



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 28, 2017 – 08:23 AM EST

PDB ID : 5OT4
Title : Legionella effector
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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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

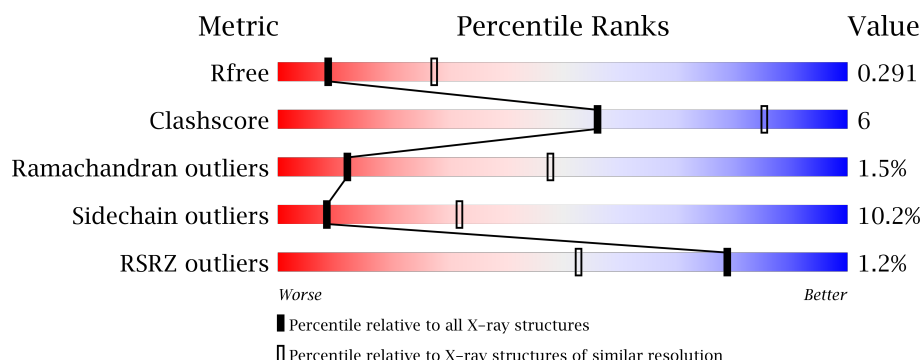
1 Overall quality at a glance

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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div> <div>0.1%</div> <div>76%</div> <div>16%</div> <div>6%</div> </div> </div>
1	B	901	<div> <div>76%</div> <div>16%</div> <div>7%</div> </div>
1	C	901	<div> <div>3%</div> <div>64%</div> <div>19%</div> <div>13%</div> </div>
1	D	901	<div> <div>74%</div> <div>16%</div> <div>7%</div> </div>

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 (three-letter code: GOL) (formula: C₃H₈O₃).

