



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:47 PM UTC

PDB ID : 4TZ4 / pdb_00004tz4
Title : Crystal Structure of Human Cereblon in Complex with DDB1 and Lenalido-
mide
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

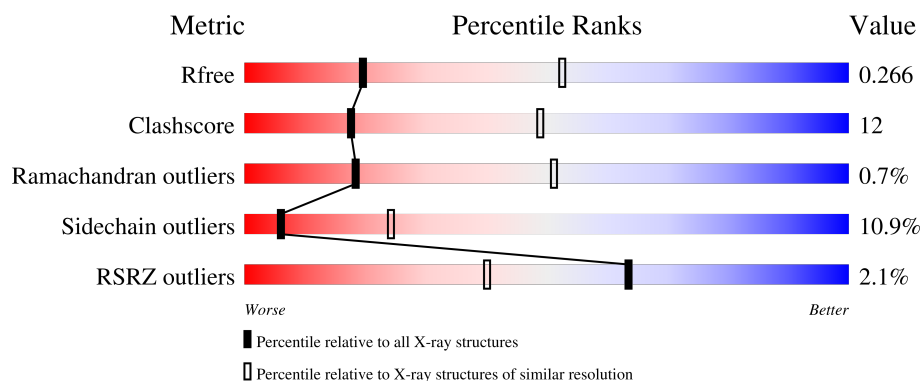
1 Overall quality at a glance

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}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (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 $\leq 5\%$. 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	 2% 68% 22% 7%
2	C	381	 % 66% 23% 6% 5%

2 Entry composition

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
1	A	1070	Total	C	N	O	S	0	0	0
			8191	5227	1367	1552	45			

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

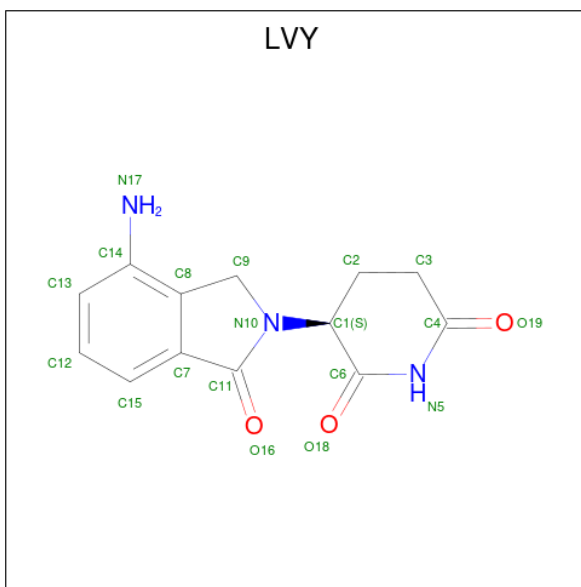
- Molecule 2 is a protein called Protein cereblon.

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is S-Lenalidomide (CCD ID: LVY) (formula: C₁₃H₁₃N₃O₃).



