



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:02 AM UTC

PDB ID : 4JW1 / pdb_00004jw1
Title : Crystal structure of N-terminal 618-residue fragment of LepB from Legionella pneumophila
Authors : Hu, L.; Yao, Q.; Zhu, Y.; Shao, F.
Deposited on : 2013-03-26
Resolution : 3.16 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

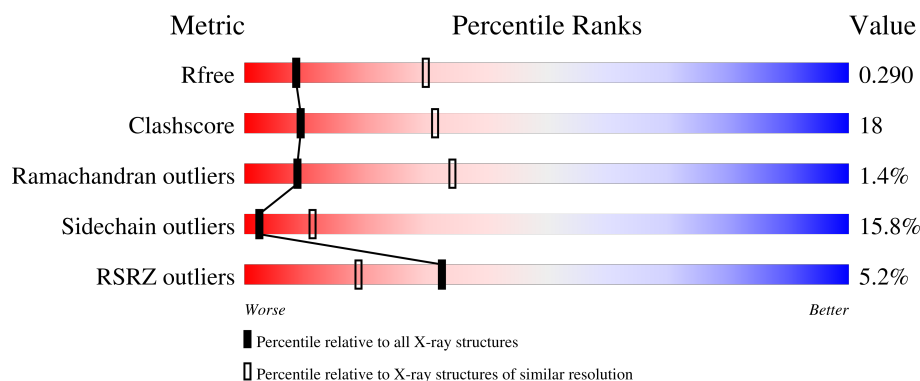
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	626	4% 50% 25% 7% 18%
1	B	626	3% 31% 17% • 49%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLC	A	702	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6745 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 Effector protein B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	Se	0	1	0
			4130	2679	676	758	7	10			
1	B	319	Total	C	N	O	S	Se	0	0	0
			2569	1670	426	467	4	2			

There are 22 discrepancies between the modelled and reference sequences:

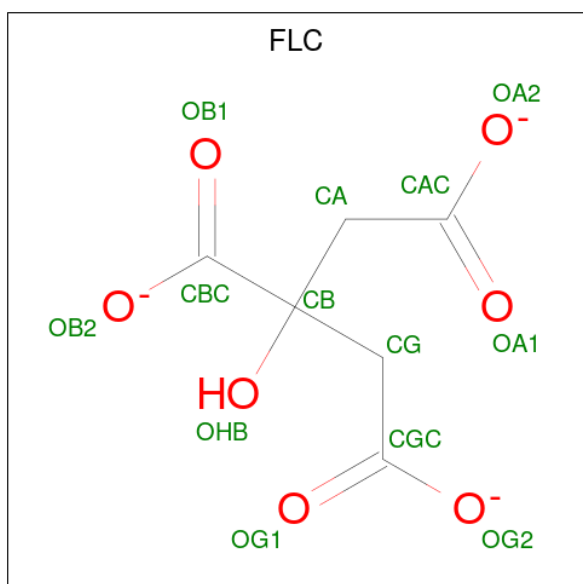
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP Q6X1Y7
A	-6	HIS	-	expression tag	UNP Q6X1Y7
A	-5	HIS	-	expression tag	UNP Q6X1Y7
A	-4	HIS	-	expression tag	UNP Q6X1Y7
A	-3	HIS	-	expression tag	UNP Q6X1Y7
A	-2	HIS	-	expression tag	UNP Q6X1Y7
A	-1	GLY	-	expression tag	UNP Q6X1Y7
A	0	PRO	-	expression tag	UNP Q6X1Y7
A	13	ALA	LYS	conflict	UNP Q6X1Y7
A	14	ALA	GLU	conflict	UNP Q6X1Y7
A	15	ALA	LYS	conflict	UNP Q6X1Y7
B	-7	HIS	-	expression tag	UNP Q6X1Y7
B	-6	HIS	-	expression tag	UNP Q6X1Y7
B	-5	HIS	-	expression tag	UNP Q6X1Y7
B	-4	HIS	-	expression tag	UNP Q6X1Y7
B	-3	HIS	-	expression tag	UNP Q6X1Y7