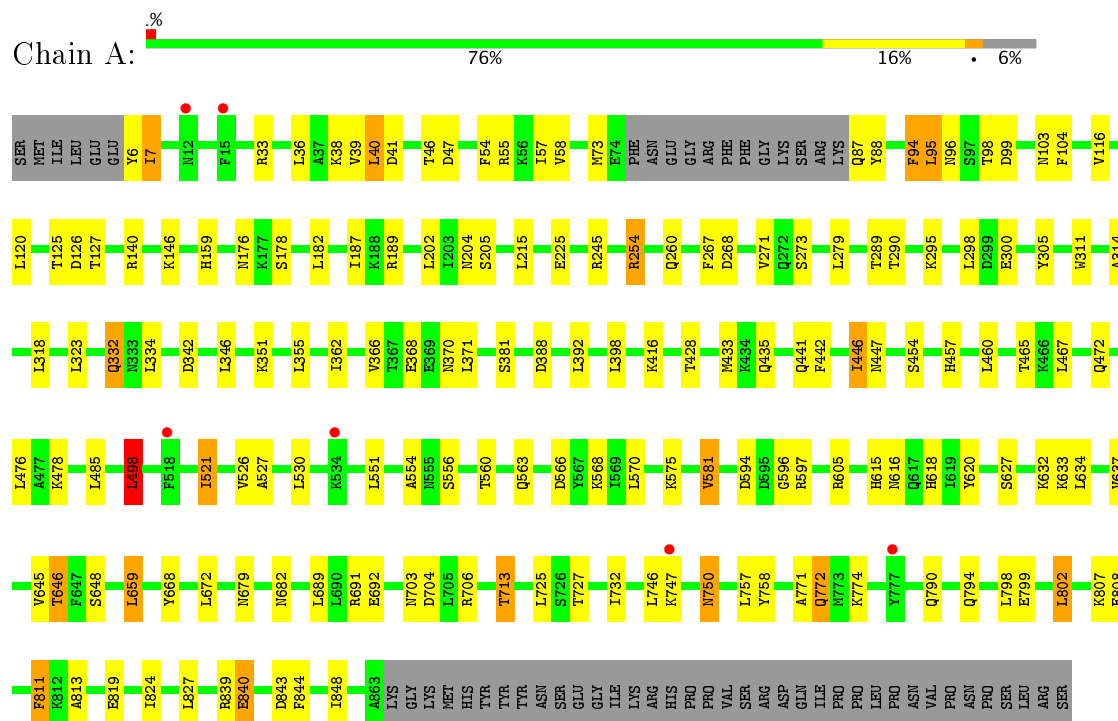


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		

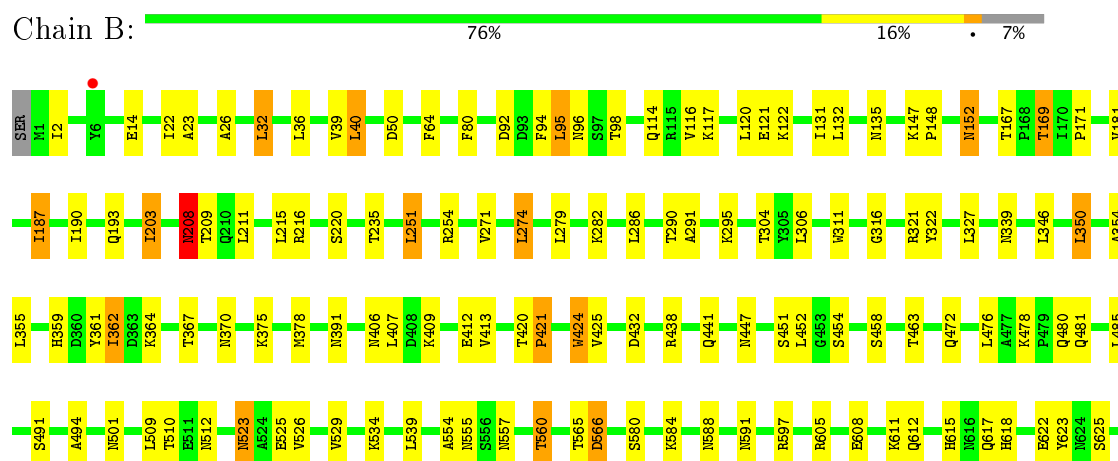
3 Residue-property plots [i](#)

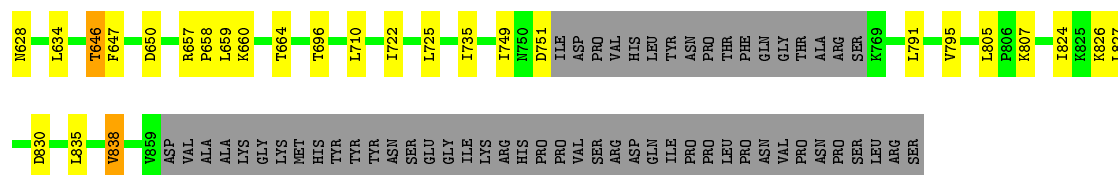
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