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

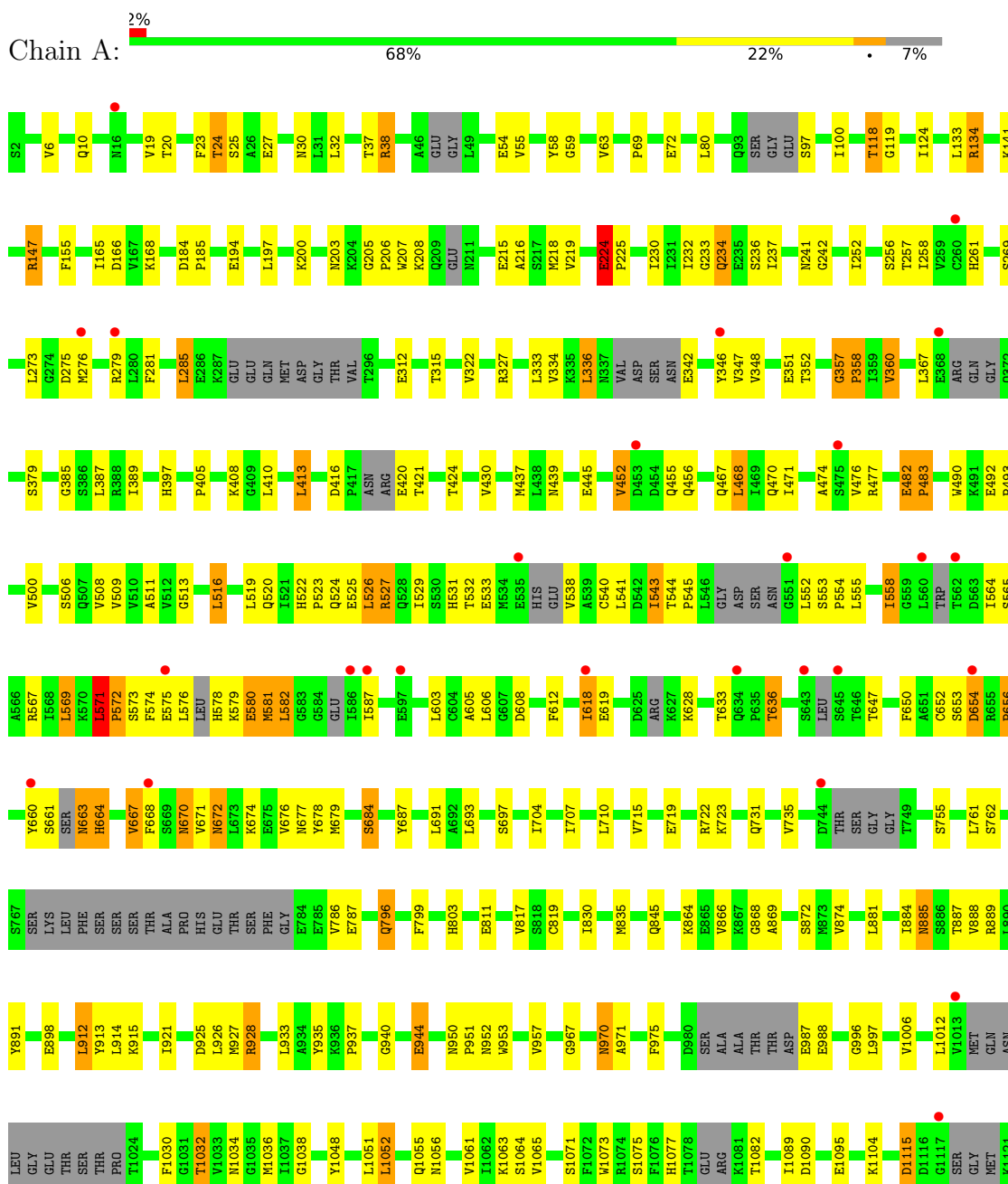
- Molecule 5 is water.

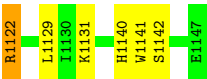
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	C	5	Total	O	0	0
			5	5		

3 Residue-property plots

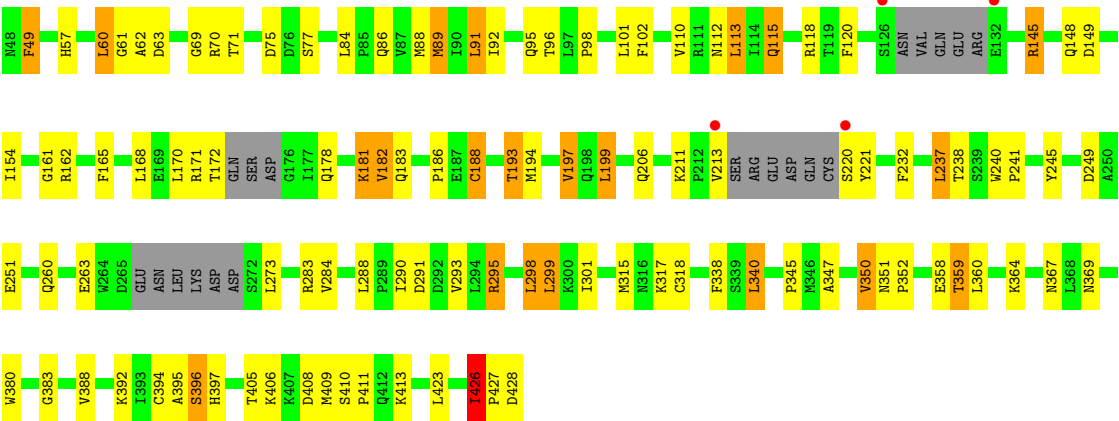
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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





