLN	Peptide
1	C	430	SER	Peptide
1	C	438	PHE	Peptide
1	C	439	VAL	Peptide
1	C	504	ILE	Peptide
1	C	93	ASN	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	3982	0	3925	175	0
1	B	3982	0	3925	194	0
1	C	3941	0	3886	413	0
2	A	43	0	32	5	0
2	B	43	0	32	4	0
2	C	43	0	33	15	0
3	A	46	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	42	0	0	5	0
3	C	36	0	0	19	0
All	All	12158	0	11833	758	0

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 32.

All (758) 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:142:ARG:NH1	1:B:307:PHE:CA	1.72	1.51
1:A:142:ARG:NH1	1:B:307:PHE:HA	1.19	1.44
1:C:429:PHE:O	1:C:501:ARG:NH1	1.65	1.29
1:A:142:ARG:HH11	1:B:307:PHE:CB	1.54	1.19
1:C:154:LEU:HD21	1:C:155:GLN:NE2	1.65	1.12
1:A:142:ARG:HH12	1:B:307:PHE:CA	1.39	1.11
1:C:429:PHE:C	1:C:501:ARG:NH1	2.03	1.10
1:C:37:VAL:HG12	1:C:120:ILE:HG22	1.30	1.09
1:C:202:LEU:HD21	1:C:452:TRP:HA	1.31	1.09
1:A:142:ARG:HH22	1:B:306:GLU:HG2	1.08	1.08
1:C:278:LYS:CD	1:C:316:LEU:HD22	1.83	1.08
1:C:429:PHE:C	1:C:501:ARG:HH11	1.56	1.07
1:C:278:LYS:HD2	1:C:316:LEU:CD2	1.87	1.04
1:C:297:VAL:HG22	1:C:301:VAL:HG13	1.40	1.04
1:A:142:ARG:HH11	1:B:307:PHE:HB2	1.22	1.04
1:C:497:ALA:HB1	1:C:501:ARG:HH22	1.13	1.02
1:C:497:ALA:CB	1:C:501:ARG:HH22	1.46	1.02
1:C:154:LEU:HD21	1:C:155:GLN:HE22	1.19	0.98
1:C:278:LYS:HD2	1:C:316:LEU:HD22	1.00	0.98
1:C:154:LEU:CD2	1:C:155:GLN:NE2	2.26	0.98
1:A:142:ARG:NH1	1:B:307:PHE:CB	2.19	0.98
1:A:401:GLU:OE2	1:A:501:ARG:NH2	1.97	0.98
1:C:168:LEU:HD11	1:C:305:CYS:SG	2.03	0.97
1:C:88:ARG:HB3	1:C:90:LYS:HE3	1.46	0.97
1:A:142:ARG:NH2	1:B:306:GLU:HG2	1.80	0.97
1:C:73:GLU:HB3	1:C:100:ARG:HG3	1.42	0.97
1:C:151:ALA:HB3	1:C:157:LEU:CD1	1.95	0.96
1:B:425:GLY:H	1:B:443:ARG:H	0.97	0.95
1:C:100:ARG:NH1	1:C:105:ASP:OD2	1.98	0.95
1:C:202:LEU:HD23	1:C:451:ASN:ND2	1.82	0.95
1:B:430:SER:HB2	1:B:433:ARG:HH12	1.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:ALA:HB1	1:C:501:ARG:NH2	1.81	0.94
1:B:13:VAL:HA	1:B:14:ASP:HB2	1.49	0.94
1:B:324:ASP:OD1	1:B:328:ARG:NH2	2.00	0.94
1:C:497:ALA:CB	1:C:501:ARG:NH2	2.31	0.94
1:C:408:ARG:NH2	1:C:421:GLU:OE1	2.02	0.92
1:C:297:VAL:CG2	1:C:301:VAL:HG13	1.99	0.92
1:C:213:ALA:HB1	1:C:217:TYR:HE2	1.32	0.92
1:C:175:ILE:HD13	1:C:187:VAL:HG13	1.51	0.92
1:C:274:ILE:HD12	1:C:306:GLU:HA	1.49	0.92
1:A:13:VAL:HA	1:A:14:ASP:HB2	1.50	0.91
1:C:456:PRO:HD2	1:C:478:TRP:CH2	2.06	0.90
1:B:169:THR:O	1:B:295:ARG:NH2	2.04	0.90
1:A:142:ARG:NH1	1:B:307:PHE:N	2.18	0.90
1:C:73:GLU:OE1	1:C:75:SER:N	2.06	0.89
1:A:43:LEU:HG	1:A:44:VAL:HG12	1.55	0.88
1:B:41:PRO:O	1:B:85:ARG:NH1	2.07	0.86
1:C:171:PHE:HE2	1:C:295:ARG:HG2	1.41	0.86
1:C:298:PRO:HD2	1:C:301:VAL:CG1	2.06	0.86
1:C:321:GLY:HA2	1:C:492:TYR:HE1	1.41	0.85
1:A:142:ARG:HH12	1:B:307:PHE:N	1.72	0.85
1:C:174:ALA:HB3	1:C:191:ALA:HB3	1.60	0.84
1:A:398:ARG:HG2	1:A:399:THR:H	1.42	0.84
1:C:471:PRO:HG2	2:C:601:BLR:H22	1.59	0.84
1:C:154:LEU:HD23	1:C:155:GLN:CD	1.98	0.83
1:C:202:LEU:HD13	1:C:202:LEU:C	1.99	0.83
1:A:142:ARG:HH11	1:B:307:PHE:CA	1.64	0.83
1:C:202:LEU:HD21	1:C:452:TRP:CA	2.09	0.83
1:C:157:LEU:HD21	3:C:706:HOH:O	1.78	0.82
1:A:69:GLY:O	1:A:77:ARG:NH1	2.12	0.82
1:B:430:SER:HB2	1:B:433:ARG:NH1	1.95	0.82
1:C:368:ALA:HA	1:C:440:LEU:HD21	1.59	0.82
1:A:42:GLY:HA3	1:A:85:ARG:HH21	1.43	0.82
1:A:192:ARG:NH2	1:C:81:GLU:OE2	2.13	0.82
1:B:330:ARG:NH1	1:B:361:GLU:OE1	2.12	0.82
1:C:37:VAL:HG12	1:C:120:ILE:CG2	2.10	0.81
1:C:276:LEU:HD11	1:C:312:MET:HG2	1.61	0.81
1:A:322:ASN:ND2	1:A:322:ASN:O	2.13	0.81
1:C:202:LEU:HB2	1:C:451:ASN:ND2	1.97	0.80
1:B:425:GLY:H	1:B:443:ARG:N	1.79	0.80
1:B:453:SER:O	1:B:472:ARG:NH2	2.14	0.80
1:C:154:LEU:HD23	1:C:155:GLN:OE1	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:NH1	1:A:196:ALA:O	2.15	0.79
1:C:161:VAL:O	1:C:165:VAL:N	2.13	0.79
1:A:142:ARG:HH12	1:B:307:PHE:HA	0.81	0.79
1:C:187:VAL:HB	1:C:202:LEU:H	1.47	0.78
1:C:452:TRP:HB2	1:C:478:TRP:CH2	2.17	0.78
1:C:113:HIS:CD2	1:C:120:ILE:HD11	2.18	0.78
1:C:213:ALA:HB1	1:C:217:TYR:CE2	2.18	0.78
1:B:410:ALA:HA	1:B:414:PRO:HA	1.67	0.77
1:A:142:ARG:NH1	1:B:307:PHE:HB2	1.89	0.77
1:C:164:GLU:O	1:C:168:LEU:HD23	1.84	0.77
1:C:204:PHE:HB2	2:C:601:BLR:H14	1.66	0.77
1:B:374:GLY:HA3	1:B:375:ARG:HB2	1.67	0.77
1:C:214:ARG:HA	1:C:217:TYR:HD2	1.50	0.77
1:A:194:ALA:HB3	1:C:78:GLU:HG2	1.67	0.77
1:C:359:LEU:HD11	1:C:441:TRP:CE2	2.20	0.77
1:C:210:PRO:HG3	2:C:601:BLR:H24	1.65	0.76
1:C:202:LEU:HD23	1:C:451:ASN:CG	2.05	0.76
1:A:502:ARG:HA	1:A:505:ILE:HD12	1.66	0.76
1:C:107:PHE:HB3	1:C:127:SER:HB3	1.65	0.76
1:C:171:PHE:CE2	1:C:295:ARG:HG2	2.21	0.76
1:C:278:LYS:HG2	1:C:283:TRP:HB2	1.67	0.76
1:C:312:MET:SD	1:C:313:SER:N	2.59	0.76
1:A:197:ASP:OD2	1:C:77:ARG:NH2	2.19	0.75
1:B:326:ASP:OD1	1:B:329:ILE:HB	1.87	0.75
1:B:408:ARG:NH1	3:B:701:HOH:O	2.18	0.75
1:C:429:PHE:N	1:C:501:ARG:HH12	1.85	0.75
1:C:16:THR:N	1:C:19:ASP:OD2	2.20	0.74
1:C:161:VAL:O	1:C:165:VAL:HG13	1.86	0.74
1:C:253:ARG:NH1	2:C:601:BLR:O2D	2.18	0.74
1:A:175:ILE:HG22	1:A:190:GLU:HB2	1.68	0.74
1:C:312:MET:O	1:C:314:SER:N	2.19	0.74
1:B:327:GLN:O	1:B:329:ILE:N	2.20	0.74
1:A:142:ARG:NH2	1:B:310:GLU:OE2	2.21	0.73
1:A:398:ARG:HG2	1:A:399:THR:N	2.03	0.73
1:B:392:ILE:HD12	1:B:393:GLU:HG3	1.70	0.73
1:C:137:PHE:O	3:C:701:HOH:O	2.05	0.73
1:C:168:LEU:CD1	1:C:305:CYS:SG	2.77	0.73
1:B:478:TRP:HZ3	1:B:480:GLU:HB2	1.54	0.72
1:C:208:ASP:OD2	1:C:472:ARG:NH1	2.23	0.72
1:C:430:SER:HA	1:C:501:ARG:CD	2.19	0.72
1:C:129:ARG:NH2	1:C:296:TYR:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:ALA:HB3	1:C:157:LEU:HD12	1.70	0.72
1:C:175:ILE:HD13	1:C:187:VAL:CG1	2.19	0.72
1:C:202:LEU:HD13	1:C:202:LEU:O	1.90	0.72
1:A:398:ARG:HD3	1:A:435:ARG:HH12	1.54	0.72
1:C:446:ALA:HB2	1:C:487:LEU:HG	1.71	0.72
1:C:49:SER:HA	1:C:235:VAL:HA	1.72	0.72
2:C:601:BLR:NB	2:C:601:BLR:H4	2.04	0.72
1:B:474:SER:OG	1:B:476:GLU:OE1	2.05	0.72
1:C:187:VAL:HG21	1:C:202:LEU:O	1.90	0.71
1:B:178:ARG:NH2	1:B:320:GLU:OE2	2.23	0.71
1:C:113:HIS:NE2	1:C:120:ILE:HD11	2.05	0.71
1:C:154:LEU:CD2	1:C:155:GLN:CD	2.57	0.71
1:C:422:VAL:HG11	1:C:486:CYS:HB2	1.72	0.71
1:A:223:ARG:NH2	1:A:273:SER:OG	2.22	0.71
1:C:201:GLY:O	1:C:451:ASN:ND2	2.19	0.71
1:B:89:LEU:HA	1:B:92:LEU:HD12	1.71	0.70
1:C:192:ARG:CZ	1:C:198:PRO:HG3	2.21	0.70
1:C:321:GLY:HA2	1:C:492:TYR:CE1	2.26	0.70
1:C:447:VAL:HB	1:C:484:GLY:HA2	1.73	0.70
1:B:177:TYR:CZ	1:B:185:GLY:HA3	2.26	0.70
1:B:486:CYS:SG	3:B:731:HOH:O	2.49	0.70
1:C:100:ARG:NH2	1:C:103:GLY:O	2.24	0.70
1:A:44:VAL:H	1:A:67:PRO:HA	1.56	0.70
1:C:303:THR:O	1:C:307:PHE:N	2.24	0.70
1:A:398:ARG:HD3	1:A:435:ARG:NH1	2.07	0.70
1:C:177:TYR:HD2	1:C:285:LEU:HD13	1.56	0.69
1:C:298:PRO:HD2	1:C:301:VAL:HG12	1.73	0.69
1:C:408:ARG:O	1:C:417:GLN:NE2	2.25	0.69
