



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:13 PM UTC

PDB ID : 5OT4 / pdb_00005ot4
Title : Structure of the Legionella pneumophila effector RidL (1-866)
Authors : Romano-Moreno, M.; Rojas, A.L.; Lucas, M.; Isupov, M.N.; Hierro, A.
Deposited on : 2017-08-20
Resolution : 3.00 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
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

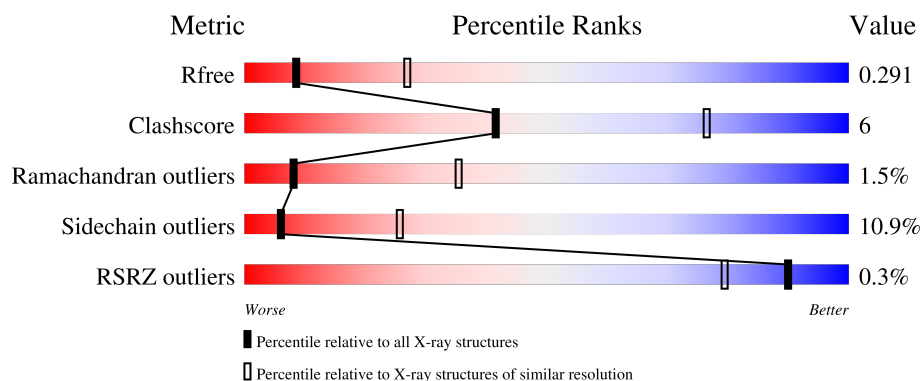
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

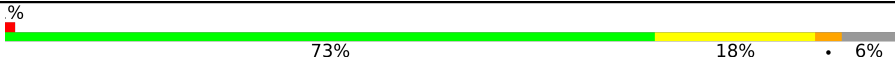
The reported resolution of this entry is 3.00 Å.

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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	901	
1	B	901	
1	C	901	
1	D	901	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26232 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 Interaptin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	846	Total	C	N	O	S	0	0	0
			6687	4198	1164	1312	13			
1	B	842	Total	C	N	O	S	0	0	0
			6673	4191	1162	1306	14			
1	C	787	Total	C	N	O	S	0	0	0
			6238	3915	1084	1225	14			
1	D	836	Total	C	N	O	S	0	0	0
			6628	4158	1151	1305	14			

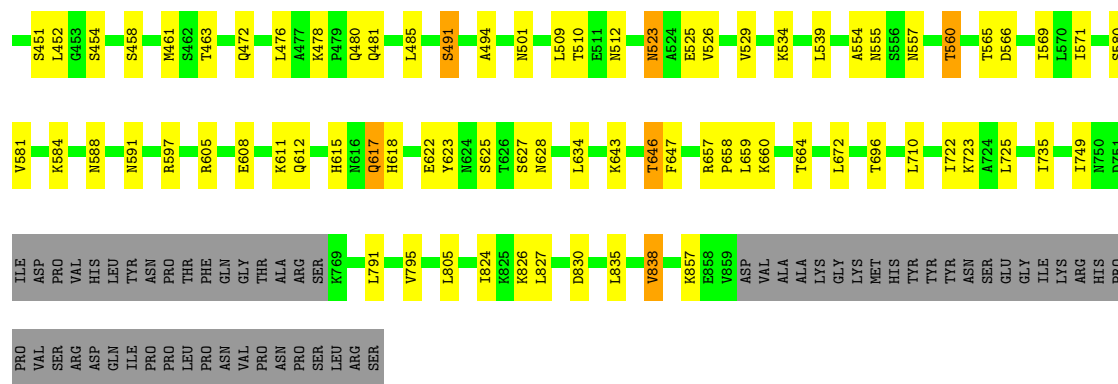
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP G8UZ99
B	0	SER	-	expression tag	UNP G8UZ99
C	0	SER	-	expression tag	UNP G8UZ99
D	0	SER	-	expression tag	UNP G8UZ99

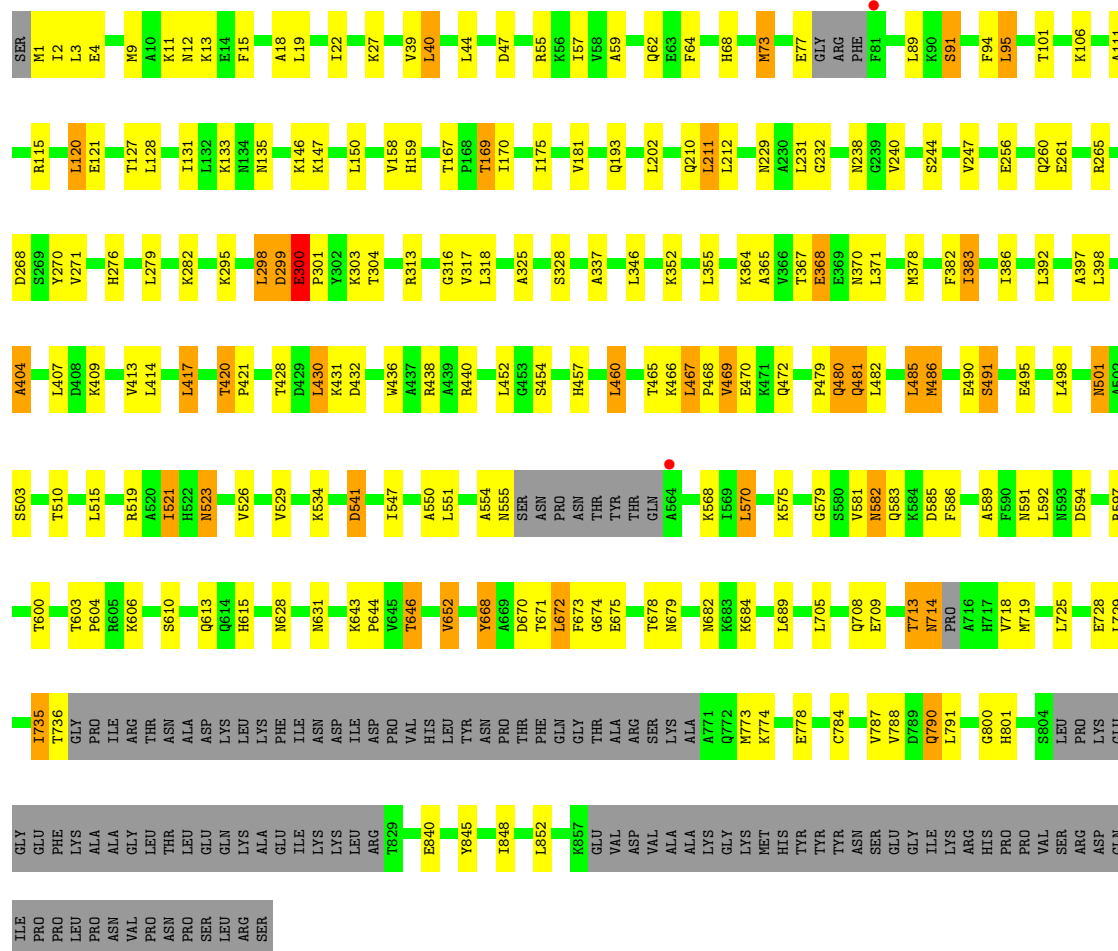
- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		