● Molecule 2: Protein cereblon



4 Data and refinement statistics

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 50.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-3.01) 99.4 (50.00-3.01)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.202 , 0.271 (Not available) , 0.266	Depositor DCC
R_{free} test set	1857 reflections (4.96%)	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)	0.29 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.78	4/8331 (0.0%)	0.90	17/11295 (0.2%)
2	C	0.80	0/2921	0.90	6/3970 (0.2%)
All	All	0.79	4/11252 (0.0%)	0.90	23/15265 (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	5
2	C	0	1
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	885	ASN	C-O	-6.34	1.18	1.24
1	A	888	VAL	C-O	-6.24	1.17	1.24
1	A	38	ARG	C-O	-5.29	1.17	1.23
1	A	656	PRO	N-CD	5.08	1.54	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLU	CA-C-N	-9.10	108.47	119.84
1	A	224	GLU	C-N-CA	-9.10	108.47	119.84
1	A	357	GLY	CA-C-N	7.94	129.76	119.84
1	A	357	GLY	C-N-CA	7.94	129.76	119.84
2	C	62	ALA	N-CA-C	7.71	119.32	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	674	LYS	N-CA-C	-7.56	100.78	110.53
1	A	1115	ASP	N-CA-C	6.89	120.08	108.02
1	A	27	GLU	N-CA-C	6.43	118.37	111.36
1	A	667	VAL	N-CA-C	6.10	116.90	108.12
1	A	677	ASN	N-CA-C	5.92	117.81	111.36
1	A	819	CYS	N-CA-C	5.88	117.08	108.14
1	A	654	ASP	N-CA-C	-5.64	105.13	111.28
1	A	1065	VAL	N-CA-C	5.60	116.06	110.23
2	C	318	CYS	N-CA-C	5.55	116.37	108.54
1	A	970	ASN	N-CA-C	5.51	118.02	110.24
1	A	312	GLU	N-CA-C	-5.42	106.34	113.12
2	C	84	LEU	CA-C-N	5.38	125.31	119.76
2	C	84	LEU	C-N-CA	5.38	125.31	119.76
1	A	256	SER	N-CA-C	5.24	114.95	108.19
2	C	426	ILE	CA-C-N	5.17	125.89	120.11
2	C	426	ILE	C-N-CA	5.17	125.89	120.11
1	A	205	GLY	CA-C-N	5.04	124.83	119.28
1	A	205	GLY	C-N-CA	5.04	124.83	119.28