1:A:367:GLY:HA2	1:A:380:GLY:HA3	1.74	0.69
1:C:299:TYR:O	1:C:303:THR:OG1	2.10	0.69
1:C:109:ASP:OD2	1:C:126:SER:OG	2.08	0.69
1:C:166:ARG:NH1	1:C:191:ALA:O	2.25	0.69
1:C:203:HIS:ND1	1:C:452:TRP:HZ3	1.91	0.69
1:A:77:ARG:O	1:A:81:GLU:HG2	1.93	0.69
1:A:386:GLU:O	1:A:389:THR:OG1	2.11	0.69
1:C:169:THR:O	1:C:295:ARG:NH2	2.26	0.68
1:C:450:VAL:HG22	1:C:451:ASN:H	1.58	0.68
1:B:423:ALA:HB2	1:B:445:GLU:HG3	1.74	0.68
1:C:203:HIS:ND1	1:C:452:TRP:CZ3	2.61	0.68
1:A:394:TRP:HB2	1:A:398:ARG:CZ	2.23	0.68
1:C:88:ARG:CB	1:C:90:LYS:HE3	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:HG13	1:A:15:LEU:HD21	1.74	0.68
1:B:408:ARG:HA	1:B:422:VAL:HG11	1.75	0.68
1:A:464:GLN:HB2	1:A:466:GLY:H	1.59	0.67
1:C:89:LEU:HD22	1:C:112:ALA:HB3	1.75	0.67
1:A:177:TYR:CZ	1:A:185:GLY:HA3	2.30	0.67
1:C:187:VAL:O	1:C:201:GLY:HA2	1.93	0.67
1:C:486:CYS:HG	1:C:489:TRP:HE1	1.38	0.67
2:C:601:BLR:H4	2:C:601:BLR:H13	1.58	0.67
1:B:37:VAL:HG12	1:B:120:ILE:HG12	1.76	0.67
1:C:429:PHE:O	1:C:501:ARG:CZ	2.41	0.67
1:B:50:GLU:OE2	1:B:236:ARG:NH1	2.28	0.67
1:C:308:LEU:HD12	3:C:732:HOH:O	1.95	0.67
1:A:142:ARG:HD2	1:B:307:PHE:HB2	1.76	0.66
1:C:316:LEU:O	1:C:320:GLU:N	2.28	0.66
1:C:430:SER:HA	1:C:501:ARG:HD2	1.76	0.66
1:A:393:GLU:O	1:A:394:TRP:CG	2.48	0.66
1:B:409:LEU:HD22	1:B:416:ALA:HB2	1.78	0.66
1:B:393:GLU:HA	1:B:396:GLY:H	1.60	0.66
1:C:202:LEU:HB2	1:C:451:ASN:HD22	1.60	0.66
1:A:346:VAL:HA	1:A:511:ARG:HE	1.61	0.66
1:C:231:GLN:OE1	1:C:231:GLN:N	2.27	0.65
1:C:37:VAL:HG21	1:C:47:HIS:ND1	2.12	0.65
1:C:464:GLN:HE22	1:C:468:ARG:HH12	1.43	0.65
1:C:184:ASN:OD1	1:C:206:ALA:N	2.29	0.65
1:C:335:HIS:NE2	1:C:499:GLU:OE2	2.29	0.65
1:C:408:ARG:NH2	1:C:484:GLY:HA3	2.11	0.65
1:B:89:LEU:HD11	1:B:112:ALA:HB3	1.77	0.65
1:B:426:LEU:HD21	1:B:428:ALA:HB2	1.79	0.65
1:C:486:CYS:SG	1:C:489:TRP:NE1	2.66	0.65
1:A:394:TRP:HB3	1:A:398:ARG:HG3	1.78	0.65
1:B:422:VAL:HG22	3:B:731:HOH:O	1.96	0.65
1:A:243:GLU:HG3	1:A:244:PRO:HD2	1.77	0.65
1:B:420:GLN:O	1:B:423:ALA:HB3	1.97	0.65
1:C:202:LEU:CD2	1:C:452:TRP:HA	2.20	0.65
1:C:509:LEU:HD12	1:C:510:GLN:NE2	2.12	0.65
2:C:601:BLR:NA	3:C:703:HOH:O	2.21	0.64
1:A:30:GLN:HE22	1:A:225:ILE:HA	1.62	0.64
1:B:425:GLY:N	1:B:443:ARG:H	1.82	0.64
1:B:423:ALA:O	1:B:444:PRO:HA	1.98	0.64
1:B:367:GLY:HA2	1:B:380:GLY:HA3	1.78	0.64
1:A:80:LEU:HD11	1:A:97:VAL:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:GLY:HA3	1:C:295:ARG:HH21	1.62	0.64
1:C:168:LEU:HG	1:C:169:THR:H	1.63	0.63
1:B:147:ARG:NH2	1:B:163:GLN:OE1	2.18	0.63
1:B:243:GLU:OE2	1:B:243:GLU:N	2.25	0.63
1:C:17:ASN:C	1:C:20:ARG:HH12	2.02	0.63
1:C:36:LEU:HD13	1:C:45:LEU:HD21	1.79	0.63
1:A:411:ARG:NH2	1:A:412:GLU:OE1	2.32	0.63
1:B:44:VAL:HA	1:B:67:PRO:HA	1.79	0.63
1:C:88:ARG:HB3	1:C:90:LYS:CE	2.26	0.63
1:B:383:PRO:O	1:B:385:ASP:N	2.32	0.63
1:C:217:TYR:OH	2:C:601:BLR:H33	1.99	0.63
1:B:392:ILE:O	1:B:395:LEU:HB2	1.98	0.63
1:A:130:GLU:HG3	1:A:133:PRO:CG	2.29	0.63
1:B:340:GLU:O	1:B:344:ARG:HG3	1.99	0.63
1:B:423:ALA:HB2	1:B:445:GLU:CG	2.29	0.62
1:C:224:ILE:CG2	1:C:302:ARG:HD3	2.29	0.62
1:A:39:SER:HB3	1:A:44:VAL:HG13	1.81	0.62
1:C:316:LEU:HG	1:C:317:ALA:N	2.14	0.62
1:C:478:TRP:NE1	1:C:480:GLU:OE1	2.33	0.62
1:C:171:PHE:HB3	1:C:173:ARG:O	1.99	0.62
1:C:101:VAL:HG21	1:C:106:ARG:NH2	2.14	0.62
1:C:209:ILE:HD11	2:C:601:BLR:H15	1.80	0.62
1:C:37:VAL:HG22	1:C:47:HIS:H	1.64	0.62
1:A:56:LEU:HD11	1:A:99:TRP:CZ2	2.34	0.62
1:B:212:GLN:OE1	1:B:212:GLN:N	2.30	0.62
1:A:394:TRP:HB2	1:A:398:ARG:NH1	2.14	0.62
1:C:396:GLY:HA3	1:C:398:ARG:HG3	1.81	0.62
1:C:162:VAL:HB	1:C:191:ALA:HB2	1.81	0.62
1:B:416:ALA:HA	1:B:419:PHE:CD2	2.34	0.61
1:C:487:LEU:HB2	1:C:489:TRP:HD1	1.65	0.61
1:A:15:LEU:HD22	1:A:19:ASP:OD2	2.00	0.61
1:A:400:GLY:O	1:A:401:GLU:HG3	2.00	0.61
1:C:320:GLU:N	1:C:321:GLY:HA3	2.15	0.61
1:A:142:ARG:NH2	1:B:306:GLU:CG	2.59	0.61
1:B:426:LEU:HA	1:B:441:TRP:O	2.01	0.61
1:C:278:LYS:CG	1:C:316:LEU:HD22	2.31	0.61
1:C:298:PRO:HB2	1:C:301:VAL:HG12	1.81	0.61
1:C:192:ARG:HD2	1:C:194:ALA:HA	1.83	0.61
1:C:492:TYR:O	1:C:496:ALA:HB2	2.01	0.61
1:B:173:ARG:NH2	1:B:197:ASP:O	2.34	0.60
1:C:93:ASN:HA	1:C:95:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LEU:HD21	1:A:121:LEU:HD13	1.82	0.60
1:C:19:ASP:HA	1:C:212:GLN:HG2	1.83	0.60
1:C:164:GLU:O	1:C:168:LEU:CD2	2.48	0.60
1:C:311:VAL:HG12	1:C:315:LEU:HD12	1.81	0.60
1:C:186:SER:HA	1:C:203:HIS:CD2	2.36	0.60
1:B:406:THR:O	1:B:489:TRP:NE1	2.32	0.60
1:B:422:VAL:HG12	1:B:484:GLY:O	2.00	0.60
1:C:430:SER:HA	1:C:501:ARG:HD3	1.82	0.60
1:B:363:VAL:HG21	1:B:441:TRP:CG	2.36	0.60
1:B:330:ARG:O	1:B:334:ILE:N	2.25	0.60
1:B:478:TRP:CZ3	1:B:480:GLU:HB2	2.37	0.60
1:C:489:TRP:HB2	1:C:494:VAL:HG22	1.84	0.60
1:C:113:HIS:CE1	1:C:120:ILE:HD11	2.37	0.59
1:C:359:LEU:HD11	1:C:441:TRP:NE1	2.16	0.59
1:B:422:VAL:CG1	1:B:484:GLY:O	2.50	0.59
1:B:495:GLU:OE1	1:B:495:GLU:N	2.32	0.59
1:B:363:VAL:HG21	1:B:441:TRP:CD1	2.38	0.59
2:A:601:BLR:NB	2:A:601:BLR:H4	2.17	0.59
1:C:364:HIS:CE1	1:C:490:LYS:HD2	2.38	0.59
1:B:328:ARG:CG	1:B:329:ILE:H	2.16	0.58
1:C:73:GLU:OE2	1:C:76:VAL:HG22	2.03	0.58
1:B:321:GLY:O	1:B:323:GLU:HG2	2.04	0.58
1:B:43:LEU:HD12	1:B:81:GLU:HG2	1.84	0.58
1:C:259:HIS:CE1	2:C:601:BLR:H9	2.39	0.58
1:A:42:GLY:O	1:A:43:LEU:HD23	2.04	0.58
1:C:19:ASP:HB3	1:C:212:GLN:NE2	2.17	0.58
1:A:130:GLU:HG3	1:A:133:PRO:HG2	1.85	0.58
1:C:209:ILE:HG12	3:C:727:HOH:O	2.02	0.58
1:A:257:PRO:HA	1:A:260:LEU:HD12	1.86	0.58
1:B:483:ARG:O	1:B:485:ARG:N	2.36	0.58
1:A:17:ASN:HA	1:A:20:ARG:HH12	1.68	0.58
1:C:175:ILE:CD1	1:C:187:VAL:CG1	2.82	0.58
1:C:217:TYR:OH	2:C:601:BLR:H1	2.04	0.57
1:C:327:GLN:NE2	1:C:493:GLU:OE1	2.35	0.57
1:A:401:GLU:HG2	3:A:707:HOH:O	2.02	0.57
1:B:166:ARG:O	1:B:170:GLY:N	2.34	0.57
1:B:338:LEU:O	1:B:342:MET:HG3	2.04	0.57
1:C:57:GLY:O	1:C:58:ASN:ND2	2.37	0.57
1:A:310:GLU:OE2	1:B:149:ARG:NH1	2.37	0.57
1:C:501:ARG:O	1:C:502:ARG:HD3	2.04	0.57
1:A:247:LEU:O	1:A:253:ARG:HD3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ARG:HH21	1:A:273:SER:HG	1.51	0.57
1:A:69:GLY:C	1:A:77:ARG:HH11	2.07	0.57
1:A:389:THR:HG22	1:A:413:TYR:HE2	1.68	0.57
1:B:384:SER:O	1:B:386:GLU:N	2.37	0.57
1:C:179:PHE:CE1	1:C:285:LEU:HD12	2.40	0.57
1:C:454:GLY:HA3	1:C:472:ARG:HD3	1.87	0.57
1:C:338:LEU:HD23	1:C:504:ILE:HG12	1.86	0.57
1:A:16:THR:O	1:A:20:ARG:NH2	2.38	0.57
1:A:389:THR:HG22	1:A:413:TYR:CE2	2.40	0.57
1:C:124:GLU:OE2	1:C:302:ARG:NH2	2.37	0.57
1:B:13:VAL:HA	1:B:14:ASP:CB	2.31	0.56
1:C:89:LEU:O	1:C:91:GLN:N	2.38	0.56
1:C:278:LYS:HB3	1:C:316:LEU:CD2	2.35	0.56
1:B:460:VAL:CG1	1:B:469:LEU:HD22	2.34	0.56
1:C:95:LEU:HD12	1:C:95:LEU:H	1.69	0.56
1:C:178:ARG:NH2	1:C:179:PHE:HB2	2.21	0.56
1:B:341:ARG:HG3	1:B:355:GLN:HE21	1.70	0.56