• Molecule 1: Interaptin



• Molecule 1: Interaptin





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	242.65Å 230.91Å 86.73Å 90.00° 90.40° 90.00°	Depositor
Resolution (Å)	167.27 – 3.00 167.27 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (167.27-3.00) 99.7 (167.27-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.229 , 0.295 0.230 , 0.291	Depositor DCC
R_{free} test set	4953 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	98.4	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26232	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9839e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL

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	0.74	0/6793	1.01	8/9163 (0.1%)
1	B	0.77	1/6777 (0.0%)	1.03	7/9130 (0.1%)
1	C	0.87	1/6330 (0.0%)	1.07	12/8523 (0.1%)
1	D	0.78	1/6729 (0.0%)	1.02	5/9067 (0.1%)
All	All	0.79	3/26629 (0.0%)	1.03	32/35883 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	355	LEU	CA-C	6.25	1.55	1.52
1	D	364	LYS	CA-C	6.12	1.58	1.53
1	C	170	ILE	CA-CB	5.85	1.57	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	SER	N-CA-C	6.76	120.40	110.59
1	B	104	PHE	N-CA-C	6.58	118.45	111.28
1	B	366	VAL	N-CA-C	6.14	118.48	109.63
1	B	82	GLY	N-CA-C	6.11	119.22	111.09
1	D	386	ILE	N-CA-CB	6.10	117.17	110.53
1	A	579	GLY	N-CA-C	6.09	120.91	113.79
1	C	352	LYS	CA-C-N	6.02	126.19	119.32
1	C	352	LYS	C-N-CA	6.02	126.19	119.32
1	B	581	VAL	N-CA-C	5.86	118.61	108.95
1	A	366	VAL	N-CA-C	5.84	116.99	108.58
1	C	3	LEU	N-CA-C	5.71	119.07	111.30
1	C	713	THR	N-CA-C	5.66	119.77	112.86
1	B	248	VAL	N-CA-CB	5.54	117.04	110.55
1	A	645	VAL	N-CA-CB	-5.48	106.31	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	THR	CA-C-N	5.39	124.64	120.33
1	C	169	THR	C-N-CA	5.39	124.64	120.33
1	C	300	GLU	CA-C-N	-5.37	113.20	119.32
1	C	300	GLU	C-N-CA	-5.37	113.20	119.32
1	D	22	ILE	CB-CA-C	-5.33	105.06	111.88
1	C	300	GLU	N-CA-C	5.32	121.57	109.81
1	D	22	ILE	N-CA-CB	5.31	116.41	110.51
1	A	807	LYS	N-CA-C	5.25	117.69	107.71
1	A	803	LYS	N-CA-C	-5.23	105.50	111.14
1	B	672	LEU	N-CA-C	5.21	116.64	111.07
1	C	652	VAL	N-CA-C	-5.20	106.06	111.58
1	A	467	LEU	CA-C-N	-5.20	114.88	120.03
1	A	467	LEU	C-N-CA	-5.20	114.88	120.03
1	A	325	ALA	N-CA-C	5.19	116.62	111.07
1	D	422	ALA	N-CA-C	5.16	121.78	110.80
1	D	67	GLU	N-CA-C	5.06	116.80	111.28
1	C	787	VAL	N-CA-C	5.05	116.38	110.62
1	B	332	GLN	N-CA-C	5.03	116.59	110.41

There are no chirality outliers.

There are no planarity outliers.

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	6687	0	6729	74	0
1	B	6673	0	6726	80	0
1	C	6238	0	6270	97	0
1	D	6628	0	6666	83	0
2	B	6	0	8	0	0
All	All	26232	0	26399	334	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 6.