B	-2	HIS	-	expression tag	UNP Q6X1Y7
B	-1	GLY	-	expression tag	UNP Q6X1Y7
B	0	PRO	-	expression tag	UNP Q6X1Y7
B	13	ALA	LYS	conflict	UNP Q6X1Y7
B	14	ALA	GLU	conflict	UNP Q6X1Y7
B	15	ALA	LYS	conflict	UNP Q6X1Y7

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



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

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

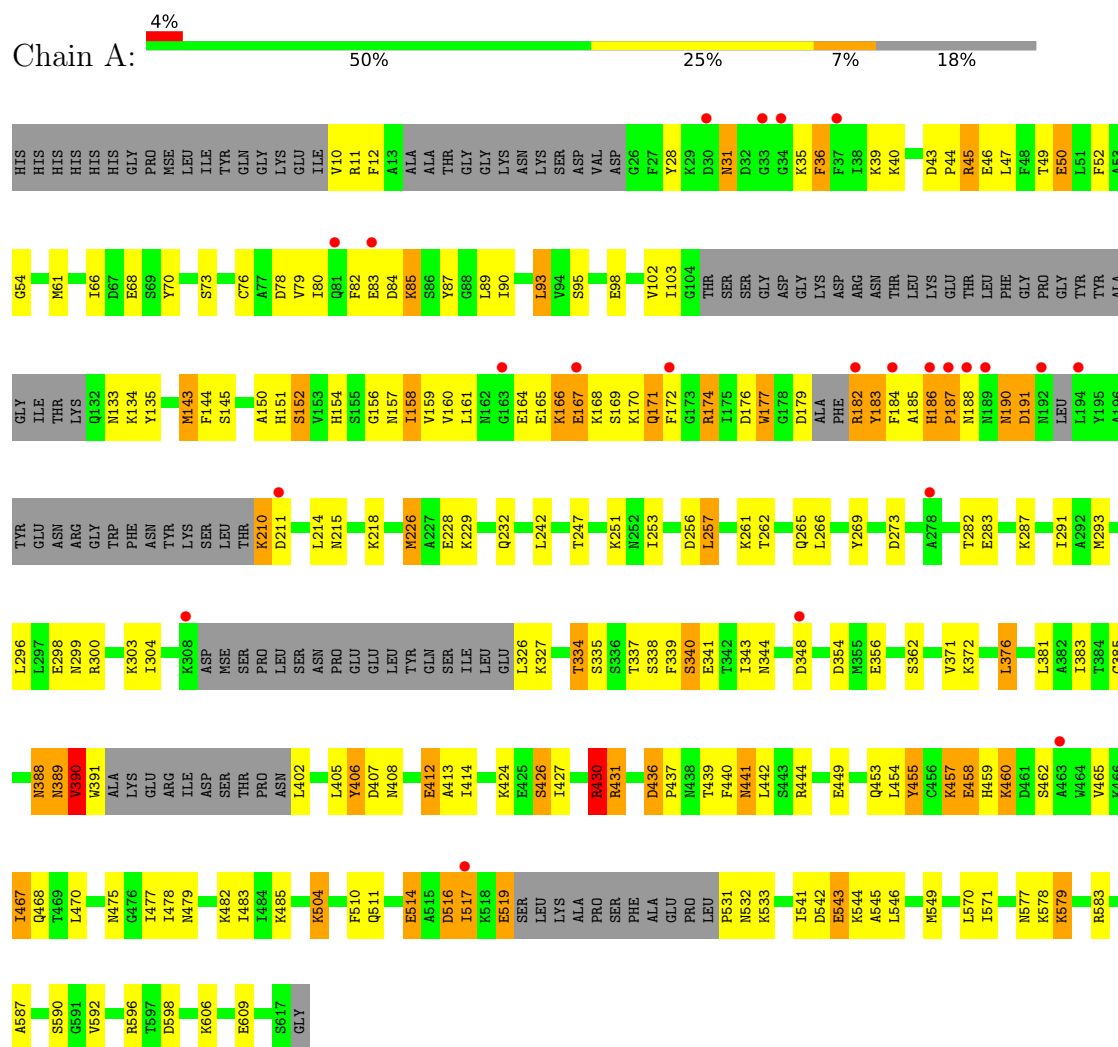
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	1	Total	O	0	0
			1	1		

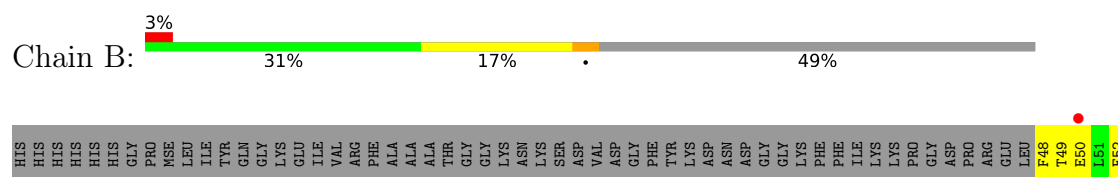
3 Residue-property plots

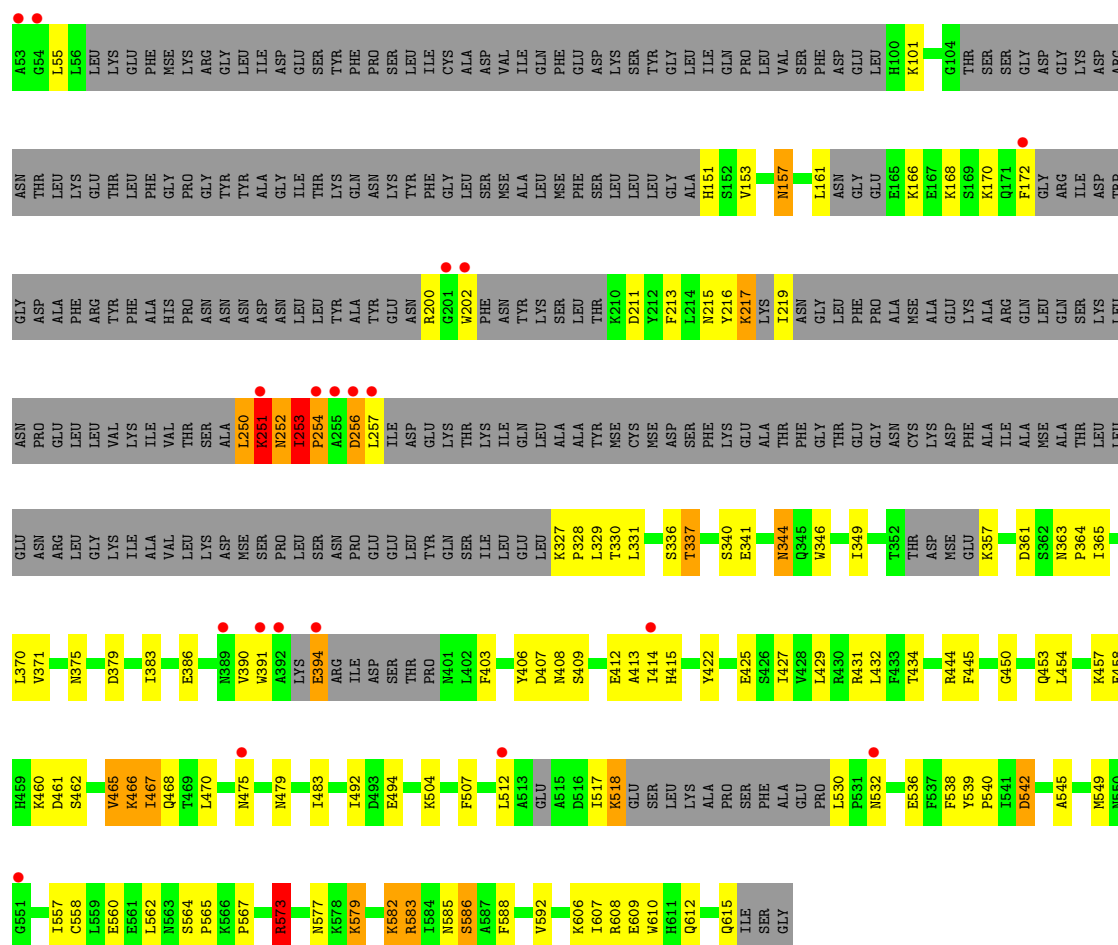
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Effector protein B





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	101.54Å 159.42Å 181.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 3.16 19.95 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.95-3.16) 99.0 (19.95-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.94 (at 3.15Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.264 , 0.283 0.251 , 0.290	Depositor DCC
R_{free} test set	1269 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	6745	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: FLC, 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	0.65	2/4207 (0.0%)	0.90	8/5644 (0.1%)
1	B	0.70	2/2615 (0.1%)	0.92	5/3512 (0.1%)
All	All	0.67	4/6822 (0.1%)	0.91	13/9156 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	424	LYS	C-O	-5.90	1.16	1.23
1	B	370	LEU	CA-C	-5.83	1.45	1.52
1	B	573	ARG	CA-C	-5.25	1.45	1.52
