Full wwPDB X-ray Structure Validation Report (i)

Jul 31, 2023 – 06:50 AM EDT

PDB ID	:	1RT5
Title	:	HIV-1 REVERSE TRANSCRIPTASE COMPLEXED WITH UC10
Authors	:	Ren, J.; Stammers, D.K.; Stuart, D.I.
Deposited on	:	1998-07-29
Resolution	:	2.90 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:

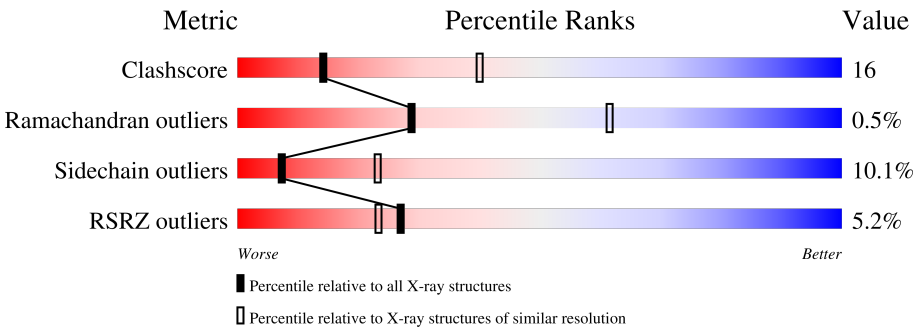
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	560	7%, 59%, 33%, • •
2	B	440	3%, 62%, 27%, •, 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7780 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 HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	537	4396	2847	732	809	8	0	0	0

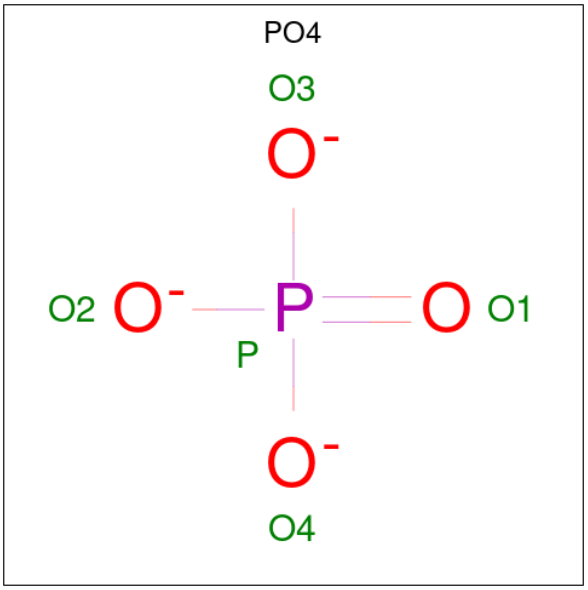
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	modified residue	UNP P04585

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

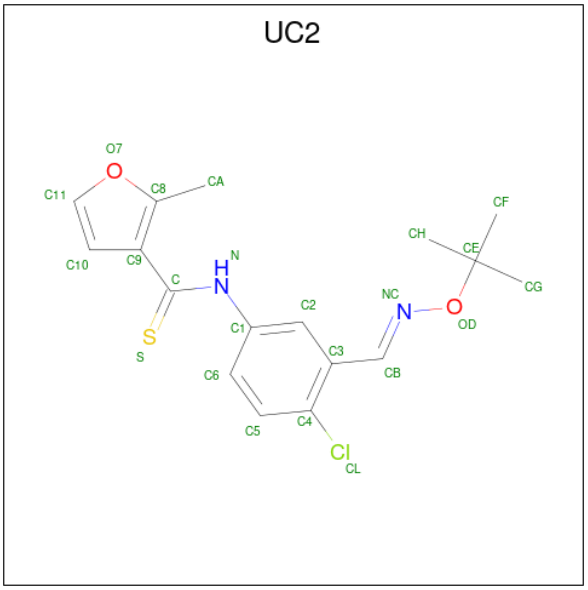
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	406	3351	2175	558	611	7	0	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	A	1	5	4	1	0	0

- Molecule 4 is N-[4-CLORO-3-(T-BUTYLOXOME)PHENYL-2-METHYL-3-FURAN-CARBOTHIAMIDE (three-letter code: UC2) (formula: $C_{17}H_{19}ClN_2O_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
4	A	1	23	17	1	2	2	1	0	0

- Molecule 5 is water.