1:C:17:ASN:HA	1:C:20:ARG:HH12	1.71	0.56
1:A:88:ARG:NH2	1:B:150:ASP:O	2.39	0.56
1:A:429:PHE:CD1	1:A:501:ARG:HG3	2.41	0.56
1:C:329:ILE:HD13	1:C:332:LYS:HZ3	1.69	0.56
1:C:173:ARG:NH2	1:C:199:TYR:CE1	2.73	0.56
1:C:175:ILE:CD1	1:C:187:VAL:HG13	2.29	0.56
1:C:276:LEU:O	1:C:283:TRP:N	2.37	0.56
1:A:388:LEU:O	1:A:392:ILE:HG22	2.06	0.56
1:A:452:TRP:CD2	1:A:456:PRO:HG3	2.41	0.56
1:C:297:VAL:CG2	1:C:301:VAL:CG1	2.81	0.56
1:C:310:GLU:N	1:C:312:MET:HG3	2.20	0.56
1:A:359:LEU:HD23	1:A:379:LEU:HD12	1.86	0.56
1:C:152:ARG:O	1:C:322:ASN:HB3	2.06	0.56
1:C:202:LEU:C	1:C:202:LEU:CD1	2.73	0.56
1:B:120:ILE:HD11	1:B:245:LEU:HD11	1.88	0.55
1:C:278:LYS:HD3	1:C:313:SER:HA	1.87	0.55
1:B:100:ARG:HH11	1:B:105:ASP:CG	2.08	0.55
1:B:258:ILE:CD1	2:B:601:BLR:H24	2.37	0.55
1:C:202:LEU:HD21	1:C:452:TRP:N	2.21	0.55
1:C:307:PHE:O	1:C:310:GLU:HG3	2.07	0.55
1:C:318:ALA:O	1:C:319:LYS:HG3	2.06	0.55
1:A:455:ASN:OD1	1:A:457:THR:OG1	2.24	0.55
1:A:253:ARG:NH2	2:A:601:BLR:O2D	2.33	0.55
1:C:154:LEU:CD2	1:C:155:GLN:HE22	2.00	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HB3	1:A:19:ASP:OD2	2.07	0.55
1:C:451:ASN:CA	1:C:480:GLU:HG2	2.37	0.55
1:C:129:ARG:HD3	1:C:298:PRO:HG3	1.89	0.55
1:B:374:GLY:CA	1:B:375:ARG:HB2	2.36	0.55
1:A:371:HIS:ND1	1:A:376:THR:HG22	2.22	0.55
1:B:44:VAL:HG22	1:B:67:PRO:HB3	1.90	0.55
1:B:326:ASP:CG	1:B:327:GLN:HA	2.28	0.54
1:C:122:GLU:OE1	1:C:251:VAL:N	2.39	0.54
1:B:330:ARG:HA	1:B:333:SER:HB3	1.89	0.54
1:B:337:ALA:O	1:B:341:ARG:HG2	2.07	0.54
1:C:372:PHE:CE2	1:C:437:ASN:HB2	2.43	0.54
1:C:381:GLN:HG2	1:C:382:ALA:H	1.72	0.54
1:C:429:PHE:HB3	1:C:498:SER:HB3	1.88	0.54
1:C:429:PHE:CA	1:C:501:ARG:NH1	2.69	0.54
1:C:120:ILE:O	1:C:120:ILE:HD12	2.08	0.54
1:C:144:GLY:HA3	1:C:308:LEU:HD11	1.89	0.54
1:C:198:PRO:HG2	1:C:200:LEU:CD1	2.38	0.54
1:C:451:ASN:N	1:C:480:GLU:HG2	2.23	0.54
1:C:173:ARG:NH2	1:C:199:TYR:CZ	2.70	0.54
1:C:178:ARG:NH2	1:C:283:TRP:O	2.39	0.54
1:A:16:THR:OG1	1:A:17:ASN:N	2.33	0.54
1:A:142:ARG:CD	1:B:307:PHE:HB2	2.38	0.54
1:B:328:ARG:CG	1:B:329:ILE:N	2.71	0.54
1:C:179:PHE:HD1	1:C:284:GLY:HA2	1.72	0.54
1:C:187:VAL:HB	1:C:202:LEU:N	2.19	0.54
1:C:456:PRO:HD2	1:C:478:TRP:CZ2	2.41	0.54
1:A:80:LEU:HD13	3:A:718:HOH:O	2.08	0.54
1:A:81:GLU:O	1:A:85:ARG:HD2	2.08	0.54
1:A:142:ARG:HH11	1:B:307:PHE:HA	1.34	0.54
1:B:407:ASP:O	1:B:485:ARG:HA	2.08	0.54
1:B:413:TYR:CE2	1:B:415:GLU:HB2	2.43	0.53
1:C:505:ILE:HG12	1:C:506:ASP:H	1.72	0.53
1:C:487:LEU:H	1:C:487:LEU:HD12	1.73	0.53
1:C:158:CYS:SG	1:C:176:ILE:HD13	2.48	0.53
1:C:277:MET:O	1:C:278:LYS:HD3	2.09	0.53
1:C:451:ASN:HA	1:C:480:GLU:HG2	1.90	0.53
1:B:500:LEU:O	1:B:504:ILE:HG13	2.09	0.53
1:C:101:VAL:HG21	1:C:106:ARG:CZ	2.39	0.53
1:C:162:VAL:HA	1:C:165:VAL:HG22	1.90	0.53
1:C:171:PHE:CD1	1:C:288:CYS:HB3	2.43	0.53
1:C:429:PHE:CA	1:C:501:ARG:HH12	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:SER:HA	1:C:285:LEU:HA	1.91	0.53
1:A:30:GLN:HG2	1:A:230:TYR:CZ	2.44	0.53
1:B:32:HIS:CE1	1:B:226:PRO:HG2	2.44	0.53
1:B:60:ALA:O	1:B:64:LEU:HD12	2.09	0.53
1:C:432:SER:O	1:C:434:GLY:N	2.38	0.53
1:C:487:LEU:HB2	1:C:489:TRP:CD1	2.43	0.53
1:A:394:TRP:HB3	1:A:398:ARG:CG	2.37	0.53
1:C:278:LYS:HG2	1:C:283:TRP:CB	2.37	0.53
1:A:42:GLY:HA3	1:A:85:ARG:NH2	2.20	0.52
1:B:460:VAL:HG11	1:B:469:LEU:HD22	1.92	0.52
1:C:148:LEU:HD11	1:C:161:VAL:HG11	1.91	0.52
1:C:178:ARG:HD2	1:C:179:PHE:H	1.73	0.52
1:B:45:LEU:HD22	1:B:63:LEU:HB3	1.91	0.52
1:C:202:LEU:CB	1:C:451:ASN:ND2	2.71	0.52
1:C:88:ARG:NH2	1:C:90:LYS:HD3	2.25	0.52
1:C:162:VAL:O	1:C:165:VAL:HG22	2.09	0.52
1:A:131:ALA:HA	1:B:134:PHE:CE1	2.44	0.52
1:C:183:TRP:HE3	1:C:214:ARG:HH21	1.57	0.52
1:A:214:ARG:HB3	1:A:282:LEU:HD23	1.91	0.52
1:C:78:GLU:HG3	3:C:709:HOH:O	2.09	0.52
1:C:111:ILE:HD12	1:C:299:TYR:CZ	2.45	0.52
1:C:261:GLU:O	1:C:264:HIS:HB3	2.09	0.52
1:C:408:ARG:HH21	1:C:421:GLU:CD	2.13	0.52
1:B:274:ILE:HB	1:B:286:ILE:HB	1.91	0.52
1:B:501:ARG:O	1:B:505:ILE:HG13	2.10	0.52
1:C:138:PHE:N	3:C:710:HOH:O	2.42	0.52
1:C:214:ARG:HA	1:C:217:TYR:CD2	2.39	0.52
1:C:509:LEU:HD12	1:C:509:LEU:O	2.09	0.52
1:C:155:GLN:HA	1:C:158:CYS:HB2	1.92	0.52
1:B:419:PHE:C	1:B:421:GLU:H	2.13	0.51
1:C:140:ALA:O	1:C:144:GLY:N	2.41	0.51
1:A:152:ARG:HG3	1:A:156:GLU:CD	2.31	0.51
1:B:114:ARG:HA	1:B:118:ARG:O	2.10	0.51
1:C:319:LYS:HA	1:C:322:ASN:HB2	1.93	0.51
1:C:349:VAL:HG12	1:C:375:ARG:NH1	2.25	0.51
1:C:440:LEU:HD22	1:C:441:TRP:H	1.76	0.51
1:B:409:LEU:H	1:B:422:VAL:HB	1.74	0.51
1:A:464:GLN:N	1:A:465:GLY:HA2	2.26	0.51
1:C:217:TYR:CD1	1:C:223:ARG:NH1	2.78	0.51
1:B:48:ALA:O	1:B:236:ARG:N	2.43	0.51
1:A:160:ALA:O	1:A:164:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:ILE:HD11	1:C:375:ARG:HH11	1.75	0.51
1:A:32:HIS:NE2	1:A:226:PRO:HG2	2.26	0.51
1:C:175:ILE:HD11	1:C:188:ILE:N	2.26	0.51
1:A:78:GLU:OE2	1:A:81:GLU:HG3	2.11	0.51
1:C:100:ARG:NH1	1:C:105:ASP:CG	2.65	0.51
1:C:221:TRP:CD1	1:C:277:MET:HE2	2.46	0.51
1:C:447:VAL:HG22	1:C:482:VAL:HG13	1.94	0.51
1:A:142:ARG:HD2	1:B:307:PHE:CD1	2.47	0.50
1:B:409:LEU:CD2	1:B:413:TYR:HB3	2.40	0.50
1:B:486:CYS:SG	1:B:487:LEU:N	2.83	0.50
1:C:312:MET:SD	1:C:313:SER:OG	2.53	0.50
1:C:143:ASP:OD1	1:C:146:SER:HB2	2.10	0.50
1:C:152:ARG:C	1:C:319:LYS:HG2	2.31	0.50
1:C:360:LEU:HD13	1:C:366:HIS:CE1	2.47	0.50
1:A:19:ASP:C	1:A:20:ARG:HD2	2.32	0.50
1:A:208:ASP:OD2	1:A:472:ARG:NH1	2.44	0.50
1:C:278:LYS:NZ	1:C:316:LEU:HB3	2.26	0.50
1:C:307:PHE:O	1:C:309:GLY:N	2.44	0.50
1:A:78:GLU:N	1:A:79:PRO:HD2	2.26	0.50
1:B:431:MET:HB2	1:B:437:ASN:HB2	1.94	0.50
1:C:17:ASN:CA	1:C:20:ARG:HH12	2.24	0.50
1:C:509:LEU:CD1	1:C:510:GLN:NE2	2.74	0.50
1:C:192:ARG:HG3	1:C:198:PRO:HB3	1.93	0.50
1:C:270:ALA:HB3	1:C:290:GLN:HB3	1.93	0.50
1:C:278:LYS:HB3	1:C:316:LEU:HD21	1.93	0.50
1:B:177:TYR:OH	1:B:204:PHE:HB2	2.11	0.50
1:C:37:VAL:HG22	1:C:47:HIS:N	2.27	0.50
1:C:224:ILE:HG21	1:C:302:ARG:HD3	1.93	0.50
1:C:314:SER:N	1:C:316:LEU:HD23	2.27	0.50
1:B:366:HIS:HB2	1:B:444:PRO:HD3	1.94	0.50
2:B:601:BLR:H4	2:B:601:BLR:NB	2.26	0.50
1:C:220:ASN:OD1	1:C:221:TRP:N	2.42	0.50
1:C:243:GLU:CD	1:C:243:GLU:H	2.15	0.50
1:C:202:LEU:O	1:C:202:LEU:CD1	2.58	0.50
1:C:157:LEU:O	1:C:161:VAL:HG22	2.12	0.49
1:A:395:LEU:HA	1:A:398:ARG:HD2	1.94	0.49
1:A:461:GLU:HB3	1:A:470:HIS:O	2.13	0.49
1:C:115:HIS:CD2	1:C:116:GLN:HG2	2.47	0.49
1:C:137:PHE:HB3	3:C:710:HOH:O	2.11	0.49
1:C:342:MET:HG2	1:C:504:ILE:HG23	1.94	0.49
1:C:492:TYR:O	1:C:493:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ALA:O	1:A:340:GLU:HG2	2.11	0.49
1:B:324:ASP:CG	1:B:328:ARG:NH2	2.66	0.49
1:B:325:TYR:CG	1:B:325:TYR:O	2.65	0.49
1:C:335:HIS:HA	3:C:726:HOH:O	2.12	0.49
1:A:370:ILE:O	1:A:376:THR:HA	2.13	0.49
1:B:15:LEU:HD13	1:B:19:ASP:HB3	1.95	0.49
1:C:421:GLU:HG3	1:C:422:VAL:N	2.27	0.49