1	A	430	ARG	C-O	-5.03	1.18	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	LYS	N-CA-C	-9.62	100.47	112.88
1	A	167	GLU	N-CA-C	6.33	116.59	108.24
1	A	158	ILE	CA-C-N	-6.14	115.54	122.48
1	A	158	ILE	C-N-CA	-6.14	115.54	122.48
1	A	257	LEU	N-CA-C	5.97	118.27	111.11
1	A	436	ASP	CA-C-N	5.83	125.31	119.24
1	A	436	ASP	C-N-CA	5.83	125.31	119.24
1	B	532	ASN	N-CA-C	5.53	118.49	110.42
1	B	337	THR	N-CA-C	5.46	115.50	108.34
1	A	36	PHE	N-CA-C	5.38	117.37	109.24
1	B	253	ILE	CA-C-N	-5.33	113.18	119.84
1	B	253	ILE	C-N-CA	-5.33	113.18	119.84
1	A	356	GLU	N-CA-C	-5.22	108.67	114.62

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	4130	0	4151	166	0
1	B	2569	0	2573	77	0
2	A	6	0	8	0	0
2	B	24	0	32	0	0
3	A	13	0	5	2	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
All	All	6745	0	6769	244	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 18.

All (244) 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:B:168:LYS:NZ	1:B:172:PHE:CE2	1.88	1.34
1:A:431:ARG:CG	1:A:431:ARG:HH21	1.67	1.06
1:A:161:LEU:HD12	1:A:165:GLU:HG2	1.07	1.06
1:A:98:GLU:HA	1:A:159:VAL:HG12	1.38	1.05
1:A:431:ARG:HH21	1:A:431:ARG:HG2	1.20	1.05
1:A:390:VAL:HG22	1:A:391:TRP:H	1.21	1.01
1:A:161:LEU:CD1	1:A:165:GLU:HG2	1.89	1.01
1:A:174:ARG:HH11	1:A:174:ARG:CG	1.81	0.93
1:A:390:VAL:CG2	1:A:391:TRP:H	1.81	0.93
1:B:217:LYS:O	1:B:219:ILE:N	2.03	0.90
1:B:168:LYS:HZ1	1:B:172:PHE:HE2	0.93	0.88
1:A:431:ARG:HG2	1:A:431:ARG:NH2	1.85	0.87
1:B:151:HIS:O	1:B:151:HIS:ND1	2.07	0.86
1:B:549:MSE:O	1:B:583:ARG:NH1	2.10	0.84
1:B:200:ARG:NH1	1:B:200:ARG:HB2	1.94	0.82
1:A:389:ASN:OD1	1:A:389:ASN:N	2.13	0.81