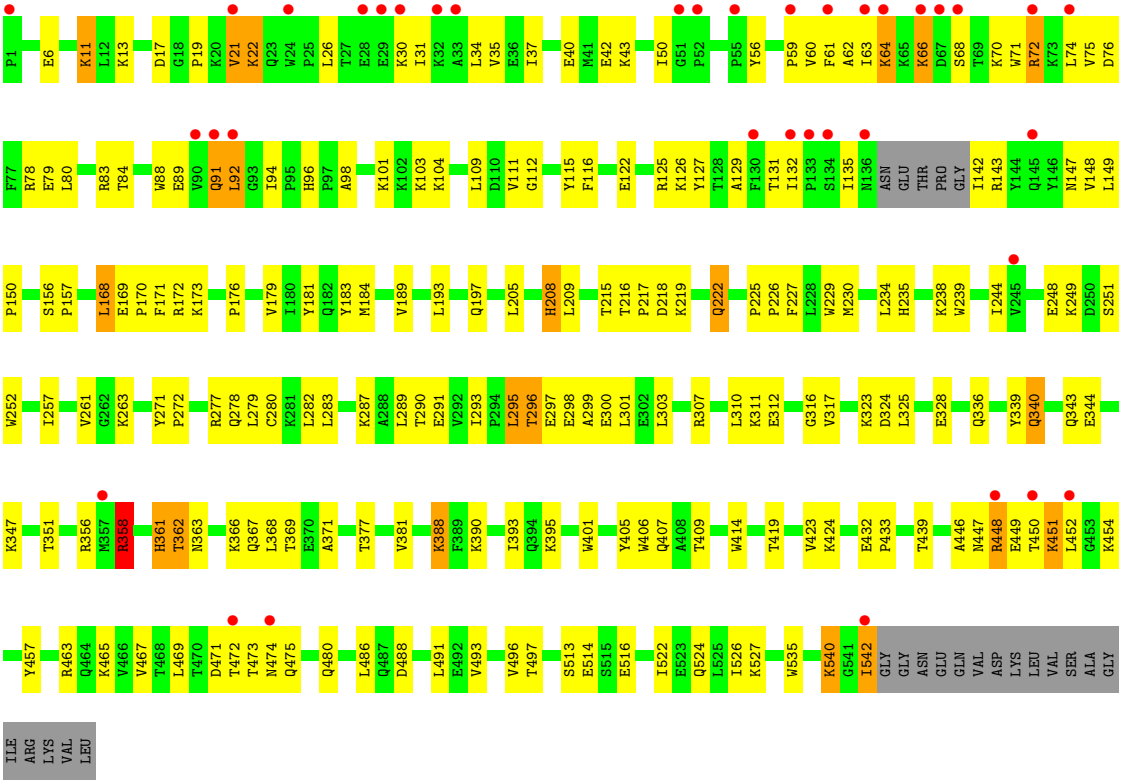
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	4	4	4	0	0
5	B	1	1	1	0	0

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.

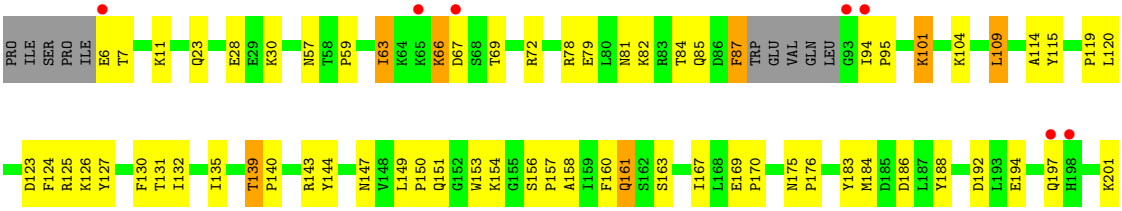
• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE

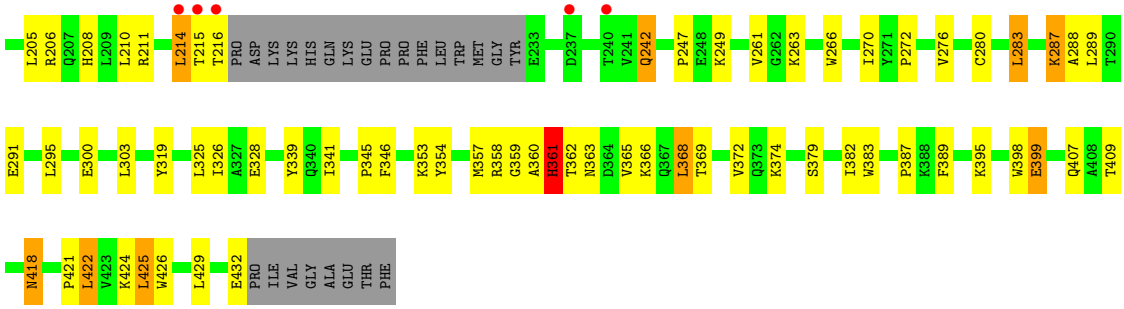
Chain A: 7% 59% 33%



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE

Chain B: 3% 62% 27% 8%




L205 R206 Q207 H208 L209 L210 R211 L214 T215 T216 PRO ASP LYS LYS HIS GLN LYS GLU PRO PRO PHE LEU TRP MET GLY TYR E233 D237 T240 V241 Q242 P247 E248 K249 V261 G262 K263 W266 I270 Y271 P272 V276 C280 L283 K287 A288 L289 T290
E291 L295 E300 L303 Y319 L325 I326 A327 E328 Y339 Q340 I341 P345 F346 K353 Y354 M357 R358 G359 A360 H361 T362 N363 D364 V365 K366 Q367 L368 T369 V372 Q373 K374 S379 I382 W383 P387 K388 F389 K395 W398 E399 Q407 A408 T409
N418 P421 L422 V423 K424 L425 W426 L429 E432 PRO ILE VAL GLY ALA GLU THR PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	140.30Å 111.00Å 73.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.65 – 2.90	Depositor EDS
% Data completeness (in resolution range)	86.1 (30.00-2.90) 87.2 (29.65-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 2.90Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.231 , 0.291 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 83.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7780	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: PO4, CSD, UC2

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	0.34	0/4503	0.63	1/6117 (0.0%)
2	B	0.33	0/3442	0.62	0/4672
All	All	0.34	0/7945	0.63	1/10789 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	388	LYS	N-CA-C	-5.14	97.13	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4396	0	4451	151	0
2	B	3351	0	3386	93	0
3	A	5	0	0	0	0
4	A	23	0	19	5	0
5	A	4	0	0	1	0
5	B	1	0	0	0	0
All	All	7780	0	7856	243	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 16.