All (334) 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:D:229:ASN:HD21	1:D:238:ASN:HD22	1.19	0.88
1:C:365:ALA:HA	1:C:370:ASN:HD22	1.48	0.79
1:A:337:ALA:HB3	1:A:378:MET:HE1	1.64	0.78
1:C:212:LEU:HD23	1:C:231:LEU:HD11	1.65	0.78
1:C:229:ASN:HD21	1:C:238:ASN:HD21	1.33	0.76
1:B:116:VAL:HG21	1:B:190:ILE:HD13	1.70	0.73
1:A:750:ASN:HD21	1:A:848:ILE:HD12	1.51	0.73
1:A:747:LYS:HB2	1:A:844:PHE:CZ	2.24	0.72
1:A:95:LEU:HD21	1:A:104:PHE:CE1	2.25	0.72
1:A:95:LEU:HD21	1:A:104:PHE:HE1	1.54	0.72
1:A:337:ALA:CB	1:A:378:MET:HE1	2.21	0.70
1:C:295:LYS:C	1:C:298:LEU:HD11	2.17	0.69
1:A:351:LYS:HG3	1:A:362:ILE:HD11	1.74	0.69
1:A:747:LYS:HD2	1:A:848:ILE:HD11	1.74	0.69
1:A:691:ARG:NH2	1:A:692:GLU:OE2	2.26	0.69
1:B:407:LEU:HD21	1:B:425:VAL:HG23	1.74	0.68
1:C:337:ALA:HB3	1:C:378:MET:HE1	1.75	0.66
1:D:619:ILE:HD11	1:D:639:LEU:HB3	1.77	0.66
1:C:11:LYS:O	1:C:13:LYS:N	2.29	0.66
1:C:365:ALA:HA	1:C:370:ASN:ND2	2.11	0.65
1:C:298:LEU:N	1:C:298:LEU:HD12	2.11	0.65
1:A:366:VAL:H	1:A:370:ASN:HD22	1.43	0.65
1:D:388:ASP:HB3	1:D:393:LYS:HG3	1.81	0.62
1:B:187:ILE:HA	1:B:190:ILE:HG12	1.82	0.62
1:B:420:THR:HG23	1:B:421:PRO:HD3	1.82	0.62
1:C:383:ILE:HD11	1:C:436:TRP:HB2	1.82	0.61
1:C:615:HIS:HA	1:C:646:THR:HG23	1.81	0.61
1:D:120:LEU:HD21	1:D:131:ILE:CD1	2.30	0.61
1:B:282:LYS:O	1:B:286:LEU:HD12	2.00	0.61
1:B:327:LEU:HD23	1:B:378:MET:CG	2.30	0.61
1:C:404:ALA:HB1	1:C:409:LYS:HB3	1.81	0.61
1:A:46:THR:HG21	1:A:54:PHE:HA	1.83	0.60
1:C:295:LYS:HA	1:C:298:LEU:HD11	1.82	0.60
1:C:268:ASP:OD1	1:C:313:ARG:NH2	2.35	0.60
1:D:15:PHE:CE1	1:D:72:LEU:HD23	2.35	0.60
1:D:537:ILE:HD11	1:D:578:SER:O	2.02	0.60
1:A:679:ASN:HB3	1:A:682:ASN:HD22	1.66	0.60
1:B:722:ILE:HG23	1:B:827:LEU:HD22	1.83	0.59
1:A:55:ARG:HD2	1:A:58:VAL:HG13	1.83	0.59
1:B:215:LEU:HD12	1:B:251:LEU:HD13	1.84	0.59
1:D:208:ASN:C	1:D:208:ASN:HD22	2.10	0.59
1:D:772:GLN:NE2	1:D:773:MET:HE2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:GLN:HE21	1:A:772:GLN:C	2.12	0.57
1:D:401:LEU:HD23	1:D:413:VAL:HG23	1.86	0.57
1:A:747:LYS:HB2	1:A:844:PHE:HZ	1.66	0.57
1:B:120:LEU:HD21	1:B:131:ILE:CD1	2.34	0.57
1:D:195:ARG:NE	1:D:196:ASP:OD2	2.37	0.57
1:A:790:GLN:HE21	1:A:794:GLN:HE21	1.51	0.57
1:D:575:LYS:HB3	1:D:586:PHE:CE2	2.40	0.57
1:B:279:LEU:HD21	1:B:322:TYR:HA	1.87	0.57
1:A:267:PHE:CE2	1:A:314:ALA:HB1	2.40	0.56
1:C:397:ALA:HB1	1:C:417:LEU:HD21	1.87	0.56
1:D:719:MET:HE3	1:D:820:GLN:HG3	1.88	0.56
1:D:615:HIS:HA	1:D:646:THR:HG22	1.87	0.56
1:B:478:LYS:HB2	1:B:481:GLN:HE21	1.70	0.56
1:C:271:VAL:HG11	1:C:317:VAL:HG12	1.87	0.56
1:C:298:LEU:HD12	1:C:298:LEU:H	1.71	0.56
1:C:270:TYR:OH	1:C:299:ASP:HB2	2.06	0.55
1:C:300:GLU:O	1:C:301:PRO:C	2.45	0.55
1:B:722:ILE:HD13	1:B:824:ILE:HG12	1.88	0.55
1:C:554:ALA:HB2	1:C:570:LEU:HD21	1.87	0.55
1:A:747:LYS:CD	1:A:848:ILE:HD11	2.35	0.55
1:D:401:LEU:HD23	1:D:413:VAL:CG2	2.37	0.55
1:C:211:LEU:HD12	1:C:211:LEU:C	2.31	0.55
1:D:44:LEU:HB3	1:D:158:VAL:HG13	1.87	0.55
1:B:337:ALA:CB	1:B:378:MET:HE1	2.37	0.55
1:D:129:VAL:O	1:D:133:LYS:HB2	2.06	0.55
1:D:554:ALA:HB2	1:D:570:LEU:HD11	1.89	0.55
1:B:523:ASN:C	1:B:523:ASN:OD1	2.49	0.55
1:C:316:GLY:HA2	1:C:364:LYS:HB2	1.89	0.55
1:C:521:ILE:HG21	1:C:526:VAL:HG13	1.89	0.55
1:D:457:HIS:CE1	1:D:515:LEU:HD13	2.42	0.55
1:C:298:LEU:HD13	1:C:303:LYS:HA	1.89	0.54
1:D:618:HIS:HB2	1:D:647:PHE:O	2.08	0.54
1:C:120:LEU:HD11	1:C:131:ILE:HD12	1.90	0.54
1:C:467:LEU:HD22	1:C:468:PRO:HD2	1.89	0.54
1:A:668:TYR:CZ	1:A:672:LEU:HD11	2.43	0.54
1:C:670:ASP:O	1:C:674:GLY:N	2.39	0.54
1:D:229:ASN:ND2	1:D:238:ASN:HD22	1.99	0.54
1:B:36:LEU:CD2	1:B:40:LEU:HD13	2.38	0.53
1:D:518:PHE:HA	1:D:521:ILE:HD13	1.91	0.53
1:C:120:LEU:HD12	1:C:128:LEU:HD23	1.89	0.53
1:D:39:VAL:HG11	1:D:64:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:735:ILE:HD12	1:C:790:GLN:HE21	1.72	0.53