1:A:247:THR:HG22	1:A:251:LYS:NZ	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ASP:O	1:B:466:LYS:NZ	2.12	0.81
1:A:470:LEU:HD22	1:A:517:ILE:HD13	1.61	0.81
1:A:247:THR:HG22	1:A:251:LYS:HZ1	1.46	0.80
1:B:168:LYS:NZ	1:B:172:PHE:CZ	2.50	0.79
1:B:256:ASP:OD1	1:B:256:ASP:N	2.12	0.78
1:A:444:ARG:NH1	1:A:449:GLU:OE1	2.16	0.78
1:B:573:ARG:HH11	1:B:573:ARG:HB3	1.48	0.78
1:A:174:ARG:HH11	1:A:174:ARG:HG2	1.47	0.77
1:A:161:LEU:HD12	1:A:165:GLU:CG	2.03	0.77
1:A:340:SER:O	1:A:344:ASN:ND2	2.17	0.77
1:A:449:GLU:O	1:A:453:GLN:HG3	1.85	0.77
1:B:394:GLU:OE2	1:B:425:GLU:HB2	1.84	0.77
1:B:585:ASN:OD1	1:B:608:ARG:NH1	2.20	0.75
1:A:543:GLU:OE1	1:A:544:LYS:N	2.19	0.75
1:A:390:VAL:HG22	1:A:391:TRP:N	2.00	0.74
1:B:394:GLU:OE1	1:B:394:GLU:N	2.21	0.74
1:A:427:ILE:O	1:A:430:ARG:HG3	1.88	0.73
1:B:168:LYS:NZ	1:B:172:PHE:CD2	2.48	0.73
1:B:391:TRP:H	1:B:391:TRP:CD1	2.06	0.72
1:A:174:ARG:HH11	1:A:174:ARG:HG3	1.54	0.72
1:B:200:ARG:HB2	1:B:200:ARG:HH11	1.51	0.72
1:B:151:HIS:CE1	1:B:172:PHE:CE2	2.78	0.71
1:A:183:TYR:HB3	1:A:184:PHE:HA	1.73	0.70
1:A:190:ASN:N	1:A:190:ASN:OD1	2.24	0.69
1:A:514:GLU:HA	1:A:517:ILE:HD12	1.74	0.69
1:A:532:ASN:O	1:A:533:LYS:NZ	2.25	0.69
1:A:12:PHE:HZ	1:A:35:LYS:HE2	1.59	0.68
1:B:394:GLU:N	1:B:394:GLU:CD	2.51	0.68
1:A:61:MSE:HG2	1:A:66:ILE:HD11	1.76	0.67
1:B:151:HIS:CE1	1:B:172:PHE:CD2	2.83	0.67
1:B:151:HIS:ND1	1:B:172:PHE:CE2	2.62	0.67
1:A:426:SER:O	1:A:430:ARG:CD	2.42	0.67
1:A:431:ARG:HH21	1:A:431:ARG:HG3	1.59	0.65
1:B:432:LEU:HD23	1:B:445:PHE:HB3	1.77	0.65
1:A:390:VAL:CG2	1:A:391:TRP:N	2.55	0.65
1:A:177:TRP:O	1:A:183:TYR:OH	2.15	0.64