All (243) 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:34:LEU:HD11	1:A:62:ALA:HB2	1.27	1.16
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.16	1.07
1:A:540:LYS:HG2	2:B:280:CYS:SG	1.95	1.05
1:A:22:LYS:H	1:A:22:LYS:HD3	1.33	0.94
1:A:219:LYS:HD3	1:A:222:GLN:HE22	1.34	0.89
1:A:244:ILE:HG23	1:A:310:LEU:HD13	1.56	0.87
1:A:34:LEU:CD1	1:A:62:ALA:HB2	2.06	0.84
2:B:109:LEU:HG	2:B:216:THR:HG21	1.57	0.84
2:B:422:LEU:HD23	2:B:422:LEU:H	1.44	0.82
1:A:132:ILE:HB	1:A:142:ILE:HB	1.61	0.81
1:A:358:ARG:HG2	1:A:358:ARG:NH1	1.87	0.79
1:A:344:GLU:HB2	1:A:347:LYS:HD3	1.64	0.78
1:A:356:ARG:HH22	1:A:371:ALA:HB2	1.50	0.77
1:A:219:LYS:HD3	1:A:222:GLN:NE2	2.00	0.77
2:B:66:LYS:HG2	2:B:407:GLN:OE1	1.84	0.76
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.65	0.76
2:B:247:PRO:HB2	2:B:249:LYS:HZ1	1.49	0.76
1:A:193:LEU:HD13	1:A:197:GLN:HG3	1.68	0.76
2:B:242:GLN:HA	2:B:242:GLN:HE21	1.52	0.74
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.22	0.74
2:B:84:THR:HG22	2:B:154:LYS:HE2	1.69	0.74
2:B:266:TRP:CD1	2:B:422:LEU:HD12	2.25	0.71
2:B:101:LYS:HD2	2:B:382:ILE:HG23	1.72	0.71
2:B:157:PRO:HG2	2:B:184:MET:HA	1.72	0.71
2:B:214:LEU:H	2:B:214:LEU:HD23	1.56	0.71
2:B:247:PRO:HB2	2:B:249:LYS:NZ	2.05	0.70
1:A:89:GLU:HB2	1:A:92:LEU:HD22	1.73	0.69
1:A:257:ILE:O	1:A:261:VAL:HG23	1.92	0.69
1:A:358:ARG:HH11	1:A:358:ARG:CG	2.02	0.69
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.75	0.68
1:A:235:HIS:HB2	1:A:238:LYS:O	1.93	0.67
2:B:354:TYR:HD1	2:B:374:LYS:HZ1	1.42	0.67
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.30	0.67
1:A:448:ARG:CZ	1:A:448:ARG:H	2.07	0.67
2:B:72:ARG:HH21	2:B:409:THR:HG22	1.60	0.66
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.78	0.66
1:A:171:PHE:HB2	1:A:208:HIS:HD2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.78	0.66
1:A:62:ALA:HB1	1:A:71:TRP:CE3	2.31	0.65
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.11	0.65
1:A:540:LYS:HB3	1:A:542:ILE:HD12	1.81	0.63
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.81	0.62
2:B:109:LEU:CG	2:B:216:THR:HG21	2.29	0.61
2:B:158:ALA:O	2:B:161:GLN:HB2	2.01	0.61
1:A:22:LYS:H	1:A:22:LYS:CD	2.05	0.61
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.35	0.61
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.36	0.60
2:B:263:LYS:HE2	2:B:425:LEU:HB3	1.84	0.60
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.00	0.60
2:B:109:LEU:HG	2:B:216:THR:CG2	2.31	0.60
1:A:62:ALA:HB1	1:A:71:TRP:HE3	1.66	0.59
1:A:448:ARG:HB3	1:A:448:ARG:HH11	1.67	0.59
1:A:17:ASP:O	1:A:83:ARG:HD3	2.03	0.59
1:A:31:ILE:O	1:A:35:VAL:HG23	2.03	0.59
1:A:542:ILE:HD12	1:A:542:ILE:H	1.66	0.59
4:A:999:UC2:H2	4:A:999:UC2:C9	2.34	0.58
1:A:344:GLU:CB	1:A:347:LYS:HD3	2.32	0.58
1:A:168:LEU:HD11	1:A:209:LEU:HD21	1.84	0.58
1:A:68:SER:C	1:A:70:LYS:H	2.06	0.57
2:B:206:ARG:HG3	2:B:216:THR:O	2.05	0.57
1:A:30:LYS:O	1:A:34:LEU:HD13	2.05	0.57
1:A:287:LYS:HG2	1:A:291:GLU:OE1	2.05	0.57
1:A:21:VAL:HG22	1:A:59:PRO:HD3	1.86	0.57
1:A:104:LYS:NZ	1:A:104:LYS:HB3	2.20	0.57
1:A:249:LYS:HG3	1:A:252:TRP:CE2	2.40	0.57
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.86	0.56
2:B:120:LEU:HD12	2:B:150:PRO:HD3	1.87	0.56
1:A:50:ILE:HG13	1:A:143:ARG:HB3	1.88	0.56
1:A:216:THR:HG23	1:A:217:PRO:HD2	1.86	0.56
1:A:66:LYS:H	1:A:66:LYS:HD2	1.71	0.56
1:A:26:LEU:HD22	1:A:30:LYS:HE2	1.88	0.56
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.41	0.56
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.89	0.55
1:A:340:GLN:CB	1:A:351:THR:HG22	2.37	0.55
2:B:197:GLN:O	2:B:201:LYS:HB2	2.06	0.55
1:A:11:LYS:NZ	1:A:11:LYS:HB3	2.21	0.55
2:B:206:ARG:O	2:B:210:LEU:HD13	2.05	0.55
1:A:92:LEU:HD23	1:A:92:LEU:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:LEU:O	2:B:372:VAL:HG23	2.06	0.55
1:A:278:GLN:HG2	1:A:298:GLU:HB3	1.88	0.54
1:A:356:ARG:HB2	1:A:367:GLN:NE2	2.23	0.54
1:A:451:LYS:HG3	1:A:472:THR:O	2.08	0.54
1:A:432:GLU:HB2	1:A:433:PRO:HD2	1.91	0.53
1:A:122:GLU:H	1:A:122:GLU:CD	2.12	0.53