1:C:784:CYS:SG	1:C:848:ILE:HG23	2.49	0.53
1:A:771:ALA:O	1:A:774:LYS:HB3	2.08	0.53
1:A:332:GLN:HG3	1:A:355:LEU:HD23	1.91	0.53
1:B:375:LYS:HB3	1:B:424:TRP:CZ3	2.44	0.53
1:D:295:LYS:NZ	1:D:304:THR:O	2.43	0.52
1:B:167:THR:HB	1:B:169:THR:HG22	1.91	0.52
1:C:668:TYR:HA	1:C:671:THR:HG22	1.90	0.52
1:C:295:LYS:CA	1:C:298:LEU:HD11	2.39	0.52
1:B:584:LYS:HG2	1:B:588:ASN:HD21	1.74	0.52
1:B:406:ASN:HD22	1:B:409:LYS:HD3	1.74	0.52
1:B:835:LEU:HA	1:B:838:VAL:HG12	1.91	0.52
1:C:39:VAL:HG21	1:C:64:PHE:CD2	2.44	0.52
1:B:39:VAL:HG21	1:B:64:PHE:CD2	2.44	0.52
1:B:555:ASN:ND2	1:B:617:GLN:HE22	2.08	0.52
1:C:491:SER:OG	1:C:495:GLU:OE2	2.25	0.52
1:C:521:ILE:CG2	1:C:526:VAL:HG13	2.39	0.52
1:B:615:HIS:HA	1:B:646:THR:HB	1.92	0.51
1:C:59:ALA:HA	1:C:73:MET:CE	2.40	0.51
1:C:668:TYR:CE1	1:C:672:LEU:HD23	2.45	0.51
1:A:95:LEU:HD22	1:A:95:LEU:C	2.36	0.51
1:A:442:PHE:O	1:A:446:ILE:HG23	2.11	0.51
1:A:6:TYR:O	1:A:7:ILE:HD13	2.11	0.51
1:A:485:LEU:HD21	1:A:498:LEU:HD13	1.92	0.51
1:C:256:GLU:O	1:C:260:GLN:HG3	2.10	0.51
1:C:167:THR:HG23	1:C:169:THR:HG22	1.93	0.51
1:D:460:LEU:HD12	1:D:508:LEU:HD13	1.92	0.51
1:D:567:TYR:HE2	1:D:592:LEU:HD22	1.75	0.51
1:A:435:GLN:HE22	1:A:472:GLN:HE22	1.58	0.50
1:B:565:THR:HA	1:B:597:ARG:NE	2.26	0.50
1:D:540:ASN:C	1:D:540:ASN:OD1	2.54	0.50
1:A:260:GLN:HA	1:A:305:TYR:O	2.11	0.50
1:A:616:ASN:O	1:A:620:TYR:HD2	1.95	0.50
1:B:36:LEU:HD23	1:B:40:LEU:HD13	1.93	0.50
1:D:452:LEU:HD13	1:D:452:LEU:N	2.25	0.50
1:B:337:ALA:HB3	1:B:378:MET:HE1	1.94	0.50
1:B:359:HIS:O	1:B:362:ILE:HD11	2.10	0.50
1:D:229:ASN:HD21	1:D:238:ASN:ND2	1.98	0.50
1:D:300:GLU:HB2	1:D:301:PRO:HD3	1.93	0.50
1:D:619:ILE:HD11	1:D:639:LEU:CB	2.42	0.50
1:B:354:ALA:C	1:B:355:LEU:HD23	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:788:VAL:HG12	1:C:845:TYR:HB3	1.94	0.50
1:D:540:ASN:N	1:D:543:GLN:HE21	2.09	0.50
1:D:560:THR:HG23	1:D:561:TYR:CD2	2.46	0.50
1:A:615:HIS:CD2	1:A:646:THR:HA	2.47	0.50
1:B:555:ASN:HD21	1:B:617:GLN:HE22	1.60	0.50
1:A:351:LYS:HG3	1:A:362:ILE:CD1	2.41	0.50
1:A:526:VAL:HG22	1:A:530:LEU:HD12	1.94	0.49
1:B:96:ASN:OD1	1:B:98:THR:HG22	2.11	0.49
1:B:36:LEU:HD22	1:B:40:LEU:HD22	1.95	0.49
1:C:337:ALA:CB	1:C:378:MET:HE1	2.42	0.49
1:A:366:VAL:N	1:A:370:ASN:HD22	2.09	0.49
1:B:116:VAL:HG21	1:B:190:ILE:CD1	2.42	0.49
1:C:120:LEU:HD11	1:C:131:ILE:CD1	2.43	0.49
1:D:27:LYS:HD2	1:D:121:GLU:CD	2.36	0.49
1:A:447:ASN:OD1	1:A:454:SER:N	2.42	0.49
1:B:525:GLU:HG3	1:B:608:GLU:HB3	1.95	0.49
1:C:430:LEU:O	1:C:431:LYS:C	2.56	0.49
1:D:120:LEU:O	1:D:121:GLU:C	2.55	0.49
1:C:316:GLY:HA2	1:C:364:LYS:CB	2.43	0.49
1:D:140:ARG:NH2	1:D:182:LEU:O	2.45	0.49
1:B:409:LYS:O	1:B:412:GLU:HB2	2.13	0.48
1:B:438:ARG:HH21	1:B:472:GLN:NE2	2.10	0.48
1:B:591:ASN:HD21	1:B:605:ARG:H	1.61	0.48
1:D:615:HIS:HA	1:D:646:THR:HA	1.95	0.48
1:C:420:THR:OG1	1:C:421:PRO:HD3	2.14	0.48
1:C:575:LYS:CD	1:C:581:VAL:HG11	2.43	0.48
1:D:208:ASN:OD1	1:D:211:LEU:HD12	2.13	0.48
1:B:279:LEU:HD11	1:B:321:ARG:HB3	1.95	0.48
1:A:55:ARG:CZ	1:A:94:PHE:HZ	2.26	0.48
1:C:568:LYS:HB3	1:C:592:LEU:HD21	1.95	0.48
1:C:211:LEU:CD1	1:C:231:LEU:HG	2.43	0.48
1:D:362:ILE:HD12	1:D:362:ILE:H	1.79	0.48
1:A:839:ARG:O	1:A:840:GLU:C	2.56	0.48
1:B:710:LEU:HD13	1:B:805:LEU:HD12	1.94	0.48
1:D:441:GLN:HG3	1:D:476:LEU:HD23	1.96	0.48
1:D:157:ASN:N	1:D:157:ASN:OD1	2.47	0.48
1:C:295:LYS:O	1:C:298:LEU:HD11	2.14	0.47
1:D:355:LEU:N	1:D:355:LEU:HD23	2.29	0.47
1:A:633:LYS:O	1:A:637:VAL:HG13	2.13	0.47
1:D:331:THR:HG22	1:D:331:THR:O	2.14	0.47
1:D:401:LEU:HD22	1:D:410:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:GLN:NE2	1:A:566:ASP:OD2	2.46	0.47
1:D:601:SER:OG	1:D:602:SER:N	2.45	0.47
1:B:291:ALA:HA	1:B:311:TRP:CD1	2.49	0.47
1:C:15:PHE:O	1:C:19:LEU:HD12	2.14	0.47