1:A:247:THR:O	1:A:251:LYS:NZ	2.30	0.64
1:A:431:ARG:CG	1:A:431:ARG:NH2	2.39	0.64
1:B:48:PHE:HB2	1:B:50:GLU:HG3	1.78	0.63
1:A:485:LYS:HE2	3:A:702:FLC:HG1	1.80	0.63
1:A:174:ARG:CG	1:A:174:ARG:NH1	2.48	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:LEU:HD12	1:B:512:LEU:O	1.99	0.63
1:B:431:ARG:NH1	1:B:560:GLU:OE1	2.31	0.62
1:B:542:ASP:OD1	1:B:542:ASP:N	2.31	0.62
1:B:475:ASN:O	1:B:479:ASN:ND2	2.32	0.62
1:A:426:SER:O	1:A:430:ARG:HD2	2.00	0.61
1:A:412:GLU:OE1	1:A:413:ALA:N	2.34	0.61
1:B:168:LYS:CE	1:B:172:PHE:CE2	2.84	0.60
1:A:457:LYS:O	1:A:460:LYS:HG3	2.00	0.60
1:B:151:HIS:CE1	1:B:172:PHE:HE2	2.19	0.60
1:A:166:LYS:C	1:A:167:GLU:CG	2.75	0.59
1:A:166:LYS:C	1:A:167:GLU:HG2	2.28	0.59
1:A:174:ARG:HG3	1:A:174:ARG:NH1	2.16	0.59
1:B:215:ASN:OD1	1:B:216:TYR:N	2.36	0.59
1:B:371:VAL:O	1:B:375:ASN:ND2	2.29	0.59
1:B:379:ASP:O	1:B:383:ILE:HG12	2.02	0.58
1:B:327:LYS:HB3	1:B:328:PRO:HD3	1.85	0.58
1:A:408:ASN:O	1:A:408:ASN:ND2	2.34	0.58
1:A:183:TYR:CB	1:A:184:PHE:HA	2.33	0.58
1:A:215:ASN:ND2	1:A:218:LYS:NZ	2.51	0.58
1:A:215:ASN:ND2	1:A:218:LYS:HZ3	2.02	0.57
1:A:261:LYS:HE3	1:A:265:GLN:HE21	1.67	0.57
1:A:166:LYS:NZ	1:A:166:LYS:HB3	2.19	0.57
1:B:341:GLU:OE1	1:B:344:ASN:ND2	2.36	0.57
1:A:45:ARG:HG3	1:A:266:LEU:HD21	1.87	0.57
1:A:441:ASN:OD1	1:A:441:ASN:N	2.38	0.57
1:B:394:GLU:C	1:B:429:LEU:HD12	2.31	0.56
1:B:573:ARG:HB3	1:B:573:ARG:NH1	2.20	0.56
1:B:465:VAL:HA	1:B:468:GLN:HG2	1.87	0.56
1:A:184:PHE:HA	1:A:303:LYS:HZ2	1.71	0.55
1:A:371:VAL:HG22	1:A:478:ILE:HD13	1.88	0.55
1:B:391:TRP:H	1:B:391:TRP:HD1	1.54	0.55
1:A:511:GLN:HA	1:A:514:GLU:HG2	1.88	0.55