1:A:44:VAL:N	1:A:67:PRO:HA	2.26	0.49
1:A:395:LEU:CA	1:A:398:ARG:HD2	2.43	0.49
1:B:433:ARG:C	1:B:435:ARG:N	2.66	0.49
1:C:450:VAL:HG22	1:C:451:ASN:N	2.28	0.49
1:C:359:LEU:HD12	1:C:359:LEU:O	2.13	0.48
1:C:447:VAL:HG23	1:C:482:VAL:HG22	1.94	0.48
1:A:19:ASP:OD1	1:A:210:PRO:HB3	2.13	0.48
1:A:142:ARG:HH12	1:B:306:GLU:C	2.15	0.48
1:B:63:LEU:HD23	1:B:71:PHE:CZ	2.48	0.48
1:C:202:LEU:CD2	1:C:451:ASN:ND2	2.66	0.48
1:C:134:PHE:HB2	1:C:135:LEU:HD22	1.96	0.48
1:C:276:LEU:HG	1:C:312:MET:CE	2.44	0.48
1:C:315:LEU:HD13	3:C:706:HOH:O	2.13	0.48
1:C:489:TRP:CE3	1:C:494:VAL:HG13	2.49	0.48
1:B:425:GLY:O	1:B:442:PHE:HA	2.14	0.48
1:B:483:ARG:NH1	1:B:483:ARG:HB2	2.29	0.48
1:C:285:LEU:HD21	3:C:727:HOH:O	2.13	0.48
1:C:440:LEU:CD2	1:C:441:TRP:H	2.26	0.48
1:C:471:PRO:CG	2:C:601:BLR:H22	2.38	0.48
1:C:489:TRP:HE3	1:C:494:VAL:HG22	1.77	0.48
1:C:217:TYR:HD1	1:C:223:ARG:NH1	2.12	0.48
1:C:238:LEU:O	1:C:241:HIS:HB2	2.14	0.48
1:A:385:ASP:C	1:A:387:ALA:H	2.16	0.48
1:C:72:ILE:O	1:C:72:ILE:HG13	2.13	0.48
1:A:44:VAL:HA	1:A:67:PRO:HA	1.96	0.48
1:B:450:VAL:HG13	1:B:452:TRP:HE1	1.78	0.48
1:C:350:SER:OG	1:C:375:ARG:NH2	2.47	0.48
1:B:463:ASP:HB3	1:B:466:GLY:HA3	1.96	0.48
1:C:277:MET:HE3	3:C:705:HOH:O	2.13	0.48
1:A:210:PRO:HB2	1:A:212:GLN:OE1	2.13	0.48
1:A:258:ILE:HG13	1:A:471:PRO:HD3	1.96	0.48
1:B:378:VAL:HG12	1:B:379:LEU:H	1.78	0.47
1:C:37:VAL:HG13	1:C:47:HIS:HB2	1.95	0.47
1:C:185:GLY:C	1:C:203:HIS:CD2	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:VAL:HG12	1:B:379:LEU:N	2.29	0.47
1:C:113:HIS:HE1	3:C:723:HOH:O	1.96	0.47
1:A:300:GLU:OE2	1:B:142:ARG:NH2	2.47	0.47
1:C:176:ILE:HD12	1:C:176:ILE:H	1.80	0.47
1:B:258:ILE:HG13	1:B:259:HIS:N	2.28	0.47
1:C:162:VAL:CB	1:C:191:ALA:HB2	2.44	0.47
1:C:359:LEU:HB2	1:C:362:LEU:HD11	1.95	0.47
1:C:361:GLU:O	3:C:702:HOH:O	2.20	0.47
1:A:177:TYR:OH	1:A:185:GLY:HA3	2.15	0.47
1:A:327:GLN:HB3	1:A:492:TYR:CZ	2.50	0.47
1:C:116:GLN:NE2	3:C:704:HOH:O	2.24	0.47
1:C:411:ARG:HA	1:C:411:ARG:CZ	2.45	0.47
1:A:44:VAL:HA	1:A:66:ALA:O	2.14	0.47
1:A:236:ARG:HD2	1:A:236:ARG:HA	1.48	0.47
1:A:436:ASN:N	3:A:708:HOH:O	2.47	0.47
1:B:419:PHE:C	1:B:421:GLU:N	2.68	0.47
1:B:455:ASN:OD1	1:B:457:THR:HG23	2.14	0.47
1:B:457:THR:OG1	1:B:458:LYS:N	2.48	0.47
1:C:169:THR:HB	1:C:171:PHE:CD2	2.50	0.47
1:C:179:PHE:HA	1:C:185:GLY:HA3	1.96	0.47
1:A:173:ARG:O	1:A:288:CYS:HA	2.14	0.47
1:B:507:VAL:O	1:B:511:ARG:HG2	2.15	0.47
1:C:124:GLU:CD	1:C:302:ARG:HH22	2.18	0.47
1:C:259:HIS:HE1	2:C:601:BLR:H9	1.80	0.47
1:C:318:ALA:O	1:C:322:ASN:HB2	2.14	0.47
1:A:20:ARG:CD	1:A:20:ARG:N	2.78	0.47
1:B:409:LEU:HD23	1:B:413:TYR:HB3	1.95	0.47
1:C:175:ILE:HD11	1:C:187:VAL:C	2.35	0.47
1:C:307:PHE:CD2	1:C:310:GLU:HG2	2.49	0.47
1:C:328:ARG:HG3	1:C:332:LYS:NZ	2.30	0.47
1:C:19:ASP:HB3	1:C:212:GLN:HE21	1.79	0.46
1:C:115:HIS:NE2	1:C:246:ASP:OD2	2.48	0.46
1:C:258:ILE:HD11	2:C:601:BLR:H27	1.97	0.46
1:A:208:ASP:HA	2:A:601:BLR:C1C	2.45	0.46
1:C:69:GLY:HA2	1:C:72:ILE:HG12	1.97	0.46
1:C:144:GLY:HA3	1:C:308:LEU:CD1	2.44	0.46
1:C:151:ALA:HB3	1:C:157:LEU:HD13	1.91	0.46
1:C:170:GLY:CA	1:C:295:ARG:HH21	2.26	0.46
1:C:328:ARG:O	1:C:332:LYS:HG3	2.14	0.46
1:C:503:SER:C	1:C:505:ILE:H	2.18	0.46
1:B:426:LEU:HD23	1:B:427:MET:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:GLU:HB3	1:C:100:ARG:CG	2.31	0.46
1:A:388:LEU:HD12	1:A:388:LEU:H	1.80	0.46
1:C:73:GLU:CD	1:C:76:VAL:H	2.19	0.46
1:C:110:GLY:HA2	1:C:122:GLU:O	2.15	0.46
1:C:495:GLU:C	1:C:497:ALA:H	2.18	0.46
1:A:399:THR:O	1:A:401:GLU:N	2.48	0.46
1:B:24:HIS:HD2	3:B:717:HOH:O	1.99	0.46
1:C:37:VAL:CG2	1:C:47:HIS:ND1	2.78	0.46
1:C:169:THR:OG1	1:C:170:GLY:N	2.48	0.46
1:C:192:ARG:NH1	1:C:198:PRO:HG3	2.30	0.46
1:A:366:HIS:HB3	3:A:741:HOH:O	2.14	0.46
1:A:395:LEU:HG	1:A:396:GLY:H	1.80	0.46
1:C:21:GLU:OE1	1:C:23:ILE:HG22	2.15	0.46
1:C:459:ALA:C	1:C:471:PRO:HB3	2.36	0.46
1:A:22:PRO:HA	3:A:740:HOH:O	2.14	0.46
1:B:49:SER:HA	1:B:235:VAL:HA	1.97	0.46
1:A:175:ILE:HD11	1:A:287:SER:HB3	1.98	0.46
1:A:365:ALA:HB1	1:A:442:PHE:O	2.15	0.46
1:C:141:VAL:HG13	3:C:701:HOH:O	2.15	0.46
1:B:187:VAL:CG2	2:B:601:BLR:H19	2.46	0.46
1:B:327:GLN:O	1:B:328:ARG:C	2.54	0.46
1:C:173:ARG:HE	1:C:173:ARG:HB2	1.49	0.46
1:A:342:MET:SD	1:A:352:LEU:HD21	2.56	0.45
1:C:94:PRO:HA	3:C:730:HOH:O	2.15	0.45
1:C:394:TRP:HZ2	1:C:426:LEU:HD21	1.82	0.45
1:A:40:GLU:HA	1:A:42:GLY:N	2.32	0.45
1:A:458:LYS:O	1:A:460:VAL:N	2.45	0.45
1:C:273:SER:HA	1:C:286:ILE:O	2.16	0.45
1:C:328:ARG:O	1:C:332:LYS:NZ	2.45	0.45
1:B:13:VAL:CA	1:B:14:ASP:HB2	2.34	0.45
1:B:503:SER:O	1:B:507:VAL:HG22	2.16	0.45
1:C:108:PHE:HA	1:C:125:PRO:HA	1.99	0.45
1:C:299:TYR:O	1:C:303:THR:N	2.36	0.45
1:C:360:LEU:HD13	1:C:366:HIS:HE1	1.80	0.45
1:A:275:SER:O	1:A:276:LEU:HD23	2.16	0.45
1:C:17:ASN:HA	1:C:20:ARG:NH1	2.31	0.45
1:C:120:ILE:HD12	1:C:120:ILE:C	2.36	0.45
1:B:377:THR:O	1:B:377:THR:OG1	2.35	0.45
1:C:140:ALA:HB3	3:C:701:HOH:O	2.15	0.45
1:C:164:GLU:O	1:C:166:ARG:N	2.49	0.45
1:A:299:TYR:CZ	1:A:303:THR:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ALA:HB1	1:B:442:PHE:O	2.16	0.45
1:B:421:GLU:O	1:B:424:ALA:N	2.34	0.45
1:C:89:LEU:HD13	1:C:113:HIS:HA	1.98	0.45
1:C:171:PHE:CZ	1:C:272:MET:HB2	2.52	0.45
1:C:408:ARG:NH2	1:C:421:GLU:CD	2.69	0.45
1:B:425:GLY:O	1:B:489:TRP:HH2	2.00	0.45
1:A:378:VAL:C	1:A:379:LEU:HD23	2.37	0.45
1:A:428:ALA:HA	1:A:439:VAL:O	2.17	0.45
1:B:328:ARG:HG2	1:B:329:ILE:H	1.81	0.45
1:C:479:LYS:H	1:C:479:LYS:HG3	1.58	0.45
1:A:147:ARG:HG2	1:A:160:ALA:HB1	1.99	0.45
1:A:197:ASP:OD2	1:C:77:ARG:NH1	2.50	0.45
1:B:502:ARG:HA	1:B:502:ARG:HD3	1.70	0.45
1:C:202:LEU:HA	1:C:202:LEU:HD22	1.62	0.45
1:C:274:ILE:HG23	1:C:274:ILE:O	2.17	0.45
1:C:429:PHE:H	1:C:497:ALA:HB3	1.81	0.45
1:A:89:LEU:HD12	1:A:113:HIS:HA	1.99	0.44
1:A:395:LEU:N	1:A:398:ARG:HD2	2.33	0.44
1:B:69:GLY:O	1:B:77:ARG:HD3	2.16	0.44
1:C:98:VAL:HG23	3:C:719:HOH:O	2.16	0.44
1:C:210:PRO:HG3	2:C:601:BLR:CAC	2.42	0.44
1:C:310:GLU:CA	1:C:312:MET:HG3	2.47	0.44
1:B:28:ALA:HB1	1:B:232:PRO:HB3	1.98	0.44
1:C:55:VAL:HG12	1:C:108:PHE:CE2	2.52	0.44
1:C:135:LEU:HA	1:C:138:PHE:HB3	1.99	0.44
1:C:179:PHE:CD1	1:C:284:GLY:HA2	2.51	0.44
1:C:202:LEU:HD21	1:C:451:ASN:C	2.38	0.44
1:A:289:HIS:CE1	2:A:601:BLR:OB	2.71	0.44
1:C:113:HIS:CD2	1:C:120:ILE:CD1	2.95	0.44
1:C:406:THR:HG23	1:C:409:LEU:HG	1.99	0.44
1:A:19:ASP:OD1	1:A:19:ASP:N	2.49	0.44
1:B:466:GLY:HA2	1:B:467:PRO:HD3	1.87	0.44
1:C:286:ILE:HG22	1:C:288:CYS:SG	2.57	0.44
1:B:34:VAL:HG11	1:B:56:LEU:HD11	1.99	0.44
1:B:384:SER:HB2	1:B:388:LEU:HB2	1.98	0.44
1:B:406:THR:C	1:B:489:TRP:HE1	2.19	0.44
1:B:502:ARG:HD2	3:B:725:HOH:O	2.17	0.44
1:C:133:PRO:HD2	1:C:136:SER:HB2	2.00	0.44
1:B:202:LEU:HD13	1:B:453:SER:HB2	1.99	0.44
1:C:311:VAL:O	1:C:314:SER:OG	2.35	0.44