1:A:40:GLU:O	1:A:43:LYS:HG2	2.09	0.53
1:A:324:ASP:O	1:A:343:GLN:HG2	2.09	0.53
2:B:163:SER:O	2:B:167:ILE:HG13	2.08	0.53
1:A:13:LYS:HG2	1:A:83:ARG:O	2.09	0.53
1:A:366:LYS:O	1:A:369:THR:HB	2.09	0.53
2:B:319:TYR:HE1	2:B:325:LEU:HD13	1.74	0.53
2:B:395:LYS:O	2:B:399:GLU:HG2	2.08	0.52
1:A:129:ALA:HB1	1:A:143:ARG:NH1	2.24	0.52
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.45	0.52
1:A:296:THR:HG23	1:A:299:ALA:HB2	1.92	0.52
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.40	0.52
1:A:516:GLU:OE1	1:A:516:GLU:HA	2.09	0.52
1:A:26:LEU:HD22	1:A:30:LYS:CE	2.41	0.51
1:A:540:LYS:CG	2:B:280:CYS:SG	2.86	0.51
2:B:360:ALA:HB2	2:B:366:LYS:HD2	1.90	0.51
1:A:37:ILE:O	1:A:40:GLU:HB3	2.10	0.51
1:A:94:ILE:HG23	1:A:229:TRP:CZ2	2.47	0.50
1:A:344:GLU:HG3	1:A:347:LYS:NZ	2.26	0.50
2:B:101:LYS:HG3	2:B:382:ILE:HA	1.94	0.50
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.91	0.50
1:A:497:THR:O	1:A:535:TRP:HA	2.11	0.50
4:A:999:UC2:C2	4:A:999:UC2:C10	2.90	0.50
1:A:22:LYS:HD3	1:A:22:LYS:N	2.14	0.50
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.46	0.50
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.93	0.50
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.12	0.50
2:B:295:LEU:HB3	2:B:300:GLU:HG2	1.93	0.50
2:B:421:PRO:O	2:B:425:LEU:HD22	2.12	0.50
1:A:448:ARG:HB3	1:A:448:ARG:NH1	2.27	0.49
2:B:354:TYR:HD1	2:B:374:LYS:NZ	2.09	0.49
1:A:362:THR:HG22	1:A:363:ASN:H	1.78	0.49
1:A:252:TRP:CD1	1:A:295:LEU:HD12	2.48	0.49
4:A:999:UC2:HA1	4:A:999:UC2:S	2.53	0.49
1:A:454:LYS:HA	1:A:467:VAL:O	2.13	0.48
1:A:91:GLN:O	1:A:91:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ARG:HH22	2:B:151:GLN:NE2	2.11	0.48
2:B:72:ARG:NH2	2:B:151:GLN:NE2	2.61	0.48
1:A:89:GLU:CB	1:A:92:LEU:HD22	2.42	0.48
1:A:173:LYS:O	1:A:176:PRO:HD3	2.13	0.48
2:B:109:LEU:CB	2:B:216:THR:HG21	2.44	0.48
2:B:125:ARG:NE	2:B:147:ASN:HA	2.27	0.48
2:B:288:ALA:O	2:B:291:GLU:HB3	2.14	0.48
2:B:365:VAL:O	2:B:369:THR:HG23	2.14	0.48
1:A:451:LYS:HD2	1:A:473:THR:HG22	1.95	0.48
1:A:94:ILE:HG23	1:A:229:TRP:HZ2	1.79	0.48
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.49	0.48
4:A:999:UC2:C9	4:A:999:UC2:C2	2.91	0.48
1:A:60:VAL:HG13	1:A:75:VAL:HG22	1.96	0.47
1:A:446:ALA:O	1:A:474:ASN:ND2	2.46	0.47
2:B:72:ARG:HG3	2:B:72:ARG:HH11	1.79	0.47
2:B:120:LEU:HD21	2:B:124:PHE:HD2	1.79	0.47
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.95	0.47
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.50	0.47
2:B:115:TYR:OH	2:B:157:PRO:HG3	2.15	0.47
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.32	0.47
1:A:13:LYS:HD3	1:A:84:THR:O	2.14	0.47
2:B:175:ASN:N	2:B:176:PRO:HD3	2.29	0.47
2:B:326:ILE:O	2:B:341:ILE:HA	2.14	0.47
2:B:66:LYS:O	2:B:67:ASP:HB2	2.15	0.47
1:A:122:GLU:HA	1:A:125:ARG:NE	2.31	0.46
1:A:325:LEU:O	1:A:388:LYS:HG3	2.14	0.46
1:A:344:GLU:HG3	1:A:347:LYS:HZ2	1.80	0.46
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.97	0.46
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.63	0.46
1:A:19:PRO:HG2	1:A:80:LEU:HB2	1.97	0.46
1:A:56:TYR:O	1:A:143:ARG:NH1	2.44	0.46
1:A:68:SER:C	1:A:70:LYS:N	2.68	0.46
1:A:248:GLU:HA	1:A:307:ARG:NH2	2.30	0.46
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.51	0.46
1:A:448:ARG:HG2	1:A:449:GLU:H	1.81	0.46
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.98	0.46
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.51	0.46
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.98	0.46
1:A:356:ARG:HH22	1:A:371:ALA:CB	2.24	0.46
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.16	0.45
1:A:26:LEU:CA	1:A:30:LYS:HZ3	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:THR:O	1:A:381:VAL:HG23	2.16	0.45
1:A:446:ALA:O	1:A:448:ARG:NH2	2.50	0.45
1:A:13:LYS:HG2	1:A:13:LYS:H	1.53	0.45
2:B:63:ILE:HD13	2:B:63:ILE:H	1.82	0.45
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.99	0.45
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.99	0.45
1:A:282:LEU:HD11	1:A:296:THR:HG22	1.98	0.45