1:A:133:ASN:OD1	1:A:134:LYS:N	2.40	0.55
1:A:183:TYR:CD1	1:A:183:TYR:N	2.73	0.54
1:A:174:ARG:HA	1:A:177:TRP:CG	2.43	0.54
1:B:251:LYS:O	1:B:253:ILE:N	2.40	0.54
1:A:183:TYR:HB3	1:A:303:LYS:HZ2	1.73	0.54
1:B:582:LYS:O	1:B:586:SER:HB3	2.07	0.54
1:A:191:ASP:OD2	1:A:191:ASP:N	2.39	0.53
3:A:702:FLC:OHB	3:A:702:FLC:OG1	2.24	0.53
1:A:12:PHE:CZ	1:A:35:LYS:HE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TYR:HB3	1:A:166:LYS:HD3	1.91	0.53
1:A:287:LYS:O	1:A:291:ILE:HG12	2.09	0.53
1:A:152:SER:HB3	1:A:172:PHE:CZ	2.44	0.53
1:A:186:HIS:N	1:A:187:PRO:HD3	2.23	0.53
1:A:531:PRO:HD2	1:A:533:LYS:NZ	2.24	0.52
1:A:341:GLU:OE1	1:A:341:GLU:N	2.34	0.52
1:A:143:MSE:HG3	1:A:144:PHE:N	2.24	0.52
1:A:80:ILE:HD12	1:A:90:ILE:HD12	1.91	0.51
1:A:427:ILE:O	1:A:430:ARG:CG	2.58	0.51
1:B:151:HIS:CE1	1:B:172:PHE:HD2	2.28	0.51
1:A:458:GLU:CD	1:A:458:GLU:H	2.19	0.51
1:A:406:TYR:HD1	1:A:454:LEU:CD1	2.23	0.51
1:B:327:LYS:HG3	1:B:357:LYS:O	2.11	0.51
1:A:158:ILE:HG13	1:A:214:LEU:HD11	1.93	0.51
1:A:516:ASP:OD1	1:A:516:ASP:N	2.43	0.51
1:A:73:SER:HG	1:A:167:GLU:CD	2.19	0.50
1:A:28:TYR:HB2	1:A:36:PHE:HB2	1.93	0.50
1:A:87:TYR:OH	1:A:256:ASP:HB3	2.11	0.50
1:A:405:LEU:O	1:A:407:ASP:N	2.44	0.50
1:A:436:ASP:OD2	1:A:439:THR:OG1	2.29	0.50
1:A:402:LEU:HD23	1:A:402:LEU:O	2.12	0.50
1:A:179:ASP:O	1:A:182:ARG:N	2.45	0.50
1:A:215:ASN:HD22	1:A:218:LYS:HZ3	1.58	0.50
1:A:247:THR:HG22	1:A:251:LYS:HZ2	1.76	0.50
1:A:334:THR:OG1	1:A:335:SER:N	2.45	0.49
1:B:479:ASN:O	1:B:483:ILE:HG12	2.12	0.49
1:A:300:ARG:O	1:A:304:ILE:HG13	2.13	0.49
1:A:371:VAL:HG21	1:A:440:PHE:HD1	1.78	0.49
1:A:413:ALA:HB3	1:A:592:VAL:HG11	1.95	0.49