1:B:349:VAL:HG21	1:B:372:PHE:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ASN:ND2	1:B:62:GLN:OE1	2.49	0.44
1:B:433:ARG:C	1:B:435:ARG:H	2.19	0.44
1:C:76:VAL:C	1:C:79:PRO:HD2	2.38	0.44
1:C:89:LEU:HD22	1:C:112:ALA:CB	2.47	0.44
1:A:463:ASP:HB2	1:A:468:ARG:HB2	2.00	0.43
1:B:483:ARG:HG2	1:B:484:GLY:N	2.32	0.43
1:C:19:ASP:C	1:C:20:ARG:HD3	2.38	0.43
1:C:169:THR:HB	1:C:171:PHE:HD2	1.83	0.43
1:C:420:GLN:O	1:C:421:GLU:HG2	2.18	0.43
1:A:129:ARG:HG3	1:B:138:PHE:CE1	2.53	0.43
2:B:601:BLR:OB	2:B:601:BLR:H18	2.17	0.43
1:C:168:LEU:HG	1:C:169:THR:N	2.31	0.43
1:C:238:LEU:HD23	1:C:239:PRO:HD2	2.00	0.43
1:C:297:VAL:O	1:C:297:VAL:HG13	2.18	0.43
1:B:90:LYS:HE2	1:B:113:HIS:HA	2.00	0.43
1:B:431:MET:HG2	1:B:504:ILE:HG21	2.00	0.43
1:C:362:LEU:HD12	1:C:363:VAL:N	2.34	0.43
1:A:13:VAL:HG22	1:A:15:LEU:HD23	1.99	0.43
1:A:515:LEU:HD23	1:A:515:LEU:HA	1.77	0.43
1:B:72:ILE:HG23	1:B:98:VAL:O	2.18	0.43
1:C:221:TRP:HB3	1:C:275:SER:O	2.18	0.43
1:C:297:VAL:HA	1:C:298:PRO:HD3	1.51	0.43
1:C:340:GLU:HA	1:C:344:ARG:HB2	1.99	0.43
1:C:72:ILE:CD1	1:C:80:LEU:HD23	2.48	0.43
1:C:166:ARG:HA	1:C:169:THR:OG1	2.19	0.43
1:C:408:ARG:NH2	1:C:445:GLU:OE1	2.51	0.43
1:A:507:VAL:O	1:A:511:ARG:HG2	2.18	0.43
1:B:173:ARG:NH2	1:B:196:ALA:HB1	2.34	0.43
1:C:365:ALA:HA	1:C:443:ARG:HD3	2.01	0.43
1:C:470:HIS:ND1	1:C:471:PRO:HD2	2.34	0.43
1:C:497:ALA:HB1	1:C:501:ARG:CZ	2.45	0.43
1:C:278:LYS:HB3	1:C:316:LEU:HD22	1.99	0.43
1:A:416:ALA:HA	1:A:419:PHE:CZ	2.54	0.43
1:B:217:TYR:N	1:B:217:TYR:CD1	2.85	0.43
1:C:36:LEU:HD13	1:C:45:LEU:CD2	2.46	0.43
1:A:29:ILE:HB	1:A:252:LEU:HB3	1.99	0.43
1:A:78:GLU:OE1	3:A:701:HOH:O	2.21	0.43
1:A:173:ARG:NH2	1:A:197:ASP:O	2.51	0.43
1:C:175:ILE:HD11	1:C:187:VAL:CA	2.49	0.43
1:C:262:TYR:HB2	1:C:470:HIS:CE1	2.54	0.43
1:B:242:GLY:N	1:B:243:GLU:OE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ARG:CD	1:C:198:PRO:HB3	2.48	0.43
1:C:463:ASP:O	1:C:465:GLY:N	2.52	0.43
1:A:101:VAL:HG11	1:A:106:ARG:CZ	2.49	0.42
1:B:175:ILE:HD13	1:B:187:VAL:HG22	2.01	0.42
1:B:273:SER:HA	1:B:286:ILE:O	2.19	0.42
1:B:451:ASN:HB3	1:B:477:LEU:CD1	2.49	0.42
1:B:80:LEU:HD12	1:B:80:LEU:HA	1.83	0.42
1:B:223:ARG:NH1	1:B:275:SER:OG	2.48	0.42
1:C:30:GLN:HA	1:C:31:PRO:HD3	1.80	0.42
1:C:490:LYS:HG3	1:C:493:GLU:OE2	2.20	0.42
1:A:30:GLN:HG3	3:A:705:HOH:O	2.20	0.42
1:B:81:GLU:O	1:B:85:ARG:HG3	2.19	0.42
1:C:335:HIS:O	1:C:503:SER:OG	2.32	0.42
1:C:505:ILE:O	1:C:507:VAL:HG22	2.20	0.42
1:A:179:PHE:CE2	1:A:282:LEU:HG	2.54	0.42
1:B:180:ASP:OD2	1:B:184:ASN:HB2	2.20	0.42
1:A:394:TRP:HB2	1:A:398:ARG:NE	2.34	0.42
1:B:328:ARG:HG3	1:B:329:ILE:N	2.34	0.42
1:C:21:GLU:HA	1:C:22:PRO:HD3	1.87	0.42
1:A:209:ILE:O	1:A:214:ARG:NH1	2.36	0.42
1:C:82:ALA:O	1:C:86:SER:OG	2.37	0.42
1:C:221:TRP:CD1	1:C:221:TRP:N	2.86	0.42
1:B:434:GLY:C	1:B:435:ARG:HG3	2.40	0.42
1:B:486:CYS:HG	1:B:487:LEU:N	2.18	0.42
1:B:73:GLU:HA	1:B:74:PRO:HD3	1.91	0.42
1:B:175:ILE:HB	1:B:187:VAL:HG13	2.02	0.42
1:B:445:GLU:CD	1:B:483:ARG:HG3	2.40	0.42
1:B:460:VAL:HG12	1:B:469:LEU:HD22	2.00	0.42
1:B:511:ARG:O	1:B:514:GLU:HB2	2.19	0.42
1:A:334:ILE:HD11	1:A:361:GLU:OE1	2.20	0.42
1:B:476:GLU:OE1	1:B:476:GLU:N	2.53	0.42
1:C:73:GLU:O	1:C:77:ARG:NE	2.53	0.42
1:C:255:VAL:CG1	1:C:260:LEU:HD11	2.50	0.42
1:C:315:LEU:O	1:C:319:LYS:N	2.53	0.42
1:C:328:ARG:C	1:C:332:LYS:HZ2	2.23	0.42
1:A:192:ARG:HH21	1:C:81:GLU:CD	2.22	0.42
1:A:340:GLU:HG3	1:A:341:ARG:N	2.35	0.42
1:C:147:ARG:NH2	1:C:160:ALA:HA	2.34	0.42
1:C:178:ARG:O	1:C:185:GLY:HA3	2.19	0.42
1:C:295:ARG:HA	1:C:295:ARG:HH11	1.84	0.42
1:B:98:VAL:HA	1:B:106:ARG:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ALA:HA	1:C:288:CYS:SG	2.60	0.41
1:C:180:ASP:N	1:C:180:ASP:OD1	2.51	0.41
1:B:140:ALA:O	1:B:144:GLY:HA3	2.20	0.41
1:B:360:LEU:HD23	1:B:360:LEU:HA	1.93	0.41
1:C:202:LEU:HD13	1:C:203:HIS:O	2.20	0.41
1:C:445:GLU:HG3	1:C:446:ALA:N	2.36	0.41
1:A:451:ASN:OD1	1:A:479:LYS:HE2	2.20	0.41
1:B:126:SER:C	1:B:129:ARG:HG3	2.40	0.41
1:C:276:LEU:HD21	1:C:278:LYS:HE2	2.01	0.41
1:C:505:ILE:HG12	1:C:506:ASP:N	2.35	0.41
1:B:175:ILE:CD1	1:B:177:TYR:HB2	2.51	0.41
1:C:55:VAL:HG12	1:C:108:PHE:HE2	1.84	0.41
1:C:436:ASN:HA	1:C:437:ASN:HA	1.85	0.41
1:A:447:VAL:O	1:A:482:VAL:O	2.39	0.41
1:B:315:LEU:HA	1:B:315:LEU:HD23	1.82	0.41
1:B:407:ASP:O	1:B:422:VAL:HG11	2.21	0.41
1:B:410:ALA:O	1:B:414:PRO:HG3	2.19	0.41
1:A:247:LEU:HD23	1:A:247:LEU:HA	1.91	0.41
1:B:59:SER:H	1:B:62:GLN:NE2	2.18	0.41
1:C:328:ARG:HG3	1:C:332:LYS:HZ2	1.85	0.41
1:C:439:VAL:HG13	1:C:500:LEU:HD23	2.01	0.41
1:A:30:GLN:OE1	1:A:226:PRO:HD2	2.21	0.41
1:C:178:ARG:CD	1:C:179:PHE:H	2.33	0.41
1:C:164:GLU:C	1:C:166:ARG:N	2.74	0.41
1:C:228:ILE:HG23	1:C:269:GLN:O	2.21	0.41
1:C:470:HIS:ND1	1:C:471:PRO:N	2.69	0.41
1:A:56:LEU:HD13	1:A:56:LEU:O	2.20	0.41
1:A:166:ARG:NH1	1:A:171:PHE:O	2.54	0.41
1:A:177:TYR:CE1	1:A:185:GLY:HA3	2.56	0.41
1:A:266:MET:HG3	1:A:475:PHE:CD2	2.56	0.41
1:A:366:HIS:O	1:A:380:GLY:HA3	2.21	0.41
1:A:394:TRP:CB	1:A:398:ARG:HG3	2.48	0.41
1:A:412:GLU:O	1:A:414:PRO:HD3	2.20	0.41
1:B:366:HIS:N	1:B:442:PHE:O	2.54	0.41
1:B:430:SER:CB	1:B:433:ARG:HH12	2.16	0.41
1:C:78:GLU:HB2	1:C:79:PRO:HD3	2.03	0.41
1:C:147:ARG:HH21	1:C:160:ALA:HA	1.86	0.41
1:C:391:LEU:O	1:C:392:ILE:HB	2.21	0.41
1:A:221:TRP:O	1:A:274:ILE:HA	2.22	0.41
1:C:88:ARG:HD2	1:C:88:ARG:HA	1.89	0.41
1:C:97:VAL:CG2	1:C:110:GLY:H	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:LEU:HD23	1:C:168:LEU:H	1.86	0.41
1:C:307:PHE:O	1:C:309:GLY:C	2.59	0.41
1:C:316:LEU:HD12	1:C:316:LEU:C	2.41	0.41
1:C:454:GLY:HA3	1:C:472:ARG:HH21	1.85	0.41
1:C:276:LEU:CD2	1:C:278:LYS:HE2	2.50	0.40
1:C:464:GLN:NE2	1:C:468:ARG:HH12	2.13	0.40
1:A:162:VAL:HG13	1:A:176:ILE:HG12	2.03	0.40
1:A:275:SER:HA	1:A:285:LEU:HD23	2.03	0.40
1:A:294:THR:O	1:A:295:ARG:HD2	2.20	0.40
1:A:464:GLN:H	1:A:466:GLY:H	1.69	0.40
1:B:324:ASP:O	1:B:326:ASP:C	2.59	0.40
1:B:427:MET:HE2	1:B:427:MET:HB2	1.83	0.40
1:C:145:LEU:HB3	1:C:146:SER:H	1.53	0.40
1:C:165:VAL:HA	1:C:168:LEU:HD21	2.03	0.40
1:A:211:ARG:HA	1:A:211:ARG:HD2	1.81	0.40
1:A:323:GLU:O	1:A:328:ARG:NH1	2.54	0.40
1:A:458:LYS:O	1:A:460:VAL:HG22	2.22	0.40
1:B:137:PHE:O	1:B:141:VAL:HG13	2.21	0.40
1:C:134:PHE:O	1:C:135:LEU:HD13	2.20	0.40
1:C:261:GLU:OE1	1:C:469:LEU:HD11	2.22	0.40
1:A:255:VAL:HG23	1:A:260:LEU:HD11	2.03	0.40
1:A:273:SER:HB3	2:A:601:BLR:O1A	2.21	0.40
1:C:190:GLU:HB2	1:C:192:ARG:HB2	2.02	0.40
1:C:297:VAL:HG23	1:C:301:VAL:CG1	2.50	0.40
1:C:322:ASN:O	1:C:492:TYR:OH	2.39	0.40
1:C:427:MET:CE	1:C:494:VAL:HA	2.51	0.40
1:C:438:PHE:O	1:C:439:VAL:HB	2.21	0.40
1:C:450:VAL:HG21	1:C:452:TRP:CH2	2.57	0.40
1:A:175:ILE:HD12	1:A:175:ILE:O	2.20	0.40
1:C:339:LEU:CD2	1:C:343:ALA:HB3	2.52	0.40

