Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 03:39 PM EST

PDB ID	:	4TZ4
Title	:	Crystal Structure of Human Cereblon in Complex with DDB1 and Lenalidomide
Authors	:	Chamberlain, P.P.; Pagarigan, B.; Delker, S.; Leon, B.; Riley, M.
Deposited on	:	2014-07-09
Resolution	:	3.01 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:

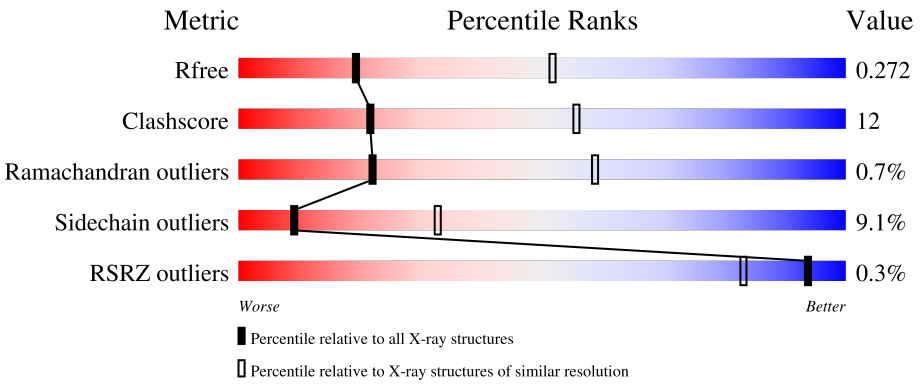
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	1146	70% 20% • 7%
2	C	381	67% 21% 6% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11081 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1070	8191	5227	1367	1552	45	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1141	TRP	-	expression tag	UNP Q16531
A	1142	SER	-	expression tag	UNP Q16531
A	1143	HIS	-	expression tag	UNP Q16531
A	1144	PRO	-	expression tag	UNP Q16531
A	1145	GLN	-	expression tag	UNP Q16531
A	1146	PHE	-	expression tag	UNP Q16531
A	1147	GLU	-	expression tag	UNP Q16531

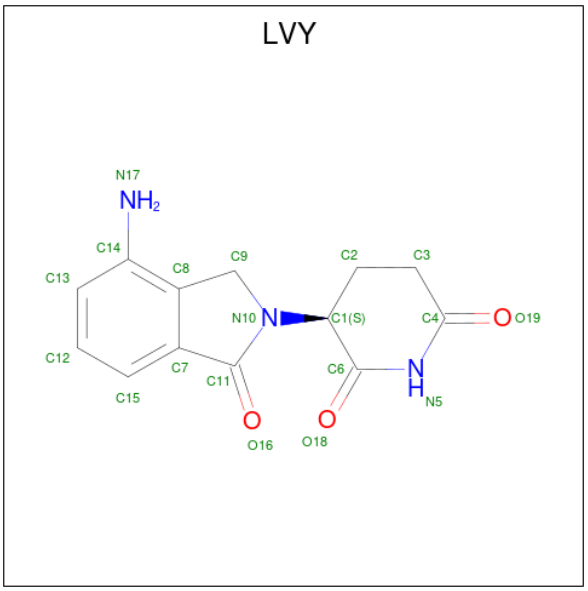
- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	361	2852	1832	485	513	22	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	C	1	1	1	0	0

- Molecule 4 is S-Lenalidomide (three-letter code: LVY) (formula: $C_{13}H_{13}N_3O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	C	1	19	13	3	3	0	0

- Molecule 5 is water.

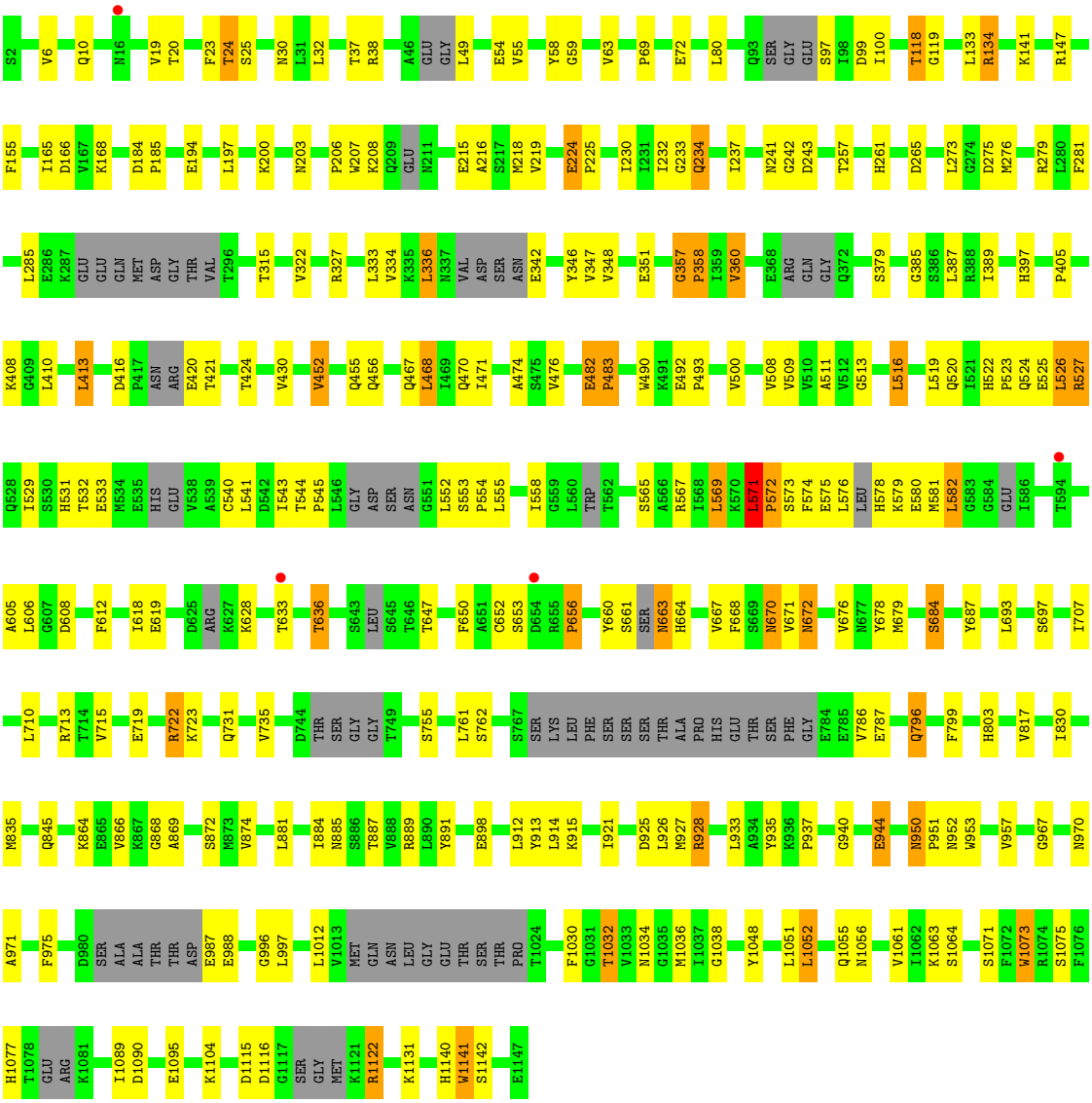
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	13	13	13	0	0
			Total	O		
5	C	5	5	5	0	0