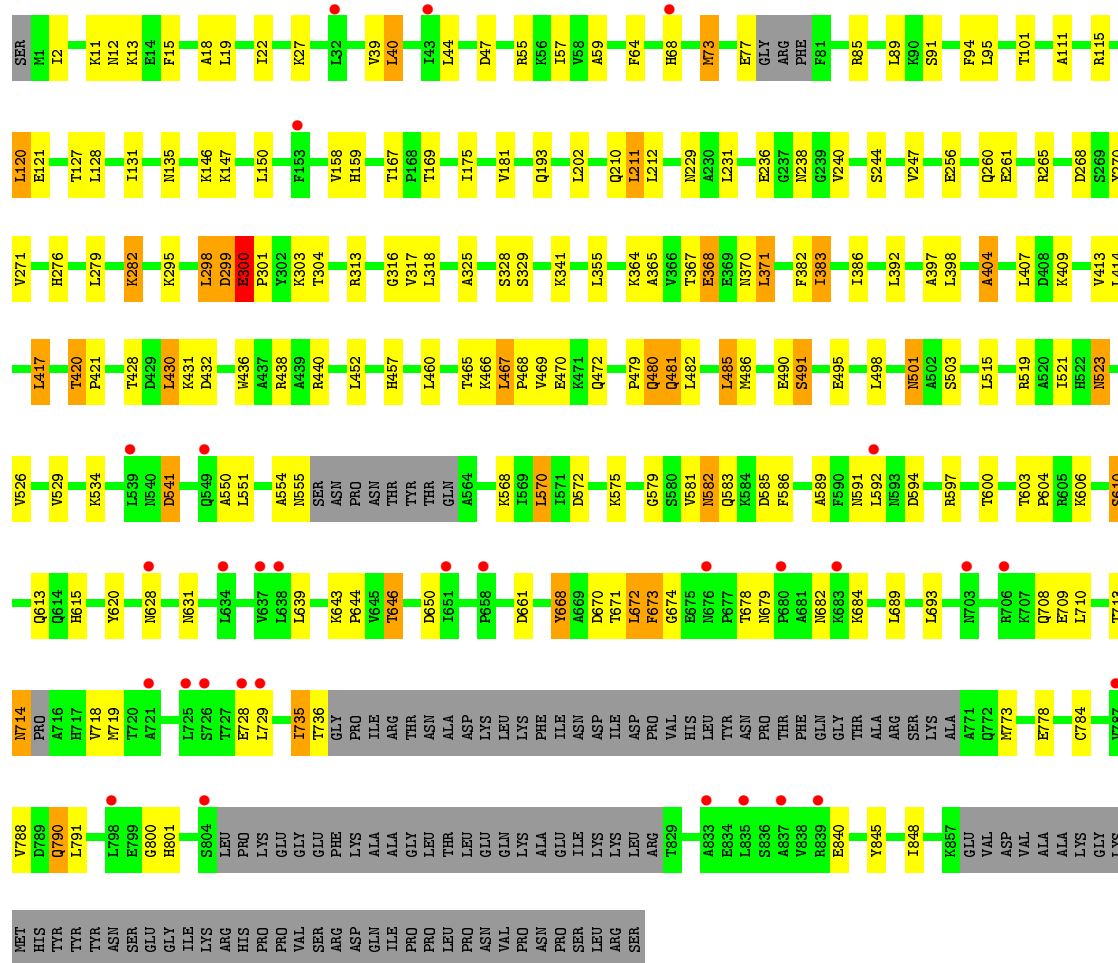


• Molecule 1: Interaptin

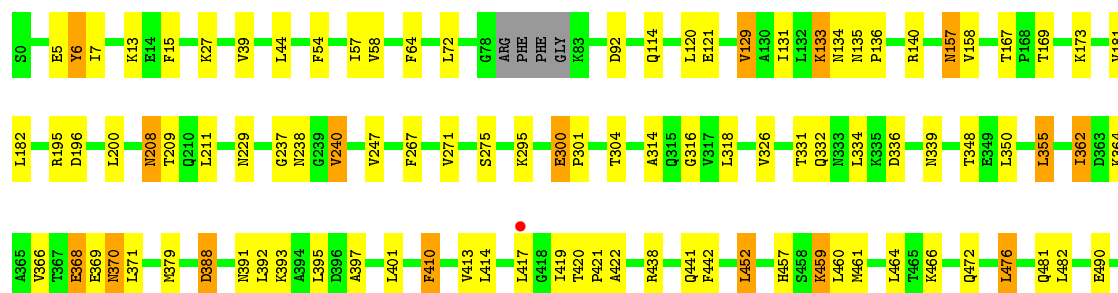


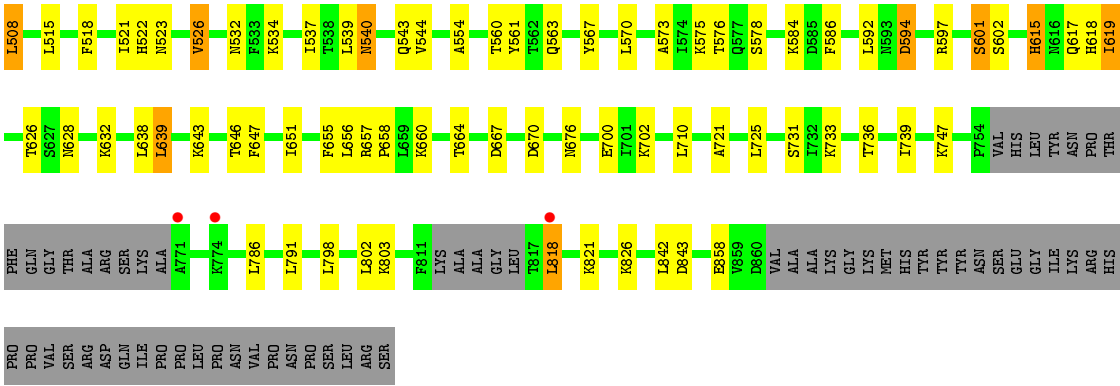


• Molecule 1: Interaptin



• 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 49.55 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (167.27-3.00) 99.8 (49.55-3.00)	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 (5.51%)	DCC
Wilson B-factor (Å ²)	98.4	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 59.4	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	0.95	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.52	0/6793	0.74	0/9163
1	B	0.52	0/6777	0.74	0/9130
1	C	0.59	0/6330	0.78	0/8523
1	D	0.53	0/6729	0.75	0/9067
All	All	0.54	0/26629	0.75	0/35883

There are no bond length outliers.

There are no bond angle outliers.