There are no symmetry-related clashes.

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	503/515 (98%)	446 (89%)	44 (9%)	13 (3%)	5 7
1	B	503/515 (98%)	444 (88%)	39 (8%)	20 (4%)	3 3
1	C	498/515 (97%)	332 (67%)	122 (24%)	44 (9%)	1 0
All	All	1504/1545 (97%)	1222 (81%)	205 (14%)	77 (5%)	2 2

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	44	VAL
1	A	389	THR
1	A	458	LYS
1	B	14	ASP
1	B	328	ARG
1	B	375	ARG
1	B	385	ASP
1	B	448	GLN
1	B	484	GLY
1	C	90	LYS
1	C	93	ASN
1	C	145	LEU
1	C	313	SER
1	C	392	ILE
1	C	414	PRO
1	C	421	GLU
1	C	439	VAL
1	C	447	VAL
1	C	470	HIS
1	A	395	LEU
1	A	448	GLN
1	A	510	GLN
1	B	128	HIS
1	B	383	PRO
1	B	463	ASP
1	C	20	ARG
1	C	94	PRO
1	C	102	ASP
1	C	282	LEU
1	C	358	GLY

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Mol	Chain	Res	Type
1	C	429	PHE
1	C	431	MET
1	C	456	PRO
1	C	462	PHE
1	C	468	ARG
1	C	471	PRO
1	A	128	HIS
1	A	386	GLU
1	A	394	TRP
1	A	400	GLY
1	A	463	ASP
1	B	195	ARG
1	B	316	LEU
1	B	384	SER
1	B	398	ARG
1	C	152	ARG
1	C	174	ALA
1	C	307	PHE
1	C	417	GLN
1	B	323	GLU
1	B	324	ASP
1	B	464	GLN
1	C	103	GLY
1	C	200	LEU
1	C	364	HIS
1	C	464	GLN
1	A	12	GLU
1	C	169	THR
1	C	226	PRO
1	C	283	TRP
1	C	340	GLU
1	C	347	ASP
1	C	444	PRO
1	C	461	GLU
1	C	467	PRO
1	B	399	THR
1	C	312	MET
1	C	460	VAL
1	C	465	GLY
1	B	22	PRO
1	B	378	VAL
1	C	26	PRO

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Mol	Chain	Res	Type
1	C	73	GLU
1	C	79	PRO
1	C	144	GLY
1	B	434	GLY

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	419/427 (98%)	405 (97%)	14 (3%)	38	54
1	B	419/427 (98%)	409 (98%)	10 (2%)	49	67
1	C	414/427 (97%)	386 (93%)	28 (7%)	16	24
All	All	1252/1281 (98%)	1200 (96%)	52 (4%)	30	45

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	20	ARG
1	A	39	SER
1	A	127	SER
1	A	142	ARG
1	A	211	ARG
1	A	223	ARG
1	A	260	LEU
1	A	322	ASN
1	A	326	ASP
1	A	356	GLU
1	A	366	HIS
1	A	395	LEU
1	A	469	LEU
1	B	73	GLU
1	B	129	ARG
1	B	166	ARG
1	B	330	ARG

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Mol	Chain	Res	Type
1	B	350	SER
1	B	377	THR
1	B	384	SER
1	B	408	ARG
1	B	417	GLN
1	B	433	ARG
1	C	20	ARG
1	C	24	HIS
1	C	83	ASP
1	C	107	PHE
1	C	129	ARG
1	C	136	SER
1	C	138	PHE
1	C	142	ARG
1	C	154	LEU
1	C	168	LEU
1	C	173	ARG
1	C	203	HIS
1	C	211	ARG
1	C	223	ARG
1	C	226	PRO
1	C	262	TYR
1	C	275	SER
1	C	278	LYS
1	C	312	MET
1	C	320	GLU
1	C	362	LEU
1	C	371	HIS
1	C	384	SER
1	C	411	ARG
1	C	453	SER
1	C	490	LYS
1	C	492	TYR
1	C	506	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	B	355	GLN
1	C	58	ASN
1	C	155	GLN

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Mol	Chain	Res	Type
1	C	364	HIS
1	C	417	GLN
1	C	510	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)

3 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	$\#\|Z\| > 2$
2	BLR	A	601	1	40,46,46	5.14	17 (42%)	44,67,67	1.57	9 (20%)
2	BLR	B	601	1	40,46,46	5.12	17 (42%)	44,67,67	1.45	9 (20%)
2	BLR	C	601	1	40,46,46	5.19	17 (42%)	44,67,67	1.60	8 (18%)

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
2	BLR	A	601	1	-	9/24/58/58	0/4/4/4
2	BLR	B	601	1	-	11/24/58/58	0/4/4/4
2	BLR	C	601	1	-	14/24/58/58	0/4/4/4

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	BLR	CHA-C4D	-24.25	1.33	1.51
2	A	601	BLR	CHA-C4D	-24.11	1.33	1.51
2	C	601	BLR	CHA-C4D	-23.42	1.33	1.51
2	C	601	BLR	C3D-C4D	10.77	1.55	1.39
2	C	601	BLR	C1B-NB	9.76	1.54	1.37
2	C	601	BLR	C4C-NC	9.72	1.54	1.37
2	A	601	BLR	C3D-C4D	9.72	1.53	1.39
2	A	601	BLR	C4C-NC	9.38	1.53	1.37
2	B	601	BLR	C3D-C4D	9.09	1.52	1.39
2	B	601	BLR	C1B-NB	9.04	1.52	1.37
2	B	601	BLR	C4C-NC	8.90	1.52	1.37
2	A	601	BLR	C1B-NB	8.82	1.52	1.37
2	C	601	BLR	C1C-NC	7.71	1.54	1.38
2	C	601	BLR	C4B-NB	7.56	1.53	1.38
2	B	601	BLR	C1C-NC	7.54	1.53	1.38
2	A	601	BLR	C1C-NC	7.32	1.53	1.38
2	A	601	BLR	C4B-NB	7.03	1.52	1.38
2	B	601	BLR	C4B-NB	6.51	1.51	1.38
2	C	601	BLR	CHA-C1A	3.93	1.54	1.51
2	B	601	BLR	C4A-CHB	3.39	1.54	1.41
2	C	601	BLR	C4A-CHB	3.35	1.54	1.41
2	B	601	BLR	C3D-C2D	3.32	1.47	1.37
2	A	601	BLR	OB-C4B	-3.15	1.17	1.23
2	B	601	BLR	OB-C4B	-3.08	1.17	1.23
2	B	601	BLR	C3C-C4C	3.06	1.50	1.45
2	A	601	BLR	C3D-C2D	3.03	1.46	1.37
2	A	601	BLR	OC-C1C	-3.01	1.17	1.23
2	A	601	BLR	C1D-CHD	3.00	1.52	1.41
2	A	601	BLR	C3C-C2C	2.97	1.43	1.37
2	B	601	BLR	C1D-CHD	2.95	1.52	1.41
2	B	601	BLR	C1B-C2B	2.93	1.50	1.45
2	B	601	BLR	C3C-C2C	2.82	1.43	1.37
2	A	601	BLR	C4A-CHB	2.80	1.52	1.41
2	B	601	BLR	OC-C1C	-2.77	1.18	1.23
2	C	601	BLR	C3D-C2D	2.77	1.45	1.37
2	A	601	BLR	CHA-C1A	2.74	1.53	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	BLR	C3B-C2B	2.73	1.42	1.37
2	C	601	BLR	C3C-C2C	2.64	1.42	1.37
2	C	601	BLR	C1D-CHD	2.62	1.51	1.41
2	A	601	BLR	C3C-C4C	2.53	1.49	1.45
2	C	601	BLR	OC-C1C	-2.52	1.18	1.23
2	A	601	BLR	C3B-C2B	2.50	1.42	1.37
2	C	601	BLR	OB-C4B	-2.47	1.18	1.23
2	B	601	BLR	CAC-C3C	2.46	1.54	1.47
2	B	601	BLR	C3B-C2B	2.45	1.42	1.37
2	A	601	BLR	CAC-C3C	2.43	1.54	1.47
2	C	601	BLR	C1B-C2B	2.42	1.49	1.45
2	C	601	BLR	CAC-C3C	2.24	1.53	1.47
2	C	601	BLR	CAB-C3B	2.14	1.53	1.47
2	B	601	BLR	CAB-C3B	2.12	1.53	1.47
2	A	601	BLR	CAB-C3B	2.07	1.53	1.47

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	BLR	CAD-C3D-C4D	4.18	130.23	127.30
2	C	601	BLR	C4C-NC-C1C	-4.07	105.48	110.67
2	A	601	BLR	CAA-C2A-C1A	4.00	130.10	127.30
2	A	601	BLR	CAD-C3D-C4D	-3.43	124.89	127.30
2	A	601	BLR	C4C-NC-C1C	-3.25	106.53	110.67
2	A	601	BLR	CBD-CAD-C3D	-3.09	107.34	112.62
2	B	601	BLR	CAA-C2A-C1A	-2.88	125.27	127.30
2	C	601	BLR	C1B-NB-C4B	-2.87	107.01	110.67
2	B	601	BLR	CAD-CBD-CGD	-2.81	105.88	113.76
2	C	601	BLR	CBA-CAA-C2A	-2.78	107.88	112.62
2	B	601	BLR	CAD-C3D-C4D	-2.77	125.35	127.30
2	B	601	BLR	C4C-NC-C1C	-2.65	107.29	110.67
2	C	601	BLR	C3B-C2B-C1B	2.57	111.14	108.03
2	A	601	BLR	C3B-C2B-C1B	2.57	111.13	108.03
2	C	601	BLR	CAD-C3D-C2D	-2.47	120.14	127.25
2	C	601	BLR	O1D-CGD-CBD	2.46	121.93	114.03
2	B	601	BLR	C1B-NB-C4B	-2.45	107.55	110.67
2	B	601	BLR	O1A-CGA-O2A	-2.37	117.39	123.30
2	A	601	BLR	C1B-NB-C4B	-2.35	107.67	110.67
2	A	601	BLR	O1A-CGA-CBA	2.21	121.12	114.03
2	A	601	BLR	CAA-C2A-C3A	-2.18	120.97	127.25
2	B	601	BLR	CMB-C2B-C1B	2.17	126.87	124.17
2	C	601	BLR	CHD-C4C-C3C	-2.10	122.48	127.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	BLR	CMB-C2B-C3B	-2.08	123.22	128.30
2	B	601	BLR	C4B-C3B-C2B	2.06	110.57	107.92
2	A	601	BLR	O1D-CGD-CBD	2.05	120.61	114.03