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 ⓘ

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	202	0
2	C	2852	0	2808	80	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	271	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 (271) 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
1:A:20:THR:HG23	1:A:315:THR:HG21	1.45	0.96
1:A:257:THR:HB	1:A:276:MET:HE3	1.49	0.94
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:257:THR:HB	1:A:276:MET:CE	2.18	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
1:A:24:THR:OG1	1:A:30:ASN:CG	2.38	0.67
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
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:383:GLY:HA3	2:C:409:MET:HE1	1.79	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:LEU:O	1:A:915:LYS:HD3	2.03	0.58
1:A:950:ASN:C	1:A:950:ASN:HD22	2.11	0.57
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
2:C:367:ASN:HD22	2:C:392:LYS:HZ2	1.54	0.56
2:C:194:MET:HE2	2:C:194:MET:HA	1.87	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:437:MET:HE2	1:A:439:ASN:ND2	2.21	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:811:GLU:HB2	1:A:835:MET:HE1	1.88	0.54
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:89:MET:HE1	2:C:358:GLU:CD	2.38	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:241:ASN:O	1:A:242:GLY:C	2.55	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:437:MET:HE2	1:A:439:ASN:HD21	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:663:ASN:ND2	1:A:663:ASN:C	2.72	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
1:A:408:LYS:HA	1:A:678:TYR:CE2	2.51	0.47
1:A:134:ARG:HD2	1:A:134:ARG:C	2.40	0.46
1:A:490:TRP:HB2	1:A:526:LEU:HD13	1.97	0.46
1:A:579:LYS:HD3	1:A:580:GLU:C	2.40	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:575:GLU:O	1:A:576:LEU:C	2.59	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
2:C:89:MET:CE	2:C:358:GLU:CD	2.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:359:THR:HG21	2:C:380:TRP:CZ3	2.51	0.45
1:A:38:ARG:HH21	1:A:54:GLU:CD	2.25	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
1:A:522:HIS:O	1:A:523:PRO:C	2.58	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: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:608:ASP:OD1	1:A:608:ASP:C	2.61	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
2:C:49:PHE:CD1	2:C:49:PHE:C	2.96	0.43
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
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:660:TYR:HB2	1:A:661:SER:HA	2.01	0.42
2:C:89:MET:HB2	2:C:89:MET:HE3	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:C:351:ASN:CB	2:C:352:PRO:CD	2.98	0.42
1:A:218:MET:HE1	1:A:258:ILE:HG22	2.02	0.41
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
1:A:950:ASN:C	1:A:950:ASN:ND2	2.78	0.41
1:A:69:PRO:HG2	1:A:72:GLU:HB2	2.02	0.41
2:C:288:LEU:HD21	2:C:315:MET:HE2	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
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
2:C:206:GLN:HA	2:C:206:GLN:OE1	2.20	0.41
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%)	16	48
2	C	351/381 (92%)	324 (92%)	26 (7%)	1 (0%)	36	68
All	All	1377/1527 (90%)	1280 (93%)	88 (6%)	9 (1%)	18	51

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
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%)	796 (90%)	86 (10%)	7	29
2	C	310/345 (90%)	266 (86%)	44 (14%)	3	15
All	All	1192/1350 (88%)	1062 (89%)	130 (11%)	6	24

All (130) 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	118	THR
1	A	124	ILE
1	A	134	ARG
1	A	147	ARG
1	A	168	LYS
1	A	197	LEU
1	A	208	LYS
1	A	234	GLN
1	A	236	SER
1	A	252	ILE
1	A	269	SER
1	A	285	LEU
1	A	336	LEU
1	A	342	GLU
1	A	346	TYR
1	A	348	VAL
1	A	352	THR
1	A	360	VAL
1	A	367	LEU
1	A	397	HIS
1	A	410	LEU
1	A	413	LEU
1	A	416	ASP
1	A	445	GLU
1	A	452	VAL
1	A	468	LEU
1	A	477	ARG
1	A	506	SER
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	538	VAL
1	A	543	ILE
1	A	544	THR
1	A	555	LEU

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Mol	Chain	Res	Type
1	A	558	ILE
1	A	564	ILE
1	A	569	LEU
1	A	571	LEU
1	A	580	GLU
1	A	581	MET
1	A	582	LEU
1	A	587	ILE
1	A	603	LEU
1	A	606	LEU
1	A	618	ILE
1	A	628	LYS
1	A	636	THR
1	A	647	THR
1	A	654	ASP
1	A	663	ASN
1	A	664	HIS
1	A	670	ASN
1	A	672	ASN
1	A	684	SER
1	A	691	LEU
1	A	704	ILE
1	A	707	ILE
1	A	761	LEU
1	A	796	GLN
1	A	864	LYS
1	A	874	VAL
1	A	898	GLU
1	A	912	LEU
1	A	944	GLU
1	A	957	VAL
1	A	1006	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	1082	THR
1	A	1115	ASP
1	A	1122	ARG
1	A	1129	LEU

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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	86	GLN
2	C	89	MET
2	C	91	LEU
2	C	96	THR
2	C	113	LEU
2	C	115	GLN
2	C	145	ARG
2	C	149	ASP
2	C	162	ARG
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	211	LYS
2	C	213	VAL
2	C	220	SER
2	C	221	TYR
2	C	237	LEU
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	340	LEU
2	C	350	VAL
2	C	359	THR
2	C	364	LYS
2	C	396	SER