1:A:262:THR:HA	1:A:265:GLN:HB2	1.94	0.49
1:A:388:ASN:OD1	1:A:388:ASN:N	2.45	0.49
1:A:531:PRO:HD2	1:A:533:LYS:HZ3	1.77	0.49
1:B:504:LYS:O	1:B:507:PHE:HB2	2.13	0.49
1:B:391:TRP:CD1	1:B:391:TRP:N	2.80	0.48
1:B:202:TRP:H	1:B:202:TRP:CD1	2.30	0.48
1:A:73:SER:OG	1:A:167:GLU:CD	2.52	0.48
1:A:406:TYR:CD1	1:A:454:LEU:HD12	2.49	0.48
1:A:587:ALA:O	1:A:590:SER:OG	2.27	0.48
1:A:470:LEU:HB2	1:A:517:ILE:HD11	1.96	0.47
1:B:407:ASP:OD1	1:B:409:SER:OG	2.29	0.47
1:A:177:TRP:CE3	1:A:300:ARG:NH1	2.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:LEU:O	1:B:252:ASN:N	2.46	0.47
1:B:256:ASP:O	1:B:257:LEU:HD23	2.14	0.47
1:A:50:GLU:HG2	1:A:171:GLN:O	2.15	0.47
1:B:409:SER:HB2	1:B:414:ILE:HD11	1.97	0.47
1:A:45:ARG:NH1	1:A:269:TYR:CE1	2.83	0.47
1:A:52:PHE:HE2	1:A:293:MSE:HE3	1.80	0.47
1:A:326:LEU:HB3	1:A:327:LYS:H	1.49	0.47
1:A:577:ASN:OD1	1:A:578:LYS:N	2.48	0.47
1:A:577:ASN:OD1	1:A:579:LYS:N	2.36	0.47
1:B:462:SER:O	1:B:466:LYS:HG2	2.14	0.47
1:A:542:ASP:OD1	1:A:545:ALA:HB3	2.15	0.47
1:A:549:MSE:O	1:A:583:ARG:NH1	2.47	0.47
1:B:151:HIS:ND1	1:B:172:PHE:CD2	2.83	0.46
1:A:35:LYS:HG3	1:A:93:LEU:HD13	1.97	0.46
1:A:152:SER:O	1:A:152:SER:OG	2.29	0.46
1:B:330:THR:OG1	1:B:331:LEU:N	2.49	0.46
1:A:390:VAL:O	1:A:391:TRP:C	2.59	0.46
1:A:459:HIS:HB3	1:A:462:SER:HB2	1.96	0.46
1:A:577:ASN:OD1	1:A:579:LYS:HB2	2.16	0.46
1:A:143:MSE:HB3	1:A:226:MSE:HG2	1.97	0.46
1:B:413:ALA:HB3	1:B:592:VAL:HG11	1.98	0.46
1:A:261:LYS:HE3	1:A:265:GLN:NE2	2.30	0.46
1:B:48:PHE:CD1	1:B:48:PHE:C	2.94	0.46
1:A:174:ARG:HG2	1:A:174:ARG:NH1	2.20	0.45
1:A:40:LYS:HD3	1:A:82:PHE:HE2	1.81	0.45