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: DNA damage-binding protein 1

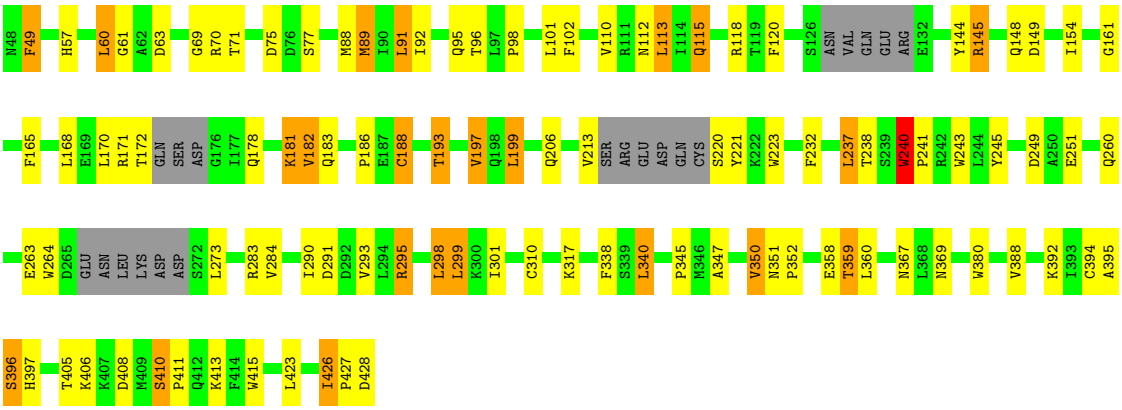
Chain A: 70% 20% • 7%



• Molecule 2: Protein cereblon

Chain C:

67%
21%
6%
5%


N48 F49 H57 L60 G61 A62 D63 G69 R70 T71 D75 D76 S77 M88 M89 I90 L91 I92 Q95 T96 L97 P98 L101 F102 V110 R111 N112 L113 I114 Q115 R118 T119 F120 S126 ASN VAL GLN GLU ARG E132 Y144 R145 Q148 D149 T154 G161
F165 L168 E169 L170 R171 T172 GLN SER ASP G176 I177 Q178 K181 V182 Q183 P186 E187 C188 T193 V197 Q198 L199 Q206 V213 SER ARG GLU ASP GLN CYS S220 Y221 K222 W223 F232 L237 T238 S239 W240 P241 R242 W243 L244 Y245 D249 A250 E251 Q260
E263 W264 D265 GLU ASN LEU LYS ASP ASP S272 L273 R283 V284 I290 D291 D292 V293 L294 R295 L298 L299 K300 I301 C310 K317 F338 S339 L340 P345 M346 A347 V350 N351 P352 E358 T359 L360 N367 L368 N369 W380 V388 K392 I393 C394 A395
S396 H397 T405 K406 K407 D408 M409 S410 P411 Q412 K413 F414 W415 L423 I426 P427 D428

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.86Å 129.12Å 198.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.01 48.70 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-3.01) 99.5 (48.70-3.01)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.202 , 0.271 0.202 , 0.272	Depositor DCC
R_{free} test set	1857 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 37.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11081	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: ZN, LVY

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	0.56	3/8331 (0.0%)	0.62	2/11295 (0.0%)
2	C	0.62	5/2921 (0.2%)	0.63	0/3970
All	All	0.58	8/11252 (0.1%)	0.63	2/15265 (0.0%)

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	5
2	C	0	1
All	All	0	6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	240	TRP	CD2-CE2	6.97	1.49	1.41
2	C	243	TRP	CD2-CE2	5.61	1.48	1.41
2	C	415	TRP	CD2-CE2	5.58	1.48	1.41
2	C	264	TRP	CD2-CE2	5.33	1.47	1.41
1	A	1141	TRP	CD2-CE2	5.23	1.47	1.41
2	C	223	TRP	CD2-CE2	5.06	1.47	1.41
1	A	1073	TRP	CD2-CE2	5.01	1.47	1.41
1	A	656	PRO	N-CD	5.00	1.54	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	357	GLY	C-N-CD	-5.30	108.94	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	49	LEU	CA-CB-CG	5.12	127.08	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	GLU	Peptide
1	A	357	GLY	Peptide
1	A	482	GLU	Peptide
1	A	571	LEU	Peptide
1	A	940	GLY	Peptide
2	C	410	SER	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	8191	0	7989	197	0
2	C	2852	0	2808	75	0
3	C	1	0	0	0	0
4	C	19	0	13	0	0
5	A	13	0	0	0	0
5	C	5	0	0	0	0
All	All	11081	0	10810	261	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 12.