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	64	0
1	B	6673	0	6726	71	0
1	C	6238	0	6270	93	0
1	D	6628	0	6666	79	0
2	B	6	0	8	0	0
All	All	26232	0	26399	307	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 (307) 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: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: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: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:C:295:LYS:C	1:C:298:LEU:HD11	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:397:ALA:HB1	1:C:417:LEU:HD21	1.87	0.56
1:A:267:PHE:CE2	1:A:314:ALA:HB1	2.40	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: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:D:44:LEU:HB3	1:D:158:VAL:HG13	1.87	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: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:208:ASN:HD22	1:D:208:ASN:C	2.10	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
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:A:772:GLN:C	1:A:772:GLN:HE21	2.12	0.52
1:B:167:THR:HB	1:B:169:THR:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:442:PHE:O	1:A:446:ILE:HG23	2.11	0.51
1:A:485:LEU:HD21	1:A:498:LEU:HD13	1.92	0.51
1:A:6:TYR:O	1:A:7:ILE:HD13	2.11	0.51
1:C:300:GLU:O	1:C:301:PRO:C	2.45	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: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: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:523:ASN:OD1	1:B:523:ASN:C	2.49	0.50
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:C:211:LEU:C	1:C:211:LEU:HD12	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:LEU:HD22	1:B:40:LEU:HD22	1.95	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: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: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: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:OD1	1:D:157:ASN:N	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:HD22	1:A:95:LEU:C	2.36	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: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:D:27:LYS:HD2	1:D:121:GLU:CD	2.36	0.46
1:D:540:ASN:OD1	1:D:540:ASN:C	2.54	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:26:ALA:HB2	1:B:32:LEU:HD23	1.97	0.45
1:B:354:ALA:C	1:B:355:LEU:HD23	2.37	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: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
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:C:430:LEU:O	1:C:431:LYS:C	2.56	0.44
1:D:120:LEU:O	1:D:121:GLU:C	2.55	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:B:295:LYS:NZ	1:B:306:LEU:O	2.45	0.43
1:C:210:GLN:NE2	1:C:210:GLN:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:839:ARG:O	1:A:840:GLU:C	2.56	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:B:316:GLY:HA2	1:B:364:LYS:HG3	2.00	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
1:A:55:ARG:HA	1:A:58:VAL:CG1	2.49	0.43
1:D:397:ALA:HB1	1:D:417:LEU:HD21	2.00	0.43
1:D:657:ARG:HB2	1:D:658:PRO:HD3	2.00	0.43
1:D:523:ASN:HB3	1:D:526:VAL:CG1	2.49	0.43
1:D:15:PHE:CD1	1:D:72:LEU:HD23	2.54	0.43
1:C:202:LEU:HD11	1:C:231:LEU:O	2.19	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:B:117:LYS:CG	1:B:190:ILE:HG22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:300:GLU:CD	1:A:300:GLU:O	2.58	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:135:ASN:O	1:D:136:PRO:C	2.58	0.42
1:D:414:LEU:HD22	1:D:419:ILE:HD11	2.02	0.42
1:C:27:LYS:HD2	1:C:121:GLU:HG3	2.02	0.42
1:C:479:PRO:O	1:C:480:GLN:C	2.58	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:420:THR:O	1:D:421:PRO:C	2.58	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
1:B:208:ASN:HD21	1:B:211:LEU:HG	1.84	0.41
1:B:612:GLN:HA	1:B:612:GLN:HE21	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:C:367:THR:O	1:C:368:GLU:C	2.59	0.41
1:D:457:HIS:HA	1:D:459:LYS:HE2	2.01	0.41
1:D:54:PHE:O	1:D:57:ILE:HG22	2.21	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: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:A:568:LYS:NZ	1:A:596:GLY:O	2.37	0.41
1:C:40:LEU:HB3	1:C:115:ARG:HG2	2.02	0.41
1:D:200:LEU:HD11	1:D:247:VAL:HA	2.03	0.41
1:C:398:LEU:HD13	1:C:440:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:LEU:N	1:C:570:LEU:HD13	2.35	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:HD22	1:C:714:ASN:N	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:438:ARG:HB3	1:C:472:GLN:HE21	1.85	0.40
1:C:44:LEU:HB3	1:C:158:VAL:HG13	2.02	0.40
1:C:529:VAL:HG21	1:C:589:ALA:HB1	2.03	0.40
1:A:96:ASN:OD1	1:A:98:THR:C	2.60	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:208:ASN:ND2	1:D:208:ASN:C	2.75	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
1:D:584:LYS:NZ	1:D:594:ASP:OD2	2.45	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%)	14	51
1	B	838/901 (93%)	780 (93%)	50 (6%)	8 (1%)	18	59
1	C	775/901 (86%)	675 (87%)	78 (10%)	22 (3%)	6	29
1	D	828/901 (92%)	759 (92%)	60 (7%)	9 (1%)	17	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3283/3604 (91%)	2971 (90%)	262 (8%)	50 (2%)	12	48

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
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

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Mol	Chain	Res	Type
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%)	656 (90%)	72 (10%)	9	34
1	B	726/779 (93%)	661 (91%)	65 (9%)	11	40
1	C	680/779 (87%)	594 (87%)	86 (13%)	5	23
1	D	725/779 (93%)	656 (90%)	69 (10%)	10	36
All	All	2859/3116 (92%)	2567 (90%)	292 (10%)	8	32

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	40	LEU
1	A	57	ILE
1	A	73	MET
1	A	87	GLN
1	A	88	TYR
1	A	94	PHE
1	A	95	LEU

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Mol	Chain	Res	Type
1	A	103	ASN
1	A	116	VAL
1	A	120	LEU
1	A	125	THR
1	A	126	ASP
1	A	127	THR
1	A	146	LYS
1	A	187	ILE
1	A	189	ARG
1	A	202	LEU
1	A	205	SER
1	A	215	LEU
1	A	245	ARG
1	A	254	ARG
1	A	268	ASP
1	A	273	SER
1	A	279	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	416	LYS
1	A	428	THR
1	A	433	MET
1	A	446	ILE
1	A	460	LEU
1	A	465	THR
1	A	467	LEU
1	A	476	LEU
1	A	478	LYS
1	A	498	LEU
1	A	521	ILE
1	A	551	LEU
1	A	556	SER
1	A	560	THR
1	A	581	VAL
1	A	594	ASP
1	A	605	ARG