1:A:289:THR:HG23	1:A:290:THR:HG23	1.96	0.47
1:C:404:ALA:HB1	1:C:409:LYS:CB	2.44	0.47
1:D:818:LEU:HA	1:D:821:LYS:HB2	1.97	0.47
1:A:446:ILE:HD11	1:A:457:HIS:HB2	1.95	0.47
1:B:22:ILE:HG23	1:B:32:LEU:HD21	1.97	0.47
1:D:135:ASN:O	1:D:136:PRO:C	2.58	0.47
1:A:300:GLU:CD	1:A:300:GLU:O	2.58	0.47
1:C:120:LEU:HD12	1:C:128:LEU:CD2	2.46	0.46
1:D:237:GLY:O	1:D:240:VAL:HG12	2.15	0.46
1:C:479:PRO:O	1:C:480:GLN:C	2.58	0.46
1:B:441:GLN:OE1	1:B:476:LEU:HD13	2.15	0.46
1:D:316:GLY:HA2	1:D:364:LYS:HB2	1.97	0.46
1:D:420:THR:O	1:D:421:PRO:C	2.58	0.46
1:A:442:PHE:HB3	1:A:461:MET:HE1	1.96	0.46
1:B:147:LYS:NZ	1:B:152:ASN:OD1	2.49	0.46
1:B:555:ASN:HD21	1:B:617:GLN:NE2	2.13	0.46
1:B:494:ALA:HB2	1:B:509:LEU:HD21	1.97	0.46
1:A:521:ILE:HG22	1:A:527:ALA:HB2	1.98	0.46
1:A:811:PHE:CE2	1:A:824:ILE:HD12	2.50	0.46
1:C:367:THR:O	1:C:368:GLU:C	2.59	0.46
1:D:736:THR:HA	1:D:739:ILE:HD11	1.98	0.46
1:C:501:ASN:HD22	1:C:501:ASN:HA	1.58	0.46
1:A:332:GLN:HG2	1:A:334:LEU:HD21	1.98	0.46
1:A:799:GLU:OE2	1:A:839:ARG:NH2	2.49	0.46
1:B:375:LYS:HZ3	1:B:424:TRP:CD1	2.34	0.46
1:A:96:ASN:OD1	1:A:99:ASP:N	2.49	0.45
1:A:725:LEU:HG	1:A:827:LEU:HD21	1.99	0.45
1:B:339:ASN:ND2	1:B:421:PRO:HD2	2.32	0.45
1:B:62:GLN:HB3	1:B:73:MET:HE2	1.99	0.45
1:B:26:ALA:HB2	1:B:32:LEU:HD23	1.97	0.45
1:B:478:LYS:HB2	1:B:481:GLN:NE2	2.31	0.45
1:C:409:LYS:O	1:C:413:VAL:HG23	2.17	0.45
1:C:18:ALA:O	1:C:22:ILE:HG12	2.17	0.45
1:D:208:ASN:C	1:D:208:ASN:ND2	2.75	0.45
1:A:96:ASN:OD1	1:A:98:THR:C	2.60	0.45
1:B:554:ALA:HB1	1:B:560:THR:HG21	1.99	0.45
1:C:120:LEU:HD22	1:C:150:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:GLU:CB	1:D:301:PRO:HD3	2.47	0.45
1:D:339:ASN:HD21	1:D:419:ILE:HA	1.82	0.45
1:C:299:ASP:O	1:C:301:PRO:HD2	2.17	0.45
1:B:346:LEU:HD12	1:B:350:LEU:HD13	1.99	0.45
1:C:382:PHE:CE1	1:C:386:ILE:HD11	2.52	0.45
1:A:96:ASN:OD1	1:A:98:THR:N	2.50	0.44
1:B:94:PHE:CE1	1:B:95:LEU:CD2	3.01	0.44
1:D:134:ASN:HD21	1:D:173:LYS:NZ	2.15	0.44
1:D:660:LYS:O	1:D:702:LYS:NZ	2.50	0.44
1:A:554:ALA:HB1	1:A:570:LEU:HD12	2.00	0.44
1:D:438:ARG:NE	1:D:472:GLN:OE1	2.45	0.44
1:A:398:LEU:HB3	1:A:441:GLN:HE21	1.82	0.44
1:C:414:LEU:O	1:C:417:LEU:N	2.44	0.44
1:C:728:GLU:OE1	1:C:801:HIS:NE2	2.44	0.44
1:B:121:GLU:O	1:B:122:LYS:HD2	2.17	0.44
1:D:135:ASN:OD1	1:D:135:ASN:C	2.60	0.44
1:B:295:LYS:NZ	1:B:306:LEU:O	2.45	0.43
1:C:210:GLN:O	1:C:210:GLN:NE2	2.51	0.43
1:C:457:HIS:CE1	1:C:515:LEU:HD11	2.53	0.43
1:C:713:THR:HG22	1:C:718:VAL:HG11	2.00	0.43
1:D:522:HIS:CG	1:D:639:LEU:HD13	2.53	0.43
1:D:573:ALA:O	1:D:576:THR:OG1	2.34	0.43
1:D:791:LEU:CD1	1:D:842:LEU:HD23	2.48	0.43
1:A:47:ASP:OD2	1:A:159:HIS:NE2	2.51	0.43
1:A:271:VAL:HG22	1:A:318:LEU:HD13	2.01	0.43
1:A:446:ILE:CD1	1:A:457:HIS:HB2	2.47	0.43
1:D:540:ASN:O	1:D:544:VAL:HG13	2.17	0.43
1:B:23:ALA:HB2	1:B:114:GLN:HE22	1.84	0.43
1:C:481:GLN:O	1:C:485:LEU:HD23	2.18	0.43
1:C:550:ALA:O	1:C:570:LEU:HD12	2.18	0.43
1:D:120:LEU:HD21	1:D:131:ILE:HD13	1.99	0.43
1:A:42:ASP:O	1:A:43:ILE:C	2.61	0.43
1:B:557:ASN:HD21	1:B:566:ASP:HB3	1.83	0.43
1:C:261:GLU:OE2	1:C:265:ARG:NH1	2.49	0.43
1:C:673:PHE:CZ	1:C:682:ASN:HB3	2.52	0.43
1:D:460:LEU:O	1:D:464:LEU:HD13	2.18	0.43
1:A:363:ASP:C	1:A:364:LYS:HD2	2.43	0.43
1:B:316:GLY:HA2	1:B:364:LYS:HG3	2.00	0.43
1:A:55:ARG:HA	1:A:58:VAL:CG1	2.49	0.43
1:A:176:ASN:OD1	1:A:178:SER:HB2	2.18	0.43
1:A:204:ASN:HA	1:A:254:ARG:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:LYS:NZ	1:A:596:GLY:O	2.37	0.43
1:D:397:ALA:HB1	1:D:417:LEU:HD21	2.00	0.43
1:B:337:ALA:HB1	1:B:378:MET:HE1	2.01	0.43
1:D:657:ARG:HB2	1:D:658:PRO:HD3	2.00	0.43
1:D:15:PHE:CD1	1:D:72:LEU:HD23	2.54	0.43
1:D:523:ASN:HB3	1:D:526:VAL:CG1	2.49	0.43
1:C:202:LEU:HD11	1:C:231:LEU:O	2.19	0.42
1:A:310:GLU:O	1:A:311:TRP:C	2.62	0.42