All (261) 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:927:MET:O	1:A:928:ARG:HB3	1.44	1.15
1:A:565:SER:OG	1:A:580:GLU:O	1.66	1.13
2:C:295:ARG:HG2	2:C:295:ARG:HH11	1.20	1.07
1:A:660:TYR:O	1:A:667:VAL:N	1.92	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:THR:HG23	1:A:315:THR:HG21	1.45	0.96
1:A:1055:GLN:HE22	1:A:1090:ASP:H	1.13	0.88
1:A:420:GLU:HG3	1:A:421:THR:HG22	1.55	0.88
1:A:24:THR:OG1	1:A:30:ASN:ND2	2.07	0.87
1:A:543:ILE:O	1:A:543:ILE:HG13	1.74	0.87
1:A:576:LEU:O	1:A:578:HIS:N	2.07	0.86
2:C:298:LEU:HA	2:C:301:ILE:HD12	1.61	0.81
2:C:295:ARG:HH11	2:C:295:ARG:CG	1.95	0.80
1:A:719:GLU:OE2	1:A:755:SER:HB3	1.82	0.79
1:A:928:ARG:HB2	1:A:952:ASN:O	1.81	0.79
1:A:866:VAL:HG11	1:A:884:ILE:HG12	1.64	0.79
2:C:57:HIS:HB3	2:C:60:LEU:HD12	1.65	0.78
1:A:1061:VAL:HG13	1:A:1104:LYS:HE3	1.66	0.76
1:A:24:THR:H	1:A:30:ASN:ND2	1.84	0.75
1:A:1032:THR:HG22	1:A:1036:MET:H	1.52	0.75
1:A:579:LYS:HD3	1:A:580:GLU:N	2.02	0.75
1:A:327:ARG:HH12	1:A:1034:ASN:ND2	1.84	0.74
1:A:257:THR:HB	1:A:276:MET:CE	2.18	0.73
2:C:367:ASN:HD22	2:C:392:LYS:NZ	1.85	0.73
1:A:206:PRO:HB2	1:A:207:TRP:CD1	2.24	0.73
1:A:1122:ARG:HG2	1:A:1122:ARG:HH21	1.53	0.73
1:A:545:PRO:HA	1:A:553:SER:HB2	1.71	0.73
1:A:579:LYS:HD3	1:A:580:GLU:CA	2.19	0.73
2:C:406:LYS:HB3	2:C:408:ASP:OD1	1.88	0.73
1:A:467:GLN:HE22	1:A:524:GLN:H	1.36	0.72
1:A:23:PHE:H	1:A:30:ASN:HD22	1.37	0.72
1:A:817:VAL:HG13	1:A:830:ILE:HB	1.72	0.71
1:A:1055:GLN:NE2	1:A:1090:ASP:H	1.86	0.71
1:A:866:VAL:CG1	1:A:884:ILE:HG21	2.21	0.70
1:A:1055:GLN:HE22	1:A:1090:ASP:N	1.90	0.69
2:C:394:CYS:SG	2:C:396:SER:HB3	2.32	0.69
2:C:295:ARG:HG2	2:C:295:ARG:NH1	1.98	0.68
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.76	0.68
2:C:168:LEU:HB2	2:C:181:LYS:HG2	1.76	0.67
1:A:928:ARG:CB	1:A:952:ASN:O	2.42	0.66
1:A:24:THR:H	1:A:30:ASN:HD21	1.38	0.66
1:A:672:ASN:O	1:A:672:ASN:ND2	2.28	0.66
1:A:24:THR:OG1	1:A:30:ASN:OD1	2.14	0.66
2:C:92:ILE:H	2:C:95:GLN:HE21	1.44	0.66
2:C:63:ASP:H	2:C:145:ARG:NH2	1.94	0.66
2:C:49:PHE:CE1	2:C:340:LEU:HD22	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:427:PRO:O	2:C:428:ASP:HB2	1.95	0.65
2:C:317:LYS:O	2:C:426:ILE:HB	1.97	0.65
1:A:37:THR:HG22	1:A:59:GLY:O	1.96	0.65
2:C:63:ASP:O	2:C:145:ARG:HG3	1.97	0.64
1:A:327:ARG:HE	2:C:199:LEU:HD12	1.62	0.64
2:C:172:THR:HG22	2:C:178:GLN:HG3	1.80	0.63
1:A:987:GLU:HG3	1:A:988:GLU:N	2.14	0.63
1:A:24:THR:OG1	1:A:30:ASN:CG	2.38	0.62
1:A:20:THR:HG23	1:A:315:THR:CG2	2.24	0.62
1:A:155:PHE:CZ	1:A:200:LYS:HG2	2.35	0.62
1:A:571:LEU:HB3	1:A:572:PRO:HD2	1.81	0.62
1:A:1032:THR:CG2	1:A:1036:MET:H	2.12	0.62
1:A:928:ARG:HD2	1:A:928:ARG:O	2.01	0.61
1:A:868:GLY:HA3	1:A:885:ASN:ND2	2.15	0.61
1:A:257:THR:HB	1:A:276:MET:HE2	1.83	0.60
2:C:69:GLY:HA2	2:C:118:ARG:NH2	2.17	0.60
2:C:112:ASN:O	2:C:115:GLN:O	2.20	0.60
1:A:912:LEU:HB2	1:A:925:ASP:HA	1.83	0.60
1:A:500:VAL:HG11	1:A:540:CYS:HA	1.84	0.60
1:A:118:THR:HG22	1:A:134:ARG:HH22	1.65	0.60
2:C:351:ASN:HB2	2:C:352:PRO:CD	2.32	0.59