2:B:28:GLU:HA	2:B:135:ILE:HD11	1.99	0.44
1:A:64:LYS:H	1:A:64:LYS:HG3	1.52	0.44
2:B:78:ARG:O	2:B:82:LYS:HG3	2.17	0.44
1:A:11:LYS:HB3	1:A:11:LYS:HZ3	1.82	0.44
2:B:426:TRP:O	2:B:429:LEU:HB2	2.18	0.44
1:A:116:PHE:O	1:A:148:VAL:HG21	2.17	0.44
1:A:300:GLU:OE1	1:A:300:GLU:HA	2.18	0.44
2:B:126:LYS:HG3	2:B:127:TYR:N	2.32	0.44
1:A:249:LYS:HG3	1:A:252:TRP:CZ2	2.52	0.44
1:A:282:LEU:HB3	1:A:293:ILE:HG21	1.98	0.44
2:B:270:ILE:O	2:B:272:PRO:HD3	2.18	0.44
1:A:361:HIS:ND1	1:A:361:HIS:N	2.65	0.43
1:A:448:ARG:HG2	1:A:449:GLU:N	2.33	0.43
1:A:72:ARG:HH21	1:A:74:LEU:CD1	2.32	0.43
2:B:422:LEU:H	2:B:422:LEU:CD2	2.18	0.43
1:A:26:LEU:HA	1:A:30:LYS:HZ3	1.82	0.43
1:A:542:ILE:H	1:A:542:ILE:CD1	2.26	0.43
1:A:184:MET:N	5:A:1004:HOH:O	2.51	0.43
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.53	0.43
1:A:277:ARG:HH11	1:A:277:ARG:HB2	1.84	0.43
2:B:328:GLU:O	2:B:339:TYR:HA	2.19	0.43
1:A:522:ILE:O	1:A:526:ILE:HG13	2.19	0.43
1:A:169:GLU:N	1:A:170:PRO:HD2	2.34	0.42
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.33	0.42
2:B:359:GLY:HA2	2:B:361:HIS:CE1	2.54	0.42
2:B:94:ILE:N	2:B:94:ILE:HD12	2.34	0.42
1:A:179:VAL:O	1:A:189:VAL:HA	2.19	0.42
2:B:261:VAL:HG22	2:B:276:VAL:HG22	2.00	0.42
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.80	0.42
1:A:296:THR:HG23	1:A:299:ALA:CB	2.49	0.42
1:A:358:ARG:H	1:A:358:ARG:HG3	1.49	0.42
1:A:109:LEU:HD23	1:A:216:THR:HG21	2.01	0.42
2:B:363:ASN:OD1	2:B:363:ASN:C	2.58	0.42
1:A:26:LEU:HB3	1:A:30:LYS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:LYS:O	2:B:85:GLN:HG2	2.19	0.42
1:A:447:ASN:HA	1:A:448:ARG:NH2	2.35	0.42
2:B:287:LYS:H	2:B:287:LYS:HG2	1.69	0.42
2:B:87:PHE:CD1	2:B:87:PHE:N	2.88	0.42
2:B:104:LYS:HB2	2:B:192:ASP:HA	2.02	0.42
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.55	0.42
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.19	0.42
1:A:184:MET:HA	1:A:184:MET:CE	2.50	0.42
1:A:463:ARG:NH1	1:A:488:ASP:O	2.52	0.41
1:A:469:LEU:HB2	1:A:472:THR:HG21	2.02	0.41
2:B:205:LEU:O	2:B:208:HIS:HB3	2.21	0.41
1:A:131:THR:OG1	1:A:143:ARG:HD3	2.20	0.41
2:B:94:ILE:HG22	2:B:94:ILE:O	2.20	0.41
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.54	0.41
1:A:234:LEU:HB3	4:A:999:UC2:CL	2.57	0.41
2:B:132:ILE:HD12	2:B:132:ILE:N	2.34	0.41
1:A:419:THR:HG23	1:A:419:THR:O	2.19	0.41
2:B:84:THR:CG2	2:B:154:LYS:HE2	2.46	0.41
1:A:103:LYS:HA	1:A:103:LYS:HD3	1.83	0.41
1:A:362:THR:HG23	1:A:366:LYS:HD3	2.01	0.41
2:B:30:LYS:HE2	2:B:30:LYS:HB3	1.88	0.41
1:A:115:TYR:O	1:A:149:LEU:HB2	2.21	0.41
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.55	0.41
2:B:183:TYR:HB3	2:B:188:TYR:HE2	1.85	0.41
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.20	0.41
1:A:542:ILE:HG13	2:B:283:LEU:HB3	2.03	0.41
1:A:116:PHE:C	1:A:148:VAL:HG21	2.41	0.41
1:A:168:LEU:O	1:A:172:ARG:HG3	2.21	0.41
2:B:79:GLU:HA	2:B:82:LYS:HE2	2.03	0.41
1:A:135:ILE:H	1:A:135:ILE:HG13	1.58	0.41
1:A:244:ILE:HD11	1:A:263:LYS:HB3	2.03	0.41
1:A:401:TRP:CZ3	1:A:409:THR:HG21	2.56	0.41
2:B:81:ASN:OD1	2:B:153:TRP:HD1	2.05	0.40
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.51	0.40
1:A:96:HIS:CD2	1:A:98:ALA:H	2.40	0.40
2:B:206:ARG:HG2	2:B:210:LEU:CD1	2.51	0.40
2:B:345:PRO:O	2:B:346:PHE:HB2	2.21	0.40
1:A:271:TYR:O	1:A:272:PRO:C	2.59	0.40
1:A:328:GLU:O	1:A:339:TYR:HA	2.22	0.40
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.57	0.40
2:B:66:LYS:H	2:B:66:LYS:HG3	1.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:LYS:HE3	2:B:353:LYS:HB2	1.93	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	532/560 (95%)	495 (93%)	34 (6%)	3 (1%)	25	58
2	B	400/440 (91%)	373 (93%)	25 (6%)	2 (0%)	29	61
All	All	932/1000 (93%)	868 (93%)	59 (6%)	5 (0%)	29	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLY
2	B	361	HIS
1	A	358	ARG
2	B	95	PRO
1	A	111	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	481/499 (96%)	426 (89%)	55 (11%)	5 17
2	B	369/400 (92%)	338 (92%)	31 (8%)	11 31
All	All	850/899 (94%)	764 (90%)	86 (10%)	7 23