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Mol	Chain	Res	Type
2	C	405	THR
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 (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	30	ASN
1	A	93	GLN
1	A	156	ASN
1	A	183	GLN
1	A	203	ASN
1	A	240	HIS
1	A	261	HIS
1	A	262	ASN
1	A	374	GLN
1	A	439	ASN
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	731	GLN
1	A	759	GLN
1	A	790	ASN
1	A	950	ASN
1	A	1034	ASN
1	A	1055	GLN
1	A	1056	ASN
1	A	1140	HIS
2	C	79	GLN
2	C	95	GLN
2	C	115	GLN
2	C	134	GLN
2	C	203	ASN
2	C	228	GLN
2	C	233	HIS
2	C	260	GLN

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Mol	Chain	Res	Type
2	C	306	GLN
2	C	335	ASN
2	C	367	ASN
2	C	369	ASN
2	C	397	HIS

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 oligosaccharides 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	1.76	5 (23%)	29,31,31	2.59	9 (31%)

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	-5.59	1.39	1.48
4	C	502	LVY	C11-N10	-2.71	1.33	1.36
4	C	502	LVY	C14-C8	-2.55	1.39	1.40
4	C	502	LVY	C4-N5	2.11	1.41	1.37
4	C	502	LVY	C6-N5	2.05	1.40	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	502	LVY	C7-C11-N10	8.25	111.66	106.42
4	C	502	LVY	C9-N10-C11	-5.60	110.79	113.15
4	C	502	LVY	C2-C1-N10	-4.28	109.35	114.03
4	C	502	LVY	C4-N5-C6	-4.18	121.18	126.69
4	C	502	LVY	C3-C4-N5	3.75	120.67	116.69
4	C	502	LVY	C1-C6-N5	2.94	120.53	116.24
4	C	502	LVY	C8-C9-N10	-2.57	101.01	101.79
4	C	502	LVY	O16-C11-C7	-2.34	124.12	128.66
4	C	502	LVY	C15-C7-C11	2.01	132.96	129.59

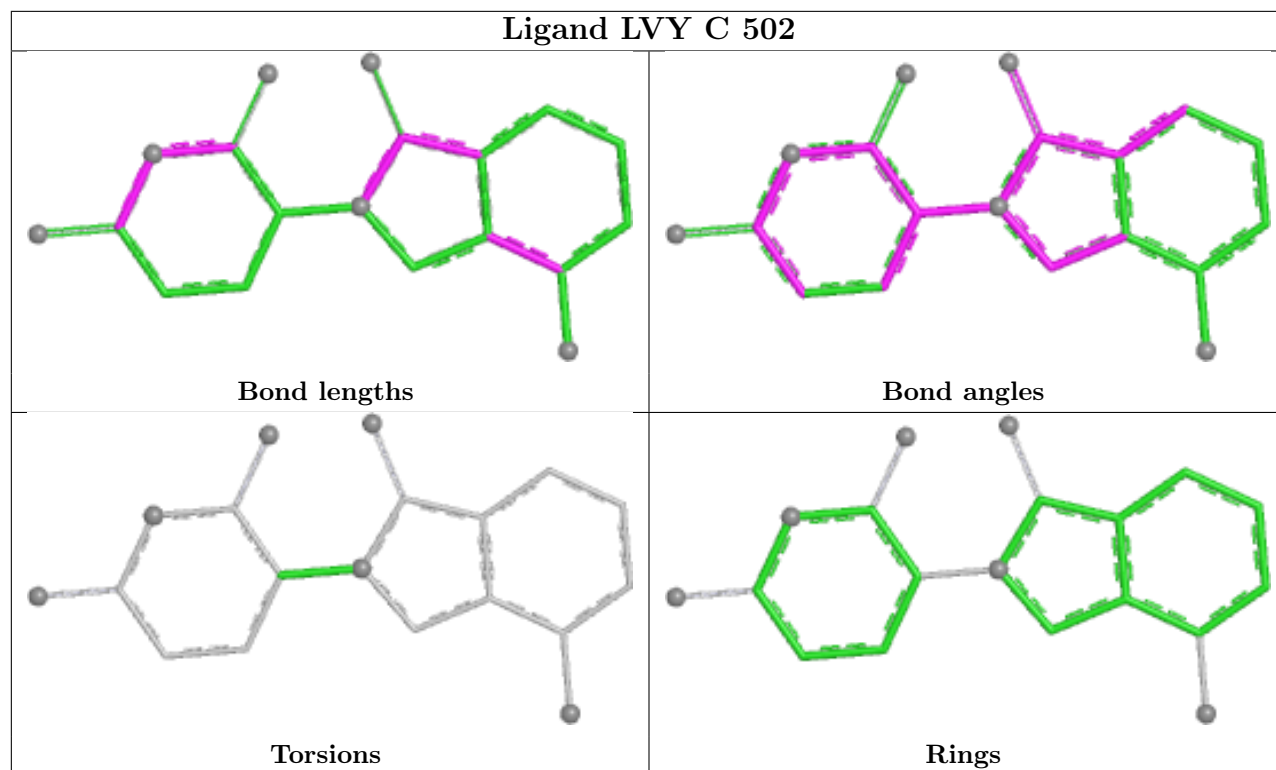
There are no chirality outliers.