1:B:282:LYS:O	1:B:283:LYS:C	2.62	0.42
1:B:618:HIS:HB2	1:B:647:PHE:O	2.19	0.42
1:B:634:LEU:HD13	1:B:659:LEU:HD21	2.01	0.42
1:A:140:ARG:NH2	1:A:182:LEU:O	2.52	0.42
1:A:713:THR:HA	1:A:813:ALA:HA	2.01	0.42
1:C:300:GLU:O	1:C:303:LYS:N	2.51	0.42
1:C:610:SER:HA	1:C:613:GLN:HB2	2.00	0.42
1:D:366:VAL:O	1:D:370:ASN:HB2	2.18	0.42
1:B:485:LEU:O	1:B:512:ASN:ND2	2.51	0.42
1:B:565:THR:HA	1:B:597:ARG:HE	1.84	0.42
1:C:55:ARG:NH1	1:C:95:LEU:O	2.52	0.42
1:C:19:LEU:HD21	1:C:111:ALA:HB2	2.02	0.42
1:C:211:LEU:HD11	1:C:231:LEU:HG	2.00	0.42
1:D:271:VAL:HG21	1:D:318:LEU:HA	2.01	0.42
1:A:574:ILE:O	1:A:575:LYS:C	2.63	0.42
1:B:117:LYS:CG	1:B:190:ILE:HG22	2.50	0.42
1:B:407:LEU:HD21	1:B:425:VAL:CG2	2.46	0.42
1:C:282:LYS:HG2	1:C:318:LEU:HD21	2.01	0.42
1:D:5:GLU:O	1:D:6:TYR:HB2	2.19	0.42
1:B:491:SER:HA	1:B:509:LEU:HD11	2.01	0.42
1:C:47:ASP:OD2	1:C:159:HIS:NE2	2.53	0.42
1:D:414:LEU:HD22	1:D:419:ILE:HD11	2.02	0.42
1:A:311:TRP:O	1:A:312:GLU:C	2.63	0.42
1:C:27:LYS:HD2	1:C:121:GLU:HG3	2.02	0.42
1:C:460:LEU:HD12	1:C:486:MET:HE1	2.02	0.42
1:A:38:LYS:HA	1:A:41:ASP:HB2	2.01	0.41
1:A:634:LEU:HD13	1:A:659:LEU:CD1	2.50	0.41
1:A:798:LEU:O	1:A:802:LEU:HD23	2.20	0.41
1:C:523:ASN:HB3	1:C:526:VAL:HG12	2.01	0.41
1:D:733:LYS:HA	1:D:736:THR:HG22	2.02	0.41
1:B:117:LYS:HG2	1:B:190:ILE:HG22	2.02	0.41
1:B:327:LEU:HD23	1:B:378:MET:HG2	2.02	0.41
1:C:581:VAL:HG13	1:C:586:PHE:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ASN:HD21	1:B:211:LEU:HG	1.84	0.41
1:B:612:GLN:HE21	1:B:612:GLN:HA	1.85	0.41
1:C:591:ASN:HB3	1:C:603:THR:HG22	2.02	0.41
1:A:618:HIS:ND1	1:A:648:SER:HA	2.36	0.41
1:D:54:PHE:O	1:D:57:ILE:HG22	2.21	0.41
1:D:457:HIS:HA	1:D:459:LYS:HE2	2.01	0.41
1:A:342:ASP:OD1	1:A:342:ASP:N	2.54	0.41
1:A:732:ILE:HG21	1:A:798:LEU:HD21	2.03	0.41
1:B:203:ILE:HD12	1:B:254:ARG:HD3	2.03	0.41
1:B:791:LEU:O	1:B:795:VAL:HG23	2.20	0.41
1:C:127:THR:HG21	1:C:146:LYS:CE	2.50	0.41
1:C:202:LEU:HD21	1:C:232:GLY:C	2.46	0.41
1:D:267:PHE:CE2	1:D:314:ALA:HB1	2.55	0.41
1:D:332:GLN:O	1:D:334:LEU:HD12	2.20	0.41
1:B:710:LEU:CD2	1:B:722:ILE:HG13	2.51	0.41
1:C:276:HIS:CD2	1:C:325:ALA:HB1	2.55	0.41
1:C:555:ASN:HD21	1:C:613:GLN:HG2	1.86	0.41
1:B:94:PHE:CE1	1:B:95:LEU:HD22	2.55	0.41
1:B:135:ASN:O	1:B:136:PRO:C	2.63	0.41
1:C:40:LEU:HB3	1:C:115:ARG:HG2	2.02	0.41
1:C:398:LEU:HD13	1:C:440:ARG:HG3	2.02	0.41
1:C:570:LEU:HD13	1:C:570:LEU:N	2.35	0.41
1:D:200:LEU:HD11	1:D:247:VAL:HA	2.03	0.41
1:D:337:ALA:CB	1:D:378:MET:HE1	2.50	0.41
1:D:710:LEU:HD21	1:D:721:ALA:HB3	2.02	0.41
1:A:36:LEU:O	1:A:40:LEU:HD22	2.20	0.41
1:B:271:VAL:HA	1:B:274:LEU:CD1	2.51	0.41
1:B:657:ARG:HB2	1:B:658:PRO:HD3	2.03	0.41
1:C:59:ALA:CB	1:C:89:LEU:HD12	2.51	0.41
1:C:714:ASN:N	1:C:714:ASN:HD22	2.19	0.41
1:C:367:THR:HG22	1:C:371:LEU:HD13	2.02	0.40
1:C:94:PHE:CD2	1:C:95:LEU:HB2	2.57	0.40
1:C:44:LEU:HB3	1:C:158:VAL:HG13	2.02	0.40
1:C:438:ARG:HB3	1:C:472:GLN:HE21	1.85	0.40
1:C:529:VAL:HG21	1:C:589:ALA:HB1	2.03	0.40
1:A:293:GLY:O	1:A:294:PHE:C	2.65	0.40
1:B:367:THR:O	1:B:368:GLU:C	2.65	0.40
1:B:406:ASN:HD22	1:B:409:LYS:CD	2.33	0.40
1:C:22:ILE:HD12	1:C:68:HIS:CG	2.57	0.40
1:D:442:PHE:CD1	1:D:464:LEU:HD23	2.57	0.40
1:D:518:PHE:CD2	1:D:539:LEU:HD12	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:584:LYS:NZ	1:D:594:ASP:OD2	2.45	0.40
1:A:404:ALA:O	1:A:434:LYS:NZ	2.40	0.40
1:B:310:GLU:O	1:B:311:TRP:C	2.64	0.40
1:C:591:ASN:HB2	1:C:606:LYS:HB2	2.04	0.40
1:D:167:THR:OG1	1:D:169:THR:HG22	2.22	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	842/901 (94%)	757 (90%)	74 (9%)	11 (1%)	9	38
1	B	838/901 (93%)	780 (93%)	50 (6%)	8 (1%)	12	45
1	C	775/901 (86%)	675 (87%)	78 (10%)	22 (3%)	4	21
1	D	828/901 (92%)	759 (92%)	60 (7%)	9 (1%)	11	43
All	All	3283/3604 (91%)	2971 (90%)	262 (8%)	50 (2%)	8	35