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Mol	Chain	Res	Type
1	A	627	SER
1	A	632	LYS
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	706	ARG
1	A	713	THR
1	A	727	THR
1	A	746	LEU
1	A	750	ASN
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	40	LEU
1	B	80	PHE
1	B	92	ASP
1	B	95	LEU
1	B	132	LEU
1	B	135	ASN
1	B	148	PRO
1	B	152	ASN
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	216	ARG
1	B	220	SER
1	B	235	THR

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Mol	Chain	Res	Type
1	B	251	LEU
1	B	274	LEU
1	B	290	THR
1	B	304	THR
1	B	350	LEU
1	B	361	TYR
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	463	THR
1	B	480	GLN
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	566	ASP
1	B	580	SER
1	B	611	LYS
1	B	622	GLU
1	B	623	TYR
1	B	625	SER
1	B	646	THR
1	B	650	ASP
1	B	660	LYS
1	B	664	THR
1	B	696	THR
1	B	725	LEU
1	B	735	ILE
1	B	749	ILE
1	B	751	ASP
1	B	807	LYS

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Mol	Chain	Res	Type
1	B	826	LYS
1	B	830	ASP
1	B	838	VAL
1	C	40	LEU
1	C	57	ILE
1	C	73	MET
1	C	77	GLU
1	C	85	ARG
1	C	91	SER
1	C	101	THR
1	C	120	LEU
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	236	GLU
1	C	240	VAL
1	C	244	SER
1	C	247	VAL
1	C	279	LEU
1	C	282	LYS
1	C	298	LEU
1	C	299	ASP
1	C	300	GLU
1	C	304	THR
1	C	328	SER
1	C	329	SER
1	C	341	LYS
1	C	355	LEU
1	C	371	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
1	C	430	LEU
1	C	452	LEU
1	C	460	LEU
1	C	465	THR

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Mol	Chain	Res	Type
1	C	466	LYS
1	C	467	LEU
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	519	ARG
1	C	523	ASN
1	C	534	LYS
1	C	541	ASP
1	C	551	LEU
1	C	570	LEU
1	C	572	ASP
1	C	582	ASN
1	C	585	ASP
1	C	600	THR
1	C	610	SER
1	C	620	TYR
1	C	631	ASN
1	C	639	LEU
1	C	643	LYS
1	C	646	THR
1	C	650	ASP
1	C	661	ASP
1	C	668	TYR
1	C	672	LEU
1	C	673	PHE
1	C	679	ASN
1	C	684	LYS
1	C	689	LEU
1	C	693	LEU
1	C	708	GLN
1	C	710	LEU
1	C	714	ASN
1	C	719	MET
1	C	729	LEU
1	C	735	ILE
1	C	736	THR

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Mol	Chain	Res	Type
1	C	773	MET
1	C	778	GLU
1	C	790	GLN
1	C	791	LEU
1	C	840	GLU
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	208	ASN
1	D	209	THR
1	D	240	VAL
1	D	275	SER
1	D	326	VAL
1	D	336	ASP
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	370	ASN
1	D	371	LEU
1	D	379	MET
1	D	388	ASP
1	D	392	LEU
1	D	395	LEU
1	D	410	PHE
1	D	452	LEU
1	D	459	LYS
1	D	461	MET
1	D	466	LYS
1	D	476	LEU
1	D	481	GLN
1	D	482	LEU
1	D	490	GLU
1	D	508	LEU
1	D	526	VAL

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Mol	Chain	Res	Type
1	D	532	ASN
1	D	534	LYS
1	D	540	ASN
1	D	563	GLN
1	D	597	ARG
1	D	615	HIS
1	D	617	GLN
1	D	619	ILE
1	D	626	THR
1	D	632	LYS
1	D	638	LEU
1	D	639	LEU
1	D	643	LYS
1	D	651	ILE
1	D	655	PHE
1	D	656	LEU
1	D	664	THR
1	D	667	ASP
1	D	670	ASP
1	D	676	ASN
1	D	700	GLU
1	D	725	LEU
1	D	731	SER
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	843	ASP
1	D	858	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
1	A	370	ASN
1	A	435	GLN
1	A	522	HIS
1	A	549	GLN
1	A	559	ASN