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 than 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

6.1 Protein, DNA and RNA chains

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%)	-0.17	26 (2%) 59 36	11, 44, 108, 136	5 (0%)
2	C	361/381 (94%)	-0.22	4 (1%) 78 57	30, 50, 78, 100	0
All	All	1431/1527 (93%)	-0.18	30 (2%) 63 40	11, 46, 102, 136	5 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	ASN	6.0
1	A	260	CYS	5.2
1	A	279	ARG	5.2
1	A	475	SER	4.9
1	A	643	SER	3.9
1	A	645	SER	3.7
1	A	668	PHE	3.7
2	C	220	SER	3.6
1	A	368	GLU	3.5
1	A	453	ASP	3.3
1	A	535	GLU	3.1
1	A	1117	GLY	2.9
1	A	597	GLU	2.9
1	A	562	THR	2.8
1	A	560	LEU	2.6
2	C	132	GLU	2.6
1	A	744	ASP	2.5
1	A	276	MET	2.4
1	A	1013	VAL	2.4
1	A	634	GLN	2.3
1	A	575	GLU	2.3
1	A	618	ILE	2.2
1	A	660	TYR	2.1
1	A	586	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	126	SER	2.1
2	C	213	VAL	2.1
1	A	346	TYR	2.1
1	A	551	GLY	2.0
1	A	654	ASP	2.0
1	A	587	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

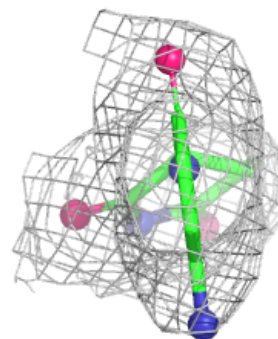
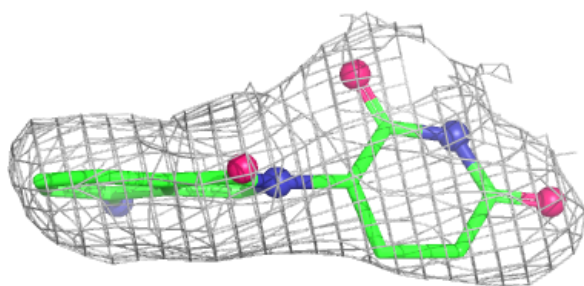
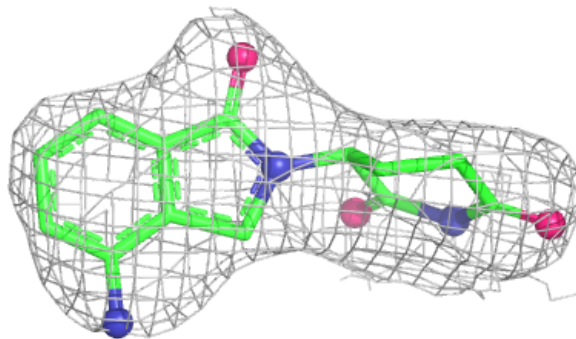
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.95	0.07	35,37,39,39	0
3	ZN	C	501	1/1	1.00	0.01	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.