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLU
1	B	50	ASP
1	B	628	ASN
1	C	12	ASN
1	C	300	GLU
1	C	541	ASP
1	C	709	GLU
1	D	300	GLU
1	D	601	SER
1	D	628	ASN

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Mol	Chain	Res	Type
1	C	2	ILE
1	C	583	GLN
1	C	594	ASP
1	D	422	ALA
1	A	388	ASP
1	A	597	ARG
1	B	169	THR
1	B	391	ASN
1	C	481	GLN
1	C	491	SER
1	C	579	GLY
1	C	628	ASN
1	C	644	PRO
1	D	6	TYR
1	D	391	ASN
1	D	594	ASP
1	A	225	GLU
1	A	311	TRP
1	A	575	LYS
1	A	808	GLU
1	B	421	PRO
1	C	368	GLU
1	C	404	ALA
1	C	582	ASN
1	C	597	ARG
1	C	604	PRO
1	C	678	THR
1	B	171	PRO
1	B	208	ASN
1	B	424	TRP
1	C	469	VAL
1	D	114	GLN
1	A	498	LEU
1	C	432	ASP
1	C	480	GLN
1	D	368	GLU
1	A	7	ILE
1	A	581	VAL
1	A	39	VAL
1	C	800	GLY

5.3.2 Protein sidechains ⓘ

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	728/779 (94%)	648 (89%)	80 (11%)	6	25
1	B	726/779 (93%)	651 (90%)	75 (10%)	7	28
1	C	680/779 (87%)	590 (87%)	90 (13%)	4	18
1	D	725/779 (93%)	657 (91%)	68 (9%)	8	32
All	All	2859/3116 (92%)	2546 (89%)	313 (11%)	6	26

All (313) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	40	LEU
1	A	57	ILE
1	A	58	VAL
1	A	73	MET
1	A	87	GLN
1	A	88	TYR
1	A	94	PHE
1	A	95	LEU
1	A	103	ASN
1	A	116	VAL
1	A	125	THR
1	A	126	ASP
1	A	127	THR
1	A	146	LYS
1	A	158	VAL
1	A	187	ILE
1	A	202	LEU
1	A	205	SER
1	A	215	LEU
1	A	243	LEU
1	A	245	ARG
1	A	248	VAL
1	A	254	ARG

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Mol	Chain	Res	Type
1	A	273	SER
1	A	279	LEU
1	A	280	LEU
1	A	295	LYS
1	A	298	LEU
1	A	323	LEU
1	A	332	GLN
1	A	346	LEU
1	A	371	LEU
1	A	381	SER
1	A	392	LEU
1	A	413	VAL
1	A	416	LYS
1	A	428	THR
1	A	446	ILE
1	A	460	LEU
1	A	465	THR
1	A	467	LEU
1	A	471	LYS
1	A	476	LEU
1	A	478	LYS
1	A	498	LEU
1	A	521	ILE
1	A	537	ILE
1	A	551	LEU
1	A	556	SER
1	A	560	THR
1	A	581	VAL
1	A	584	LYS
1	A	602	SER
1	A	605	ARG
1	A	627	SER
1	A	637	VAL
1	A	645	VAL
1	A	646	THR
1	A	659	LEU
1	A	689	LEU
1	A	703	ASN
1	A	704	ASP
1	A	705	LEU
1	A	706	ARG
1	A	713	THR

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Mol	Chain	Res	Type
1	A	727	THR
1	A	729	LEU
1	A	746	LEU
1	A	750	ASN
1	A	755	VAL
1	A	757	LEU
1	A	758	TYR
1	A	772	GLN
1	A	802	LEU
1	A	807	LYS
1	A	811	PHE
1	A	819	GLU
1	A	840	GLU
1	A	843	ASP
1	B	2	ILE
1	B	14	GLU
1	B	32	LEU
1	B	36	LEU
1	B	40	LEU
1	B	77	GLU
1	B	80	PHE
1	B	92	ASP
1	B	95	LEU
1	B	128	LEU
1	B	132	LEU
1	B	135	ASN
1	B	148	PRO
1	B	167	THR
1	B	181	VAL
1	B	187	ILE
1	B	193	GLN
1	B	203	ILE
1	B	208	ASN
1	B	209	THR
1	B	215	LEU
1	B	216	ARG
1	B	220	SER
1	B	235	THR
1	B	248	VAL
1	B	251	LEU
1	B	274	LEU
1	B	290	THR

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Mol	Chain	Res	Type
1	B	304	THR
1	B	350	LEU
1	B	355	LEU
1	B	362	ILE
1	B	367	THR
1	B	370	ASN
1	B	413	VAL
1	B	432	ASP
1	B	447	ASN
1	B	451	SER
1	B	452	LEU
1	B	454	SER
1	B	458	SER
1	B	461	MET
1	B	463	THR
1	B	480	GLN
1	B	491	SER
1	B	501	ASN
1	B	510	THR
1	B	523	ASN
1	B	526	VAL
1	B	529	VAL
1	B	534	LYS
1	B	539	LEU
1	B	560	THR
1	B	569	ILE
1	B	571	ILE
1	B	580	SER
1	B	611	LYS
1	B	617	GLN
1	B	622	GLU
1	B	623	TYR
1	B	625	SER
1	B	627	SER
1	B	643	LYS
1	B	646	THR
1	B	660	LYS
1	B	664	THR
1	B	696	THR
1	B	723	LYS
1	B	725	LEU
1	B	735	ILE

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Mol	Chain	Res	Type
1	B	749	ILE
1	B	826	LYS
1	B	830	ASP
1	B	838	VAL
1	B	857	LYS
1	C	1	MET
1	C	4	GLU
1	C	9	MET
1	C	40	LEU
1	C	57	ILE
1	C	62	GLN
1	C	73	MET
1	C	77	GLU
1	C	91	SER
1	C	95	LEU
1	C	101	THR
1	C	106	LYS
1	C	120	LEU
1	C	133	LYS
1	C	135	ASN
1	C	147	LYS
1	C	175	ILE
1	C	181	VAL
1	C	193	GLN
1	C	211	LEU
1	C	240	VAL
1	C	244	SER
1	C	247	VAL
1	C	279	LEU
1	C	298	LEU
1	C	299	ASP
1	C	300	GLU
1	C	304	THR
1	C	328	SER
1	C	346	LEU
1	C	355	LEU
1	C	383	ILE
1	C	392	LEU
1	C	407	LEU
1	C	417	LEU
1	C	420	THR
1	C	428	THR