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	11	LYS
1	A	21	VAL
1	A	22	LYS
1	A	42	GLU
1	A	61	PHE
1	A	63	ILE
1	A	64	LYS
1	A	66	LYS
1	A	72	ARG
1	A	91	GLN
1	A	92	LEU
1	A	101	LYS
1	A	168	LEU
1	A	205	LEU
1	A	208	HIS
1	A	215	THR
1	A	218	ASP
1	A	222	GLN
1	A	230	MET
1	A	251	SER
1	A	279	LEU
1	A	283	LEU
1	A	289	LEU
1	A	290	THR
1	A	295	LEU
1	A	296	THR
1	A	297	GLU
1	A	301	LEU
1	A	303	LEU
1	A	311	LYS
1	A	312	GLU

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Mol	Chain	Res	Type
1	A	317	VAL
1	A	323	LYS
1	A	336	GLN
1	A	340	GLN
1	A	358	ARG
1	A	361	HIS
1	A	362	THR
1	A	368	LEU
1	A	424	LYS
1	A	448	ARG
1	A	451	LYS
1	A	452	LEU
1	A	471	ASP
1	A	475	GLN
1	A	480	GLN
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL
1	A	513	SER
1	A	514	GLU
1	A	527	LYS
1	A	540	LYS
1	A	542	ILE
2	B	6	GLU
2	B	63	ILE
2	B	66	LYS
2	B	69	THR
2	B	87	PHE
2	B	101	LYS
2	B	109	LEU
2	B	123	ASP
2	B	139	THR
2	B	161	GLN
2	B	186	ASP
2	B	194	GLU
2	B	211	ARG
2	B	214	LEU
2	B	215	THR
2	B	242	GLN
2	B	283	LEU
2	B	287	LYS
2	B	303	LEU