1:A:10:GLN:O	1:A:1036:MET:HG2	2.03	0.59
1:A:257:THR:HB	1:A:276:MET:HE3	1.84	0.59
1:A:215:GLU:HG2	1:A:234:GLN:HG3	1.85	0.58
1:A:663:ASN:ND2	1:A:663:ASN:O	2.34	0.58
2:C:148:GLN:O	2:C:148:GLN:HG2	2.03	0.58
1:A:914:LEU:O	1:A:915:LYS:HD3	2.03	0.58
1:A:676:VAL:HG11	1:A:693:LEU:HD12	1.87	0.57
1:A:23:PHE:H	1:A:30:ASN:ND2	2.03	0.57
1:A:389:ILE:HG12	1:A:799:PHE:CZ	2.40	0.57
1:A:664:HIS:N	1:A:664:HIS:CD2	2.73	0.57
1:A:927:MET:O	1:A:928:ARG:CB	2.27	0.57
1:A:327:ARG:HG2	1:A:327:ARG:HH11	1.70	0.57
1:A:389:ILE:HD12	1:A:389:ILE:N	2.20	0.57
1:A:933:LEU:HD23	1:A:944:GLU:HA	1.86	0.57
1:A:881:LEU:HD21	1:A:921:ILE:HG12	1.87	0.57
1:A:1032:THR:HG21	1:A:1036:MET:HB3	1.86	0.57
1:A:1140:HIS:HD2	1:A:1141:TRP:O	1.86	0.56
2:C:240:TRP:HD1	2:C:241:PRO:HD3	1.70	0.56
1:A:913:TYR:CE1	2:C:240:TRP:CH2	2.94	0.56
1:A:118:THR:O	1:A:118:THR:CG2	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:367:ASN:HD22	2:C:392:LYS:HZ2	1.54	0.56
2:C:426:ILE:O	2:C:426:ILE:HG13	2.04	0.56
1:A:118:THR:CG2	1:A:134:ARG:HH22	2.20	0.55
2:C:165:PHE:HB2	2:C:182:VAL:HG13	1.86	0.55
1:A:571:LEU:HB3	1:A:572:PRO:CD	2.37	0.55
1:A:608:ASP:O	1:A:633:THR:HA	2.07	0.55
1:A:452:VAL:N	1:A:470:GLN:HE22	2.05	0.55
1:A:482:GLU:HG3	1:A:483:PRO:HD2	1.89	0.55
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.36	0.54
1:A:230:ILE:HD11	1:A:285:LEU:HD21	1.89	0.54
1:A:656:PRO:HG2	1:A:671:VAL:HB	1.90	0.54
1:A:520:GLN:HG3	1:A:529:ILE:HD12	1.89	0.54
2:C:69:GLY:HA2	2:C:118:ARG:HH22	1.73	0.54
1:A:63:VAL:HB	1:A:80:LEU:HB3	1.89	0.54
1:A:670:ASN:H	1:A:670:ASN:ND2	2.06	0.53
1:A:869:ALA:O	1:A:884:ILE:HA	2.07	0.53
1:A:1032:THR:HG22	1:A:1036:MET:N	2.21	0.53
1:A:119:GLY:O	1:A:134:ARG:NH1	2.42	0.53
1:A:1048:TYR:CE2	1:A:1052:LEU:HD12	2.44	0.53
1:A:913:TYR:CE1	2:C:240:TRP:CZ3	2.97	0.53
1:A:950:ASN:C	1:A:950:ASN:HD22	2.11	0.53
1:A:413:LEU:HB3	1:A:424:THR:HB	1.89	0.53
1:A:327:ARG:HG2	1:A:327:ARG:NH1	2.24	0.52
2:C:240:TRP:CD1	2:C:241:PRO:HD3	2.43	0.52
1:A:579:LYS:CG	1:A:580:GLU:N	2.73	0.52
1:A:579:LYS:CD	1:A:580:GLU:N	2.73	0.52
1:A:928:ARG:HB3	1:A:952:ASN:H	1.75	0.52
1:A:650:PHE:CD1	1:A:679:MET:HG2	2.45	0.52
1:A:232:ILE:HD13	1:A:237:ILE:HG12	1.90	0.52
1:A:661:SER:OG	1:A:663:ASN:OD1	2.21	0.52
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.45	0.51
1:A:786:VAL:HG22	1:A:787:GLU:N	2.25	0.51
1:A:1055:GLN:NE2	1:A:1090:ASP:N	2.53	0.51
1:A:971:ALA:HB3	1:A:1077:HIS:O	2.10	0.51
1:A:786:VAL:HG22	1:A:787:GLU:H	1.74	0.51
1:A:509:VAL:O	1:A:541:LEU:HD13	2.11	0.51
2:C:290:ILE:HD11	2:C:298:LEU:HD11	1.92	0.50
1:A:405:PRO:HA	1:A:697:SER:HA	1.93	0.50
1:A:118:THR:HG21	1:A:165:ILE:O	2.12	0.50
1:A:887:THR:HG21	1:A:889:ARG:HH21	1.76	0.50
2:C:101:LEU:CD1	2:C:110:VAL:HG21	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:427:PRO:O	2:C:428:ASP:CB	2.59	0.50
1:A:1056:ASN:N	1:A:1056:ASN:HD22	2.07	0.49
2:C:63:ASP:H	2:C:145:ARG:HH22	1.58	0.49
2:C:98:PRO:HG2	2:C:350:VAL:HG22	1.92	0.49
1:A:118:THR:O	1:A:118:THR:HG23	2.13	0.49