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Mol	Chain	Res	Type
1	C	430	LEU
1	C	452	LEU
1	C	454	SER
1	C	460	LEU
1	C	465	THR
1	C	466	LYS
1	C	467	LEU
1	C	469	VAL
1	C	470	GLU
1	C	482	LEU
1	C	485	LEU
1	C	486	MET
1	C	490	GLU
1	C	498	LEU
1	C	501	ASN
1	C	503	SER
1	C	510	THR
1	C	519	ARG
1	C	521	ILE
1	C	523	ASN
1	C	534	LYS
1	C	541	ASP
1	C	547	ILE
1	C	551	LEU
1	C	570	LEU
1	C	582	ASN
1	C	585	ASP
1	C	600	THR
1	C	631	ASN
1	C	643	LYS
1	C	646	THR
1	C	652	VAL
1	C	668	TYR
1	C	672	LEU
1	C	675	GLU
1	C	679	ASN
1	C	684	LYS
1	C	689	LEU
1	C	705	LEU
1	C	708	GLN
1	C	714	ASN
1	C	719	MET

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Mol	Chain	Res	Type
1	C	725	LEU
1	C	729	LEU
1	C	735	ILE
1	C	736	THR
1	C	773	MET
1	C	774	LYS
1	C	778	GLU
1	C	790	GLN
1	C	791	LEU
1	C	840	GLU
1	C	852	LEU
1	D	7	ILE
1	D	13	LYS
1	D	58	VAL
1	D	92	ASP
1	D	129	VAL
1	D	133	LYS
1	D	157	ASN
1	D	181	VAL
1	D	209	THR
1	D	240	VAL
1	D	275	SER
1	D	326	VAL
1	D	338	LEU
1	D	348	THR
1	D	350	LEU
1	D	355	LEU
1	D	362	ILE
1	D	368	GLU
1	D	369	GLU
1	D	371	LEU
1	D	379	MET
1	D	386	ILE
1	D	388	ASP
1	D	392	LEU
1	D	395	LEU
1	D	447	ASN
1	D	452	LEU
1	D	459	LYS
1	D	461	MET
1	D	466	LYS
1	D	476	LEU

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Mol	Chain	Res	Type
1	D	481	GLN
1	D	482	LEU
1	D	490	GLU
1	D	493	VAL
1	D	508	LEU
1	D	526	VAL
1	D	534	LYS
1	D	540	ASN
1	D	552	THR
1	D	563	GLN
1	D	592	LEU
1	D	597	ARG
1	D	617	GLN
1	D	619	ILE
1	D	626	THR
1	D	638	LEU
1	D	639	LEU
1	D	643	LYS
1	D	651	ILE
1	D	652	VAL
1	D	656	LEU
1	D	664	THR
1	D	676	ASN
1	D	700	GLU
1	D	725	LEU
1	D	731	SER
1	D	745	LYS
1	D	747	LYS
1	D	786	LEU
1	D	798	LEU
1	D	802	LEU
1	D	803	LYS
1	D	818	LEU
1	D	826	LYS
1	D	832	GLU
1	D	843	ASP
1	D	858	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN

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Mol	Chain	Res	Type
1	A	134	ASN
1	A	193	GLN
1	A	229	ASN
1	A	238	ASN
1	A	260	GLN
1	A	435	GLN
1	A	496	HIS
1	A	512	ASN
1	A	549	GLN
1	A	555	ASN
1	A	559	ASN
1	A	563	GLN
1	A	588	ASN
1	A	615	HIS
1	A	653	ASN
1	A	682	ASN
1	A	703	ASN
1	A	750	ASN
1	A	763	GLN
1	A	772	GLN
1	A	790	GLN
1	A	849	GLN
1	B	62	GLN
1	B	103	ASN
1	B	105	GLN
1	B	114	GLN
1	B	229	ASN
1	B	238	ASN
1	B	272	GLN
1	B	315	GLN
1	B	339	ASN
1	B	391	ASN
1	B	406	ASN
1	B	472	GLN
1	B	480	GLN
1	B	481	GLN
1	B	484	HIS
1	B	492	HIS
1	B	522	HIS
1	B	555	ASN
1	B	563	GLN
1	B	577	GLN

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Mol	Chain	Res	Type
1	B	588	ASN
1	B	591	ASN
1	B	593	ASN
1	B	612	GLN
1	B	631	ASN
1	B	666	GLN
1	B	676	ASN
1	B	708	GLN
1	B	801	HIS
1	C	87	GLN
1	C	108	HIS
1	C	109	GLN
1	C	134	ASN
1	C	135	ASN
1	C	204	ASN
1	C	208	ASN
1	C	210	GLN
1	C	229	ASN
1	C	324	GLN
1	C	391	ASN
1	C	472	GLN
1	C	501	ASN
1	C	555	ASN
1	C	613	GLN
1	C	653	ASN
1	C	714	ASN
1	C	790	GLN
1	D	134	ASN
1	D	229	ASN
1	D	238	ASN
1	D	333	ASN
1	D	339	ASN
1	D	385	ASN
1	D	391	ASN
1	D	441	GLN
1	D	501	ASN
1	D	543	GLN
1	D	555	ASN
1	D	559	ASN
1	D	617	GLN
1	D	618	HIS
1	D	676	ASN

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Mol	Chain	Res	Type
1	D	682	ASN
1	D	699	ASN
1	D	703	ASN
1	D	742	ASN
1	D	801	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](#)

1 ligand 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	$\# Z > 2$
2	GOL	B	1001	-	5,5,5	0.39	0	5,5,5	0.29	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
2	GOL	B	1001	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	846/901 (93%)	-0.60	6 (0%) 84 66	80, 116, 158, 196	0
1	B	842/901 (93%)	-0.69	0 100 100	78, 111, 156, 210	0
1	C	787/901 (87%)	-0.44	2 (0%) 90 79	80, 141, 193, 219	0
1	D	836/901 (92%)	-0.59	1 (0%) 92 86	69, 127, 174, 204	0
All	All	3311/3604 (91%)	-0.58	9 (0%) 90 79	69, 122, 177, 219	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	PHE	4.0
1	D	65	TRP	3.0
1	A	12	ASN	3.0
1	A	558	PRO	2.9
1	A	58	VAL	2.5
1	C	81	PHE	2.5
1	A	107	LEU	2.5
1	A	574	ILE	2.1
1	C	564	ALA	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($\text{\AA}^2$)	Q<0.9
2	GOL	B	1001	6/6	0.88	0.12	155,167,170,171	0

6.5 Other polymers [i](#)

There are no such residues in this entry.