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	BLR	C2A-C1A-CHA-C4D
2	A	601	BLR	NA-C4A-CHB-C1B
2	A	601	BLR	C3A-C4A-CHB-C1B
2	B	601	BLR	C2A-C1A-CHA-C4D
2	B	601	BLR	C3D-C4D-CHA-C1A
2	B	601	BLR	NA-C4A-CHB-C1B
2	B	601	BLR	C3A-C4A-CHB-C1B
2	B	601	BLR	C2C-C3C-CAC-CBC
2	B	601	BLR	C4C-C3C-CAC-CBC
2	C	601	BLR	C3D-C4D-CHA-C1A
2	C	601	BLR	NA-C4A-CHB-C1B
2	C	601	BLR	C3A-C4A-CHB-C1B
2	C	601	BLR	C2A-CAA-CBA-CGA
2	C	601	BLR	NB-C1B-CHB-C4A
2	C	601	BLR	NC-C4C-CHD-C1D
2	C	601	BLR	C3D-CAD-CBD-CGD
2	A	601	BLR	NB-C1B-CHB-C4A
2	B	601	BLR	NB-C1B-CHB-C4A
2	A	601	BLR	CAD-CBD-CGD-O2D
2	B	601	BLR	CAD-CBD-CGD-O1D
2	A	601	BLR	CAA-CBA-CGA-O2A
2	C	601	BLR	CAD-CBD-CGD-O2D
2	B	601	BLR	CAA-CBA-CGA-O2A
2	B	601	BLR	CAD-CBD-CGD-O2D
2	C	601	BLR	CAD-CBD-CGD-O1D
2	A	601	BLR	CAA-CBA-CGA-O1A
2	A	601	BLR	CAD-CBD-CGD-O1D
2	B	601	BLR	CAA-CBA-CGA-O1A
2	A	601	BLR	C3D-C4D-CHA-C1A
2	C	601	BLR	C2A-C1A-CHA-C4D
2	C	601	BLR	CAA-CBA-CGA-O2A
2	C	601	BLR	C2B-C1B-CHB-C4A
2	C	601	BLR	C3C-C4C-CHD-C1D
2	C	601	BLR	CAA-CBA-CGA-O1A

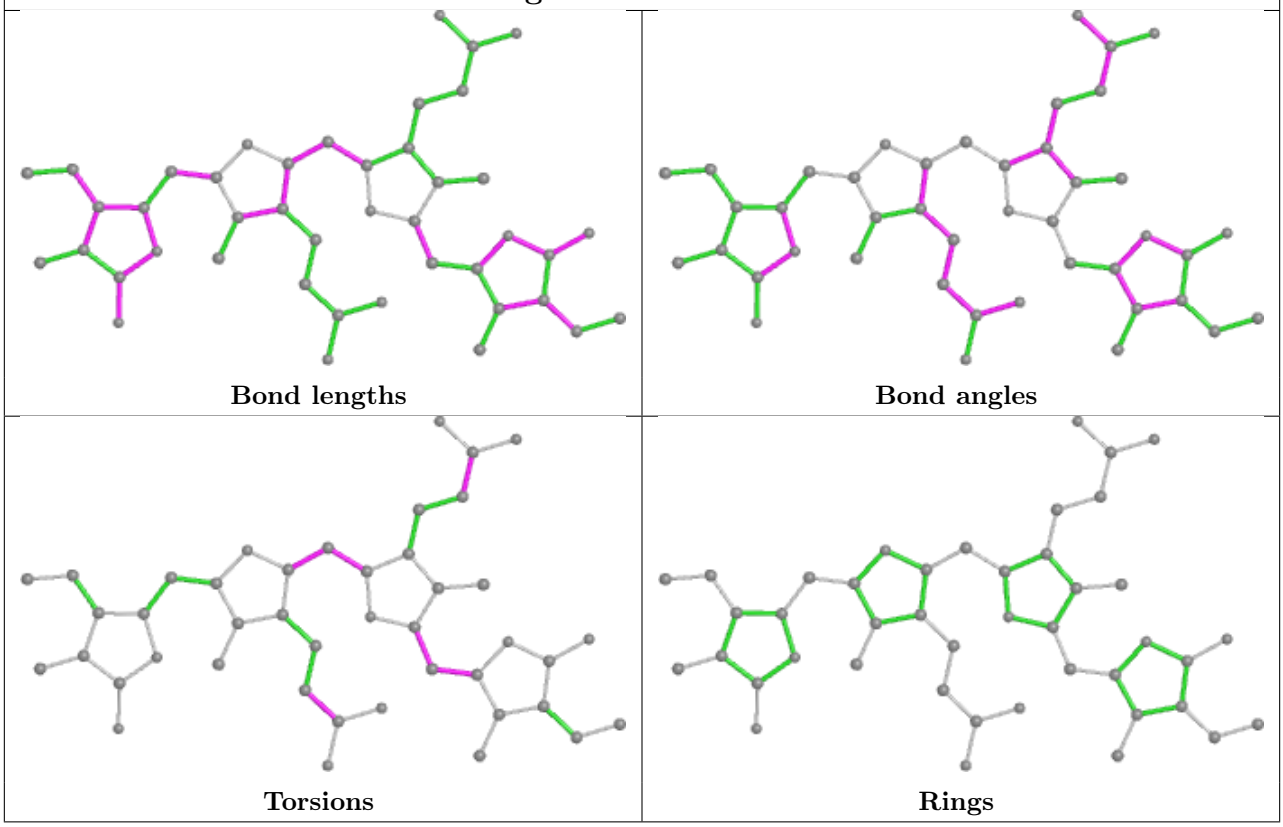
There are no ring outliers.

3 monomers are involved in 24 short contacts:

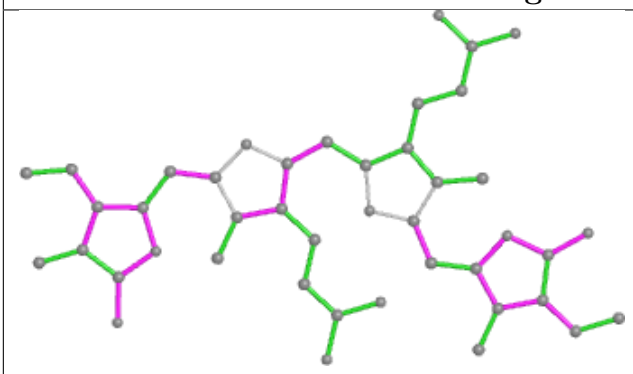
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	BLR	5	0
2	B	601	BLR	4	0
2	C	601	BLR	15	0

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.

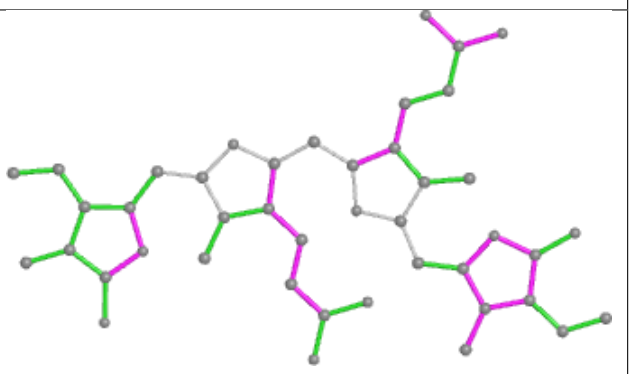
Ligand BLR A 601



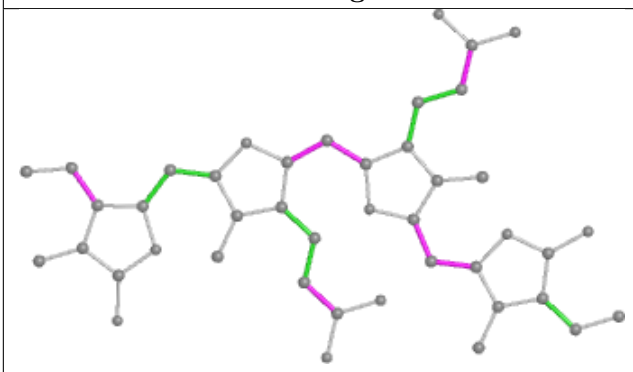
Ligand BLR B 601



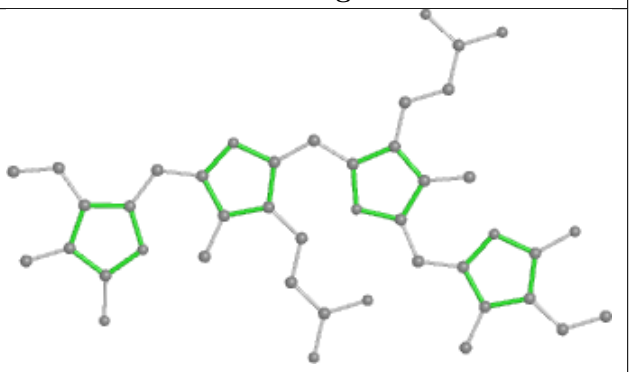
Bond lengths



Bond angles

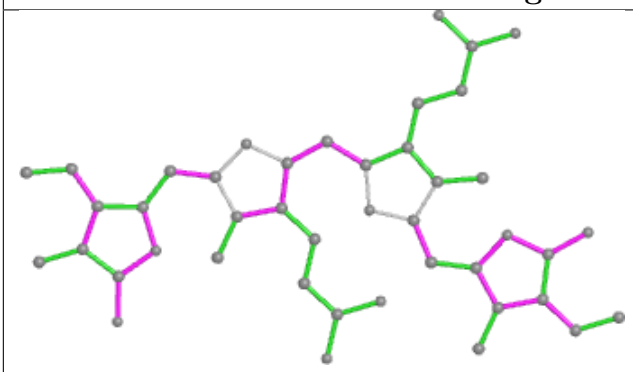


Torsions

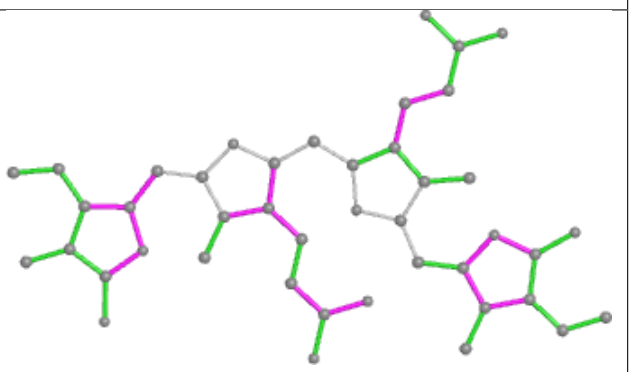


Rings

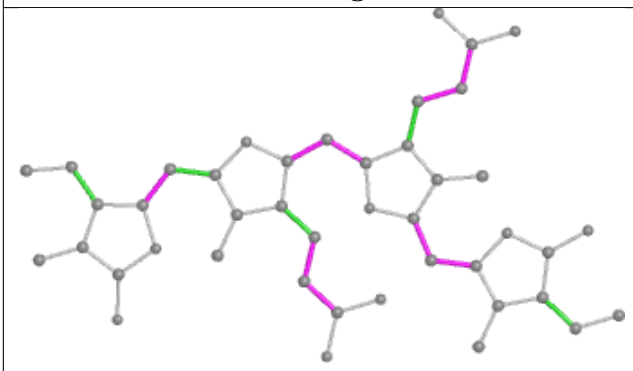
Ligand BLR C 601



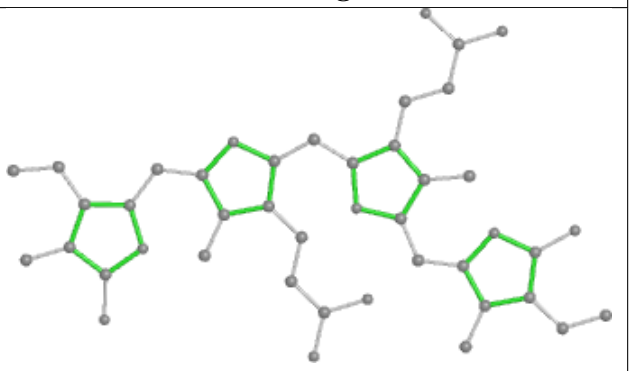
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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	505/515 (98%)	0.03	18 (3%)	42	39	35, 64, 99, 162	0
1	B	505/515 (98%)	0.05	18 (3%)	42	39	35, 69, 109, 135	1 (0%)
1	C	500/515 (97%)	2.02	167 (33%)	0	0	54, 107, 209, 230	3 (0%)
All	All	1510/1545 (97%)	0.70	203 (13%)	3	2	35, 74, 189, 230	4 (0%)

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	337	ALA	32.8
1	C	380	GLY	17.2
1	C	368	ALA	15.6
1	C	378	VAL	14.9
1	C	491	ALA	14.6
1	C	379	LEU	14.4
1	C	423	ALA	14.0
1	C	506	ASP	13.0
1	C	440	LEU	12.5
1	C	372	PHE	11.4
1	C	418	ALA	11.2
1	C	439	VAL	11.2
1	C	436	ASN	11.1
1	C	334	ILE	10.8
1	C	512	SER	10.6
1	C	358	GLY	10.4
1	C	404	PHE	9.8
1	C	488	PRO	9.7
1	C	403	VAL	9.6
1	C	132	VAL	9.5
1	C	376	THR	9.5
1	C	374	GLY	9.1
1	C	370	ILE	8.9