1:A:545:PRO:CA	1:A:553:SER:HB2	2.39	0.49
1:A:889:ARG:HD2	1:A:891:TYR:OH	2.12	0.49
1:A:573:SER:O	1:A:574:PHE:HB2	2.12	0.49
1:A:913:TYR:CZ	2:C:240:TRP:HZ3	2.30	0.49
1:A:1012:LEU:HD22	1:A:1141:TRP:CZ2	2.47	0.49
1:A:667:VAL:HG12	1:A:668:PHE:O	2.13	0.49
2:C:49:PHE:HE1	2:C:340:LEU:HD22	1.74	0.49
1:A:413:LEU:HD21	1:A:468:LEU:HD21	1.94	0.48
2:C:388:VAL:HG13	2:C:397:HIS:CD2	2.48	0.48
1:A:327:ARG:HH12	1:A:1034:ASN:HD22	1.60	0.48
2:C:77:SER:O	2:C:183:GLN:HA	2.12	0.48
2:C:291:ASP:OD1	2:C:293:VAL:CG1	2.62	0.48
1:A:216:ALA:HA	1:A:233:GLY:HA2	1.95	0.48
1:A:571:LEU:O	1:A:573:SER:N	2.44	0.48
1:A:1095:GLU:OE2	1:A:1140:HIS:HE1	1.97	0.48
1:A:652:CYS:HB3	1:A:676:VAL:O	2.14	0.48
1:A:360:VAL:HG21	1:A:722:ARG:NH1	2.29	0.48
1:A:913:TYR:CZ	2:C:240:TRP:CZ3	3.02	0.48
1:A:166:ASP:HB3	1:A:219:VAL:HG23	1.95	0.48
1:A:660:TYR:HB2	1:A:661:SER:CA	2.44	0.48
1:A:710:LEU:HD21	1:A:1141:TRP:CD2	2.48	0.47
2:C:369:ASN:ND2	2:C:392:LYS:HA	2.29	0.47
1:A:385:GLY:HA3	1:A:719:GLU:O	2.14	0.47
1:A:490:TRP:CG	1:A:519:LEU:HD21	2.49	0.47
1:A:762:SER:O	1:A:803:HIS:HA	2.13	0.47
1:A:554:PRO:HA	1:A:571:LEU:HB2	1.96	0.47
1:A:558:ILE:HG13	1:A:569:LEU:HD22	1.96	0.47
2:C:88:MET:O	2:C:89:MET:HB3	2.13	0.47
1:A:1051:LEU:HB2	1:A:1089:ILE:HD13	1.96	0.47
1:A:660:TYR:HB2	1:A:661:SER:CB	2.44	0.47
1:A:334:VAL:HB	1:A:347:VAL:HG22	1.96	0.47
1:A:579:LYS:HE2	1:A:581:MET:HB2	1.96	0.47
1:A:55:VAL:HG21	1:A:100:ILE:HD12	1.97	0.47
1:A:511:ALA:HA	1:A:516:LEU:HB3	1.96	0.47
1:A:913:TYR:CE1	2:C:240:TRP:HH2	2.33	0.47
1:A:928:ARG:HG3	1:A:950:ASN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LYS:HA	1:A:678:TYR:CE2	2.51	0.47
1:A:490:TRP:HB2	1:A:526:LEU:HD13	1.97	0.46
1:A:582:LEU:HD21	1:A:612:PHE:CE1	2.50	0.46
1:A:953:TRP:HB2	1:A:970:ASN:HB2	1.97	0.46
1:A:731:GLN:O	1:A:796:GLN:HB3	2.15	0.46
2:C:367:ASN:HD22	2:C:392:LYS:HZ1	1.61	0.46
1:A:552:LEU:O	1:A:554:PRO:HD3	2.15	0.46
1:A:684:SER:HB2	1:A:687:TYR:H	1.80	0.46
1:A:525:GLU:OE1	1:A:527:ARG:HB2	2.15	0.46
2:C:197:VAL:HG21	2:C:238:THR:HG22	1.98	0.46
1:A:387:LEU:HB2	1:A:715:VAL:HB	1.97	0.46
1:A:951:PRO:HB2	2:C:188:CYS:SG	2.56	0.45
1:A:1122:ARG:HH21	1:A:1122:ARG:CG	2.23	0.45
2:C:92:ILE:H	2:C:95:GLN:NE2	2.12	0.45
1:A:569:LEU:HG	1:A:574:PHE:O	2.16	0.45
2:C:359:THR:HG21	2:C:380:TRP:CZ3	2.51	0.45
1:A:516:LEU:HD22	1:A:541:LEU:HD21	1.99	0.45
1:A:670:ASN:ND2	1:A:670:ASN:N	2.63	0.45
2:C:61:GLY:HA3	2:C:145:ARG:HH12	1.81	0.45
2:C:75:ASP:OD1	2:C:186:PRO:HA	2.17	0.45
1:A:926:LEU:HD21	2:C:193:THR:HG21	1.99	0.45
1:A:19:VAL:HG12	1:A:32:LEU:HB2	1.98	0.44
2:C:359:THR:HG21	2:C:380:TRP:HZ3	1.81	0.44
1:A:275:ASP:HB2	1:A:279:ARG:HB2	1.98	0.44
1:A:543:ILE:O	1:A:543:ILE:CG1	2.56	0.44
1:A:579:LYS:HG2	1:A:580:GLU:H	1.81	0.44
1:A:241:ASN:O	1:A:242:GLY:C	2.55	0.44
1:A:336:LEU:HB3	1:A:347:VAL:HG23	1.99	0.44
1:A:605:ALA:HB1	1:A:636:THR:HB	1.98	0.44
2:C:113:LEU:HD21	2:C:120:PHE:HB3	2.00	0.44
2:C:291:ASP:OD1	2:C:293:VAL:HG13	2.17	0.44
1:A:275:ASP:OD1	1:A:276:MET:N	2.49	0.44
1:A:430:VAL:HA	1:A:456:GLN:HE21	1.83	0.44