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Mol	Chain	Res	Type
2	B	357	MET
2	B	358	ARG
2	B	361	HIS
2	B	362	THR
2	B	368	LEU
2	B	379	SER
2	B	399	GLU
2	B	418	ASN
2	B	422	LEU
2	B	424	LYS
2	B	425	LEU
2	B	432	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	222	GLN
1	A	235	HIS
1	A	242	GLN
1	A	315	HIS
1	A	332	GLN
1	A	373	GLN
2	B	57	ASN
2	B	85	GLN
2	B	151	GLN
2	B	161	GLN
2	B	242	GLN
2	B	269	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)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	CSD	A	280	1	3,7,8	0.82	0	1,8,10	3.49	1 (100%)

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
1	CSD	A	280	1	-	2/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	CSD	OD1-SG-CB	3.49	112.18	105.54

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
4	UC2	A	999	-	20,24,24	3.79	5 (25%)	23,34,34	1.48	4 (17%)
3	PO4	A	1001	-	4,4,4	1.75	2 (50%)	6,6,6	0.39	0

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
4	UC2	A	999	-	-	2/10/15/15	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	UC2	OD-NC	-12.76	1.16	1.42
4	A	999	UC2	CB-NC	6.60	1.40	1.27
4	A	999	UC2	C-N	5.25	1.39	1.34
4	A	999	UC2	OD-CE	-4.77	1.40	1.47
4	A	999	UC2	CA-C8	3.71	1.53	1.48
3	A	1001	PO4	P-O4	-2.16	1.48	1.54
3	A	1001	PO4	P-O2	-2.11	1.48	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	999	UC2	S-C-N	-3.78	117.91	125.23
4	A	999	UC2	CE-OD-NC	2.99	112.98	110.39
4	A	999	UC2	C3-CB-NC	-2.90	116.33	120.92
4	A	999	UC2	C5-C4-C3	-2.45	119.85	121.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	999	UC2	C9-C-N-C1
4	A	999	UC2	S-C-N-C1

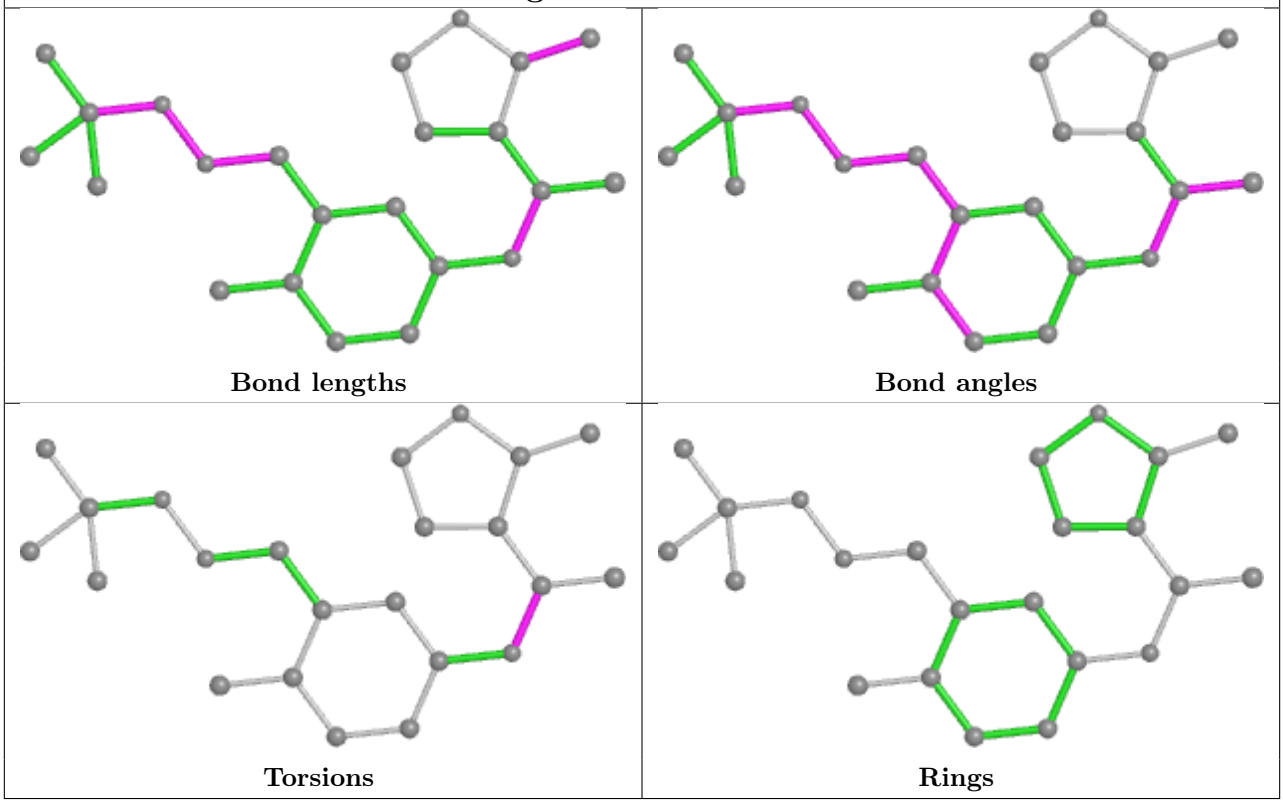
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	UC2	5	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 UC2 A 999