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Mol	Chain	Res	Type	RSRZ
1	A	13	VAL	8.5
1	C	373	HIS	8.3
1	C	413	TYR	8.2
1	C	336	ALA	8.2
1	C	391	LEU	8.1
1	A	12	GLU	7.9
1	C	431	MET	7.9
1	A	11	GLN	7.6
1	C	363	VAL	7.5
1	C	369	ALA	7.4
1	C	507	VAL	7.4
1	C	387	ALA	7.4
1	C	339	LEU	7.3
1	C	430	SER	7.3
1	C	504	ILE	7.3
1	C	333	SER	7.3
1	C	457	THR	7.3
1	C	515	LEU	7.1
1	C	346	VAL	7.1
1	C	513	GLU	7.0
1	A	15	LEU	7.0
1	C	435	ARG	6.9
1	C	326	ASP	6.8
1	C	329	ILE	6.7
1	A	462	PHE	6.6
1	C	338	LEU	6.5
1	C	377	THR	6.5
1	C	401	GLU	6.5
1	C	414	PRO	6.3
1	B	425	GLY	6.2
1	C	354	SER	6.2
1	C	500	LEU	6.0
1	B	398	ARG	6.0
1	C	381	GLN	5.9
1	C	325	TYR	5.8
1	B	423	ALA	5.7
1	C	360	LEU	5.6
1	C	490	LYS	5.6
1	C	327	GLN	5.6
1	C	402	GLY	5.6
1	C	492	TYR	5.6
1	C	400	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	499	GLU	5.5
1	C	505	ILE	5.5
1	C	411	ARG	5.4
1	C	371	HIS	5.3
1	C	503	SER	5.3
1	B	424	ALA	5.3
1	C	481	THR	5.2
1	C	399	THR	5.1
1	C	419	PHE	5.0
1	C	433	ARG	5.0
1	C	510	GLN	5.0
1	C	383	PRO	4.9
1	A	467	PRO	4.8
1	C	494	VAL	4.7
1	C	434	GLY	4.6
1	C	495	GLU	4.6
1	C	514	GLU	4.6
1	C	442	PHE	4.6
1	A	397	SER	4.6
1	C	412	GLU	4.5
1	C	316	LEU	4.5
1	A	14	ASP	4.5
1	C	424	ALA	4.5
1	C	441	TRP	4.5
1	C	386	GLU	4.4
1	C	392	ILE	4.4
1	C	330	ARG	4.4
1	C	432	SER	4.3
1	C	498	SER	4.3
1	C	395	LEU	4.3
1	C	397	SER	4.3
1	C	384	SER	4.2
1	B	422	VAL	4.2
1	B	11	GLN	4.1
1	B	464	GLN	4.1
1	C	405	CYS	4.1
1	C	130	GLU	4.1
1	B	12	GLU	4.0
1	B	400	GLY	4.0
1	C	186	SER	4.0
1	C	18	CYS	3.9
1	C	361	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	493	GLU	3.9
1	C	315	LEU	3.9
1	C	385	ASP	3.9
1	C	429	PHE	3.8
1	C	461	GLU	3.8
1	C	394	TRP	3.8
1	A	465	GLY	3.8
1	C	364	HIS	3.8
1	C	331	ALA	3.8
1	C	460	VAL	3.8
1	C	511	ARG	3.8
1	A	16	THR	3.8
1	C	508	ALA	3.7
1	C	204	PHE	3.7
1	C	443	ARG	3.6
1	C	307	PHE	3.5
1	C	390	GLY	3.4
1	C	366	HIS	3.4
1	C	509	LEU	3.4
1	C	291	VAL	3.3
1	C	466	GLY	3.3
1	C	489	TRP	3.3
1	C	101	VAL	3.2
1	C	348	PHE	3.2
1	B	13	VAL	3.2
1	A	464	GLN	3.1
1	C	340	GLU	3.1
1	C	470	HIS	3.1
1	C	17	ASN	3.1
1	C	422	VAL	3.1
1	C	487	LEU	3.0
1	C	191	ALA	3.0
1	A	399	THR	3.0
1	C	367	GLY	3.0
1	C	452	TRP	3.0
1	C	465	GLY	2.9
1	A	400	GLY	2.8
1	B	438	PHE	2.8
1	C	362	LEU	2.8
1	C	324	ASP	2.8
1	C	349	VAL	2.7
1	B	387	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	341	ARG	2.7
1	C	154	LEU	2.7
1	C	382	ALA	2.7
1	C	446	ALA	2.7
1	C	437	ASN	2.6
1	C	285	LEU	2.6
1	C	283	TRP	2.6
1	C	16	THR	2.6
1	C	133	PRO	2.6
1	B	15	LEU	2.6
1	C	375	ARG	2.6
1	A	463	ASP	2.6
1	C	357	SER	2.6
1	C	131	ALA	2.5
1	C	396	GLY	2.5
1	C	282	LEU	2.5
1	C	444	PRO	2.5
1	C	286	ILE	2.5
1	C	428	ALA	2.5
1	C	313	SER	2.5
1	C	277	MET	2.5
1	C	323	GLU	2.4
1	C	496	ALA	2.4
1	C	425	GLY	2.4
1	C	416	ALA	2.4
1	A	468	ARG	2.4
1	C	200	LEU	2.4
1	C	274	ILE	2.4
1	C	309	GLY	2.4
1	C	345	GLU	2.3
1	C	447	VAL	2.3
1	C	389	THR	2.3
1	C	410	ALA	2.3
1	C	335	HIS	2.3
1	B	436	ASN	2.3
1	C	310	GLU	2.2
1	B	419	PHE	2.2
1	C	342	MET	2.2
1	A	22	PRO	2.2
1	C	320	GLU	2.2
1	A	346	VAL	2.2
1	C	179	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	350	SER	2.2
1	C	188	ILE	2.1
1	C	20	ARG	2.1
1	B	383	PRO	2.1
1	C	306	GLU	2.1
1	C	468	ARG	2.1
1	B	14	ASP	2.1
1	C	157	LEU	2.0
1	A	461	GLU	2.0
1	C	449	THR	2.0
1	C	355	GLN	2.0
1	B	444	PRO	2.0

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)

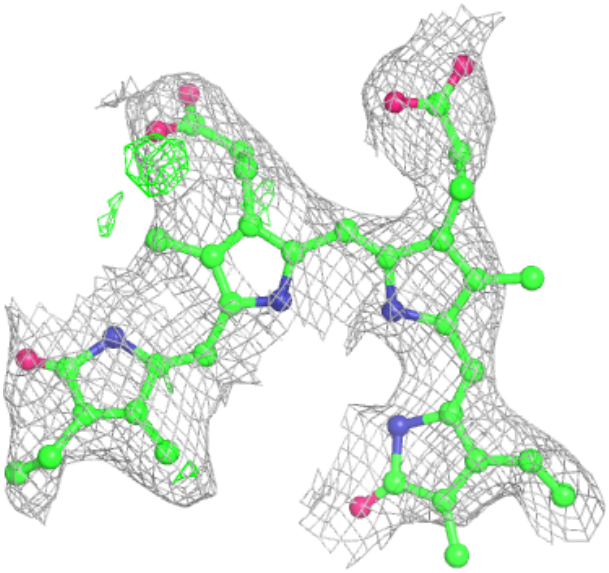
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

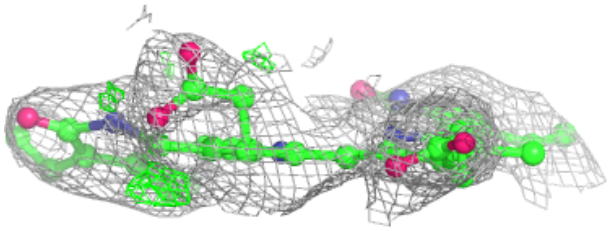
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BLR	C	601	43/43	0.78	0.24	86,97,113,118	0
2	BLR	A	601	43/43	0.94	0.20	47,60,78,94	1
2	BLR	B	601	43/43	0.95	0.18	43,51,63,67	1

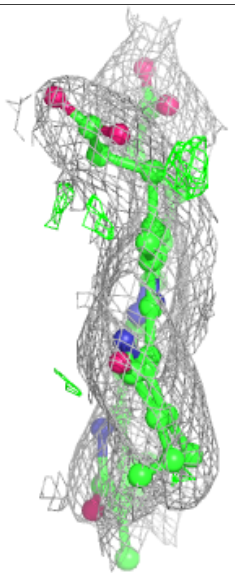
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BLR C 601:

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

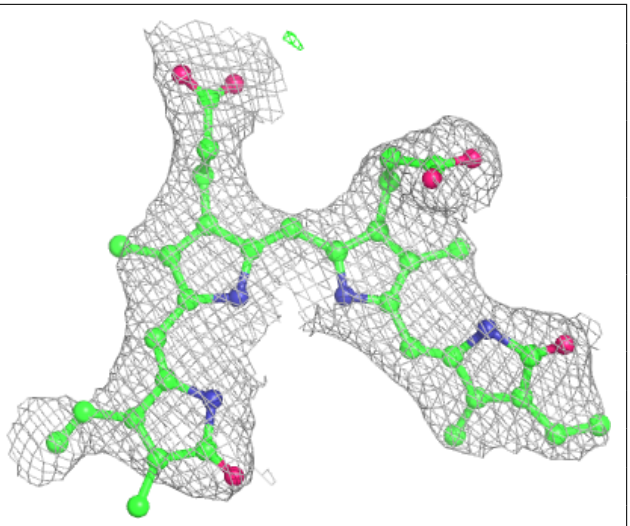


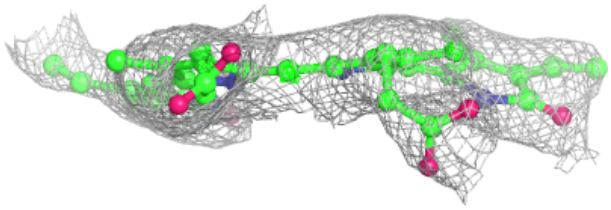


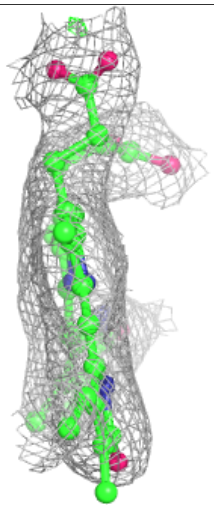


Electron density around BLR A 601:

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

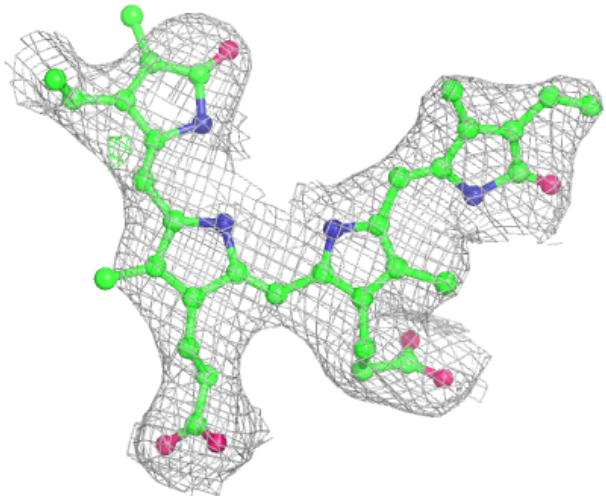


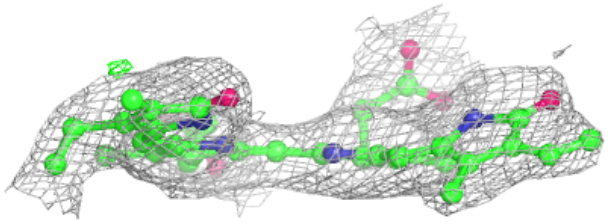


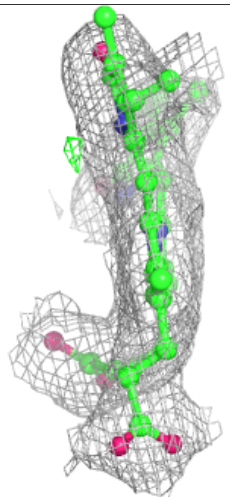


Electron density around BLR B 601:

$2mF_o$-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.