2:C:91:LEU:HD11	2:C:161:GLY:CA	2.48	0.44
1:A:358:PRO:O	1:A:379:SER:HA	2.18	0.44
1:A:1140:HIS:CD2	1:A:1141:TRP:O	2.68	0.44
1:A:579:LYS:HG2	1:A:580:GLU:N	2.33	0.44
2:C:232:PHE:HZ	2:C:249:ASP:HB2	1.83	0.44
2:C:295:ARG:HA	2:C:298:LEU:CD1	2.48	0.44
1:A:147:ARG:CZ	1:A:147:ARG:HB3	2.49	0.43
2:C:394:CYS:O	2:C:395:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:193:THR:HG21	2:C:245:TYR:HD1	1.84	0.43
1:A:133:LEU:HB2	1:A:141:LYS:HB3	2.00	0.43
1:A:327:ARG:HH12	1:A:1034:ASN:HD21	1.59	0.43
1:A:565:SER:OG	1:A:579:LYS:HE3	2.19	0.43
1:A:58:TYR:HB3	1:A:1073:TRP:CG	2.54	0.43
1:A:218:MET:SD	1:A:261:HIS:HD2	2.42	0.43
1:A:358:PRO:HG3	2:C:237:LEU:HD13	1.99	0.43
1:A:967:GLY:HA3	1:A:975:PHE:CE1	2.54	0.43
1:A:134:ARG:HD2	1:A:134:ARG:C	2.40	0.42
1:A:660:TYR:HB2	1:A:661:SER:HA	2.01	0.42
1:A:650:PHE:CG	1:A:679:MET:HG2	2.54	0.42
1:A:273:LEU:HB2	1:A:281:PHE:HB2	2.00	0.42
1:A:663:ASN:ND2	1:A:663:ASN:C	2.72	0.42
2:C:338:PHE:CZ	2:C:340:LEU:HG	2.54	0.42
2:C:347:ALA:O	2:C:358:GLU:HA	2.20	0.42
1:A:935:TYR:O	1:A:937:PRO:HD3	2.19	0.42
1:A:522:HIS:O	1:A:523:PRO:C	2.58	0.42
1:A:565:SER:HB3	1:A:567:ARG:NH1	2.35	0.42
1:A:618:ILE:HD12	1:A:619:GLU:H	1.84	0.42
1:A:913:TYR:OH	2:C:240:TRP:HZ3	2.03	0.42
2:C:299:LEU:HD22	2:C:299:LEU:HA	1.82	0.42
1:A:194:GLU:HB3	1:A:203:ASN:HB2	2.02	0.42
2:C:345:PRO:O	2:C:360:LEU:HA	2.19	0.42
1:A:575:GLU:O	1:A:576:LEU:C	2.59	0.42
2:C:351:ASN:CB	2:C:352:PRO:CD	2.98	0.42
1:A:492:GLU:HG2	1:A:493:PRO:HD2	2.01	0.41
1:A:996:GLY:O	1:A:997:LEU:HD23	2.20	0.41
1:A:322:VAL:HB	1:A:334:VAL:HG23	2.01	0.41
1:A:835:MET:HB2	1:A:845:GLN:HG3	2.03	0.41
1:A:872:SER:HB3	1:A:914:LEU:HB2	2.02	0.41
2:C:89:MET:HE3	2:C:89:MET:HB2	1.89	0.41
1:A:69:PRO:HG2	1:A:72:GLU:HB2	2.02	0.41
2:C:351:ASN:HB2	2:C:352:PRO:HD3	2.01	0.41
2:C:102:PHE:CE1	2:C:154:ILE:HD12	2.55	0.41
2:C:193:THR:HG21	2:C:245:TYR:CD1	2.54	0.41
1:A:333:LEU:HB2	1:A:351:GLU:HB2	2.02	0.41
2:C:89:MET:CE	2:C:358:GLU:CD	2.89	0.41
1:A:508:VAL:HB	1:A:519:LEU:HB2	2.02	0.41
1:A:660:TYR:HB2	1:A:661:SER:HB3	2.02	0.41
1:A:723:LYS:O	1:A:735:VAL:HA	2.20	0.41
2:C:101:LEU:HD13	2:C:110:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:206:GLN:HA	2:C:206:GLN:OE1	2.20	0.41
1:A:38:ARG:HH21	1:A:54:GLU:CD	2.25	0.40
1:A:579:LYS:HD3	1:A:580:GLU:C	2.40	0.40
1:A:913:TYR:CE1	2:C:240:TRP:HZ3	2.39	0.40
1:A:455:GLN:NE2	1:A:474:ALA:HB2	2.36	0.40
1:A:471:ILE:HG12	1:A:476:VAL:HG13	2.02	0.40
1:A:660:TYR:O	1:A:667:VAL:CA	2.65	0.40
2:C:340:LEU:HD23	2:C:340:LEU:HA	1.83	0.40
1:A:218:MET:SD	1:A:261:HIS:CD2	3.15	0.40
1:A:1056:ASN:N	1:A:1056:ASN:ND2	2.69	0.40
1:A:1122:ARG:CG	1:A:1122:ARG:NH2	2.83	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	1026/1146 (90%)	956 (93%)	62 (6%)	8 (1%)	19 55
2	C	351/381 (92%)	324 (92%)	26 (7%)	1 (0%)	41 75
All	All	1377/1527 (90%)	1280 (93%)	88 (6%)	9 (1%)	22 59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	GLU
1	A	358	PRO
1	A	483	PRO
1	A	572	PRO
2	C	411	PRO
1	A	225	PRO
1	A	513	GLY