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	536/560 (95%)	0.01	37 (6%)	16	13	11, 54, 124, 149	0
2	B	406/440 (92%)	-0.19	12 (2%)	50	45	10, 50, 108, 160	0
All	All	942/1000 (94%)	-0.08	49 (5%)	27	23	10, 52, 120, 160	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	SER	5.8
1	A	67	ASP	5.5
1	A	52	PRO	5.3
2	B	216	THR	5.0
1	A	30	LYS	4.9
1	A	29	GLU	4.5
2	B	6	GLU	4.1
1	A	132	ILE	4.1
1	A	450	THR	3.9
1	A	28	GLU	3.9
1	A	63	ILE	3.8
1	A	74	LEU	3.8
1	A	542	ILE	3.7
1	A	90	VAL	3.7
2	B	214	LEU	3.7
2	B	198	HIS	3.6
1	A	136	ASN	3.5
1	A	452	LEU	3.5
1	A	91	GLN	3.4
1	A	61	PHE	3.4
1	A	21	VAL	3.2
1	A	245	VAL	3.2
1	A	55	PRO	3.2
1	A	51	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	94	ILE	3.1
2	B	93	GLY	3.1
1	A	72	ARG	2.8
1	A	145	GLN	2.8
2	B	237	ASP	2.8
1	A	472	THR	2.7
2	B	67	ASP	2.6
1	A	130	PHE	2.6
2	B	215	THR	2.6
1	A	1	PRO	2.6
1	A	33	ALA	2.6
1	A	133	PRO	2.5
2	B	197	GLN	2.5
1	A	64	LYS	2.3
1	A	474	ASN	2.3
1	A	66	LYS	2.3
1	A	24	TRP	2.2
1	A	92	LEU	2.2
2	B	65	LYS	2.1
2	B	240	THR	2.1
1	A	134	SER	2.1
1	A	357	MET	2.1
1	A	448	ARG	2.0
1	A	59	PRO	2.0
1	A	32	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CSD	A	280	8/9	0.94	0.12	40,44,51,60	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

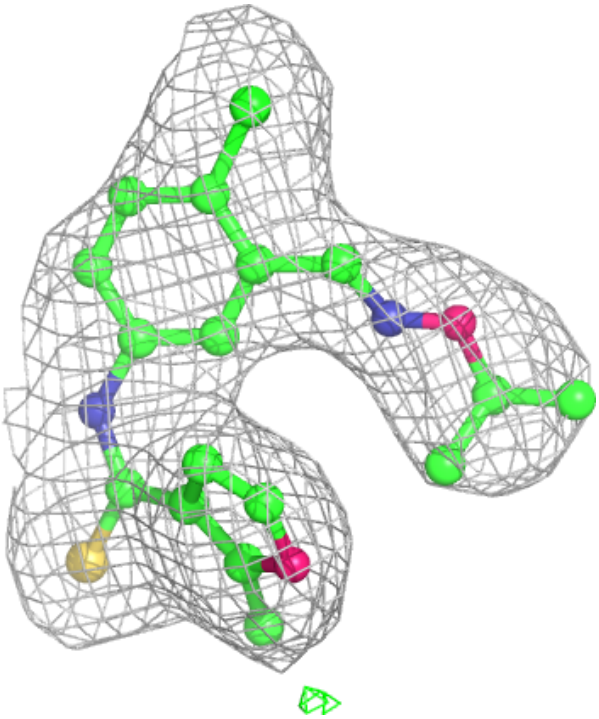
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

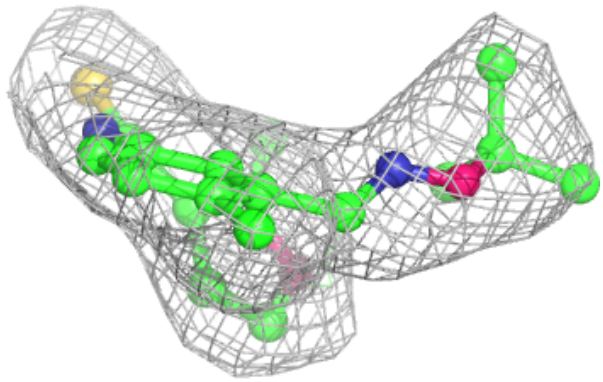
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	A	1001	5/5	0.93	0.28	100,101,108,109	0
4	UC2	A	999	23/23	0.98	0.12	8,22,34,40	0

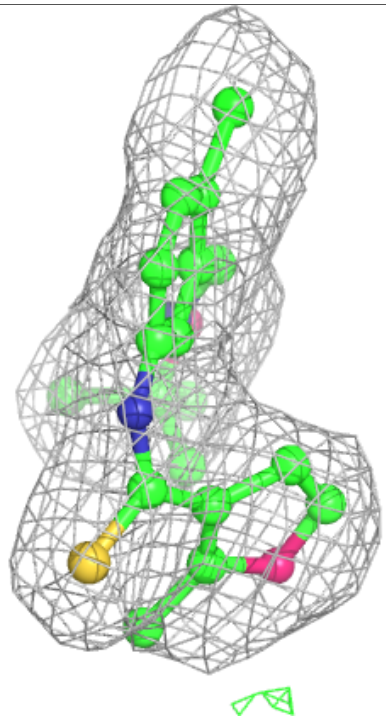
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UC2 A 999:

$2mF_o$-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.