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Mol	Chain	Res	Type
1	A	563	GLN
1	A	577	GLN
1	A	612	GLN
1	A	615	HIS
1	A	653	ASN
1	A	679	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	820	GLN
1	A	849	GLN
1	B	62	GLN
1	B	114	GLN
1	B	339	ASN
1	B	385	ASN
1	B	406	ASN
1	B	472	GLN
1	B	480	GLN
1	B	481	GLN
1	B	501	ASN
1	B	522	HIS
1	B	555	ASN
1	B	563	GLN
1	B	577	GLN
1	B	588	ASN
1	B	591	ASN
1	B	612	GLN
1	B	631	ASN
1	B	666	GLN
1	C	108	HIS
1	C	109	GLN
1	C	134	ASN
1	C	135	ASN
1	C	210	GLN
1	C	238	ASN
1	C	324	GLN
1	C	370	ASN
1	C	472	GLN
1	C	501	ASN

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Mol	Chain	Res	Type
1	C	555	ASN
1	C	613	GLN
1	C	653	ASN
1	C	679	ASN
1	C	703	ASN
1	C	714	ASN
1	C	772	GLN
1	C	790	GLN
1	D	134	ASN
1	D	208	ASN
1	D	229	ASN
1	D	238	ASN
1	D	385	ASN
1	D	391	ASN
1	D	501	ASN
1	D	522	HIS
1	D	532	ASN
1	D	543	GLN
1	D	555	ASN
1	D	613	GLN
1	D	676	ASN
1	D	679	ASN
1	D	682	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	0.34	0	5,5,5	0.28	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	0/0/0/0

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

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	846/901 (93%)	-0.32	6 (0%) 87 67	80, 116, 158, 196	0
1	B	842/901 (93%)	-0.32	1 (0%) 95 88	78, 111, 156, 210	0
1	C	787/901 (87%)	-0.09	30 (3%) 41 17	80, 141, 193, 219	0
1	D	836/901 (92%)	-0.31	4 (0%) 90 74	69, 127, 174, 204	0
All	All	3311/3604 (91%)	-0.26	41 (1%) 79 53	69, 122, 177, 219	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	771	ALA	5.2
1	C	68	HIS	3.7
1	C	726	SER	3.4
1	C	638	LEU	3.4
1	A	15	PHE	3.4
1	A	12	ASN	3.3
1	C	835	LEU	3.3
1	C	833	ALA	3.2
1	C	804	SER	3.0
1	C	798	LEU	3.0
1	C	628	ASN	3.0
1	C	725	LEU	3.0
1	C	728	GLU	3.0
1	C	637	VAL	2.9
1	C	676	ASN	2.8
1	A	518	PHE	2.8
1	C	703	ASN	2.8
1	C	43	ILE	2.7
1	D	417	LEU	2.7
1	A	747	LYS	2.6
1	C	787	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	153	PHE	2.5
1	C	680	PRO	2.5
1	C	539	LEU	2.4
1	C	839	ARG	2.4
1	C	721	ALA	2.3
1	C	634	LEU	2.3
1	C	32	LEU	2.2
1	C	592	LEU	2.2
1	A	777	TYR	2.2
1	C	658	PRO	2.2
1	C	549	GLN	2.2
1	C	729	LEU	2.2
1	D	774	LYS	2.1
1	C	651	ILE	2.1
1	A	534	LYS	2.1
1	B	6	TYR	2.0
1	C	683	LYS	2.0
1	D	818	LEU	2.0
1	C	837	ALA	2.0
1	C	706	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	B	1001	6/6	0.82	0.15	-	155,167,170,171	0

6.5 Other polymers

There are no such residues in this entry.