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Mol	Chain	Res	Type
1	A	653	SER
1	A	928	ARG

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	882/1005 (88%)	817 (93%)	65 (7%)	13 42
2	C	310/345 (90%)	266 (86%)	44 (14%)	3 15
All	All	1192/1350 (88%)	1083 (91%)	109 (9%)	9 33

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	24	THR
1	A	25	SER
1	A	97	SER
1	A	99	ASP
1	A	118	THR
1	A	134	ARG
1	A	168	LYS
1	A	197	LEU
1	A	208	LYS
1	A	234	GLN
1	A	243	ASP
1	A	265	ASP
1	A	336	LEU
1	A	342	GLU
1	A	346	TYR
1	A	348	VAL
1	A	360	VAL
1	A	397	HIS
1	A	410	LEU
1	A	413	LEU

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Mol	Chain	Res	Type
1	A	416	ASP
1	A	452	VAL
1	A	468	LEU
1	A	516	LEU
1	A	526	LEU
1	A	527	ARG
1	A	531	HIS
1	A	532	THR
1	A	533	GLU
1	A	544	THR
1	A	555	LEU
1	A	569	LEU
1	A	571	LEU
1	A	582	LEU
1	A	606	LEU
1	A	628	LYS
1	A	636	THR
1	A	647	THR
1	A	663	ASN
1	A	670	ASN
1	A	672	ASN
1	A	684	SER
1	A	707	ILE
1	A	713	ARG
1	A	722	ARG
1	A	761	LEU
1	A	796	GLN
1	A	864	LYS
1	A	874	VAL
1	A	898	GLU
1	A	944	GLU
1	A	950	ASN
1	A	957	VAL
1	A	1032	THR
1	A	1052	LEU
1	A	1063	LYS
1	A	1064	SER
1	A	1071	SER
1	A	1075	SER
1	A	1115	ASP
1	A	1116	ASP
1	A	1122	ARG

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Mol	Chain	Res	Type
1	A	1131	LYS
1	A	1142	SER
2	C	49	PHE
2	C	60	LEU
2	C	70	ARG
2	C	71	THR
2	C	89	MET
2	C	91	LEU
2	C	96	THR
2	C	113	LEU
2	C	115	GLN
2	C	144	TYR
2	C	145	ARG
2	C	149	ASP
2	C	170	LEU
2	C	171	ARG
2	C	181	LYS
2	C	182	VAL
2	C	188	CYS
2	C	193	THR
2	C	197	VAL
2	C	199	LEU
2	C	213	VAL
2	C	220	SER
2	C	221	TYR
2	C	237	LEU
2	C	240	TRP
2	C	251	GLU
2	C	260	GLN
2	C	263	GLU
2	C	273	LEU
2	C	283	ARG
2	C	284	VAL
2	C	295	ARG
2	C	298	LEU
2	C	299	LEU
2	C	310	CYS
2	C	340	LEU
2	C	350	VAL
2	C	359	THR
2	C	396	SER
2	C	405	THR

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Mol	Chain	Res	Type
2	C	410	SER
2	C	413	LYS
2	C	423	LEU
2	C	426	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	156	ASN
1	A	183	GLN
1	A	261	HIS
1	A	262	ASN
1	A	374	GLN
1	A	399	HIS
1	A	456	GLN
1	A	467	GLN
1	A	470	GLN
1	A	664	HIS
1	A	670	ASN
1	A	672	ASN
1	A	677	ASN
1	A	950	ASN
1	A	1034	ASN
1	A	1055	GLN
1	A	1056	ASN
1	A	1140	HIS
2	C	95	GLN
2	C	115	GLN
2	C	203	ASN
2	C	225	GLN
2	C	335	ASN
2	C	367	ASN
2	C	369	ASN

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)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	LVY	C	502	-	21,21,21	1.73	5 (23%)	28,31,31	2.70	10 (35%)

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	LVY	C	502	-	-	0/4/29/29	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	LVY	C7-C11	-5.53	1.39	1.48
4	C	502	LVY	C11-N10	-2.68	1.33	1.36
4	C	502	LVY	C14-C8	-2.43	1.39	1.40
4	C	502	LVY	C6-N5	2.10	1.40	1.37
4	C	502	LVY	C4-N5	2.06	1.41	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	502	LVY	C7-C11-N10	8.85	111.66	106.44
4	C	502	LVY	C9-N10-C11	-5.67	110.79	113.12
4	C	502	LVY	C2-C1-N10	-4.41	109.35	114.11
4	C	502	LVY	C4-N5-C6	-3.90	121.18	126.61
4	C	502	LVY	C3-C4-N5	3.58	120.67	116.65
4	C	502	LVY	C1-C6-N5	3.19	120.53	116.25
4	C	502	LVY	C8-C9-N10	-2.44	101.01	101.79
4	C	502	LVY	O16-C11-C7	-2.34	124.12	128.68
4	C	502	LVY	C2-C3-C4	-2.05	110.50	114.12
4	C	502	LVY	C15-C7-C11	2.04	132.96	129.63

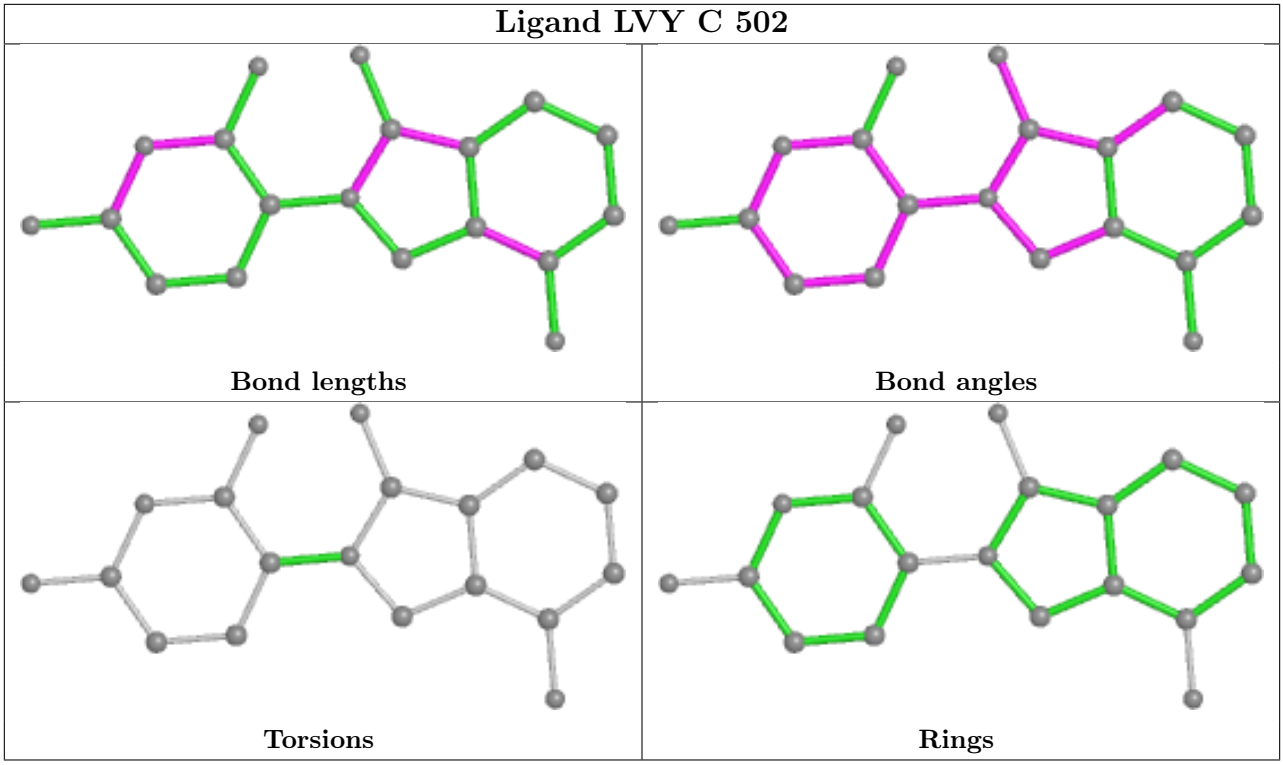
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.



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	1070/1146 (93%)	-0.39	4 (0%) 92 78	21, 44, 108, 136	5 (0%)
2	C	361/381 (94%)	-0.33	0 100 100	30, 50, 78, 100	0
All	All	1431/1527 (93%)	-0.37	4 (0%) 94 83	21, 46, 102, 136	5 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	594	THR	2.3
1	A	654	ASP	2.3
1	A	633	THR	2.1
1	A	16	ASN	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
4	LVY	C	502	19/19	0.97	0.19	35,37,39,39	0

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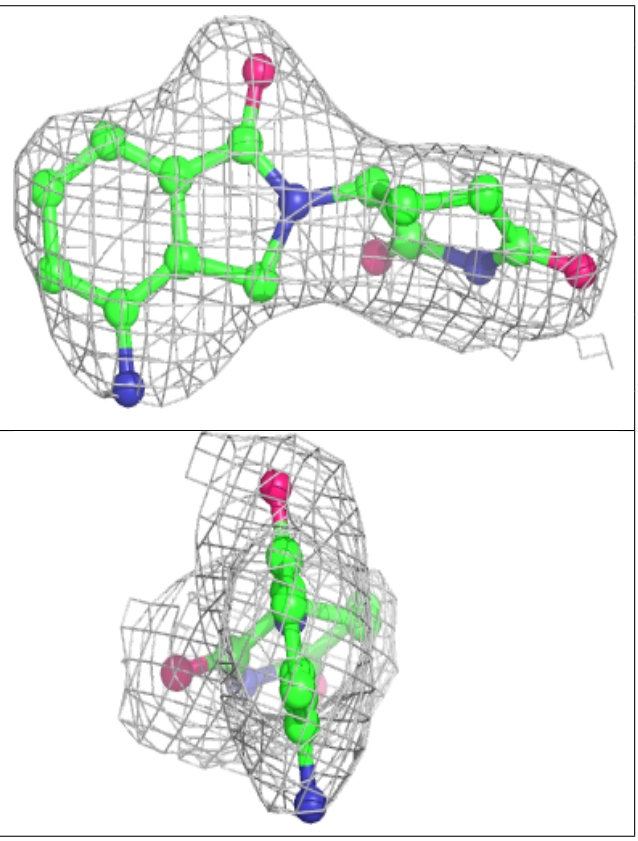
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	C	501	1/1	0.99	0.09	45,45,45,45	0

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 LVY C 502:

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.