1:A:296:LEU:O	1:A:300:ARG:HG3	2.16	0.45
1:B:518:LYS:HA	1:B:518:LYS:HD3	1.38	0.45
1:A:543:GLU:HG3	1:A:544:LYS:HD2	1.98	0.45
1:A:70:TYR:O	1:A:73:SER:HB2	2.16	0.45
1:A:11:ARG:HG2	1:A:12:PHE:N	2.29	0.45
1:A:102:VAL:HG23	1:A:103:ILE:HG23	1.99	0.44
1:A:183:TYR:N	1:A:183:TYR:HD1	2.14	0.44
1:A:402:LEU:HD23	1:A:402:LEU:C	2.42	0.44
1:A:170:LYS:HE2	1:A:170:LYS:HB2	1.76	0.44
1:A:228:GLU:O	1:A:232:GLN:HB2	2.17	0.44
1:A:362:SER:O	1:A:485:LYS:NZ	2.50	0.44
1:A:372:LYS:HB2	1:A:372:LYS:HE3	1.78	0.44
1:A:47:LEU:HD12	1:A:89:LEU:HG	1.98	0.44
1:A:381:LEU:HD23	1:A:381:LEU:HA	1.88	0.44
1:A:479:ASN:O	1:A:482:LYS:HB2	2.18	0.44
1:B:457:LYS:HA	1:B:460:LYS:NZ	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:CYS:HB3	1:B:607:ILE:HD13	2.00	0.44
1:B:504:LYS:HE3	1:B:504:LYS:HB3	1.78	0.43
1:A:517:ILE:O	1:A:519:GLU:N	2.39	0.43
1:A:542:ASP:OD1	1:A:542:ASP:C	2.59	0.43
1:A:152:SER:O	1:A:157:ASN:ND2	2.51	0.43
1:A:35:LYS:HG2	1:A:93:LEU:HD22	2.01	0.43
1:B:539:TYR:O	1:B:540:PRO:C	2.59	0.43
1:B:467:ILE:O	1:B:470:LEU:HB3	2.18	0.43
1:A:78:ASP:OD1	1:A:79:VAL:N	2.50	0.43
1:A:385:CYS:HB3	1:A:391:TRP:CZ2	2.54	0.43
1:A:177:TRP:HZ2	1:A:293:MSE:SE	2.51	0.43
1:B:432:LEU:CD2	1:B:445:PHE:HB3	2.47	0.43
1:A:158:ILE:HA	1:A:167:GLU:O	2.19	0.43
1:A:455:TYR:N	1:A:458:GLU:OE1	2.48	0.42
1:B:538:PHE:CE2	1:B:557:ILE:HG23	2.54	0.42
1:A:151:HIS:HB3	1:A:188:ASN:HD22	1.85	0.42
1:A:84:ASP:O	1:A:85:LYS:HB3	2.19	0.42
1:A:31:ASN:OD1	1:A:31:ASN:N	2.52	0.42
1:A:467:ILE:HG22	1:A:468:GLN:N	2.34	0.42
1:B:151:HIS:ND1	1:B:172:PHE:HE2	2.13	0.42
1:B:213:PHE:O	1:B:492:ILE:HG23	2.19	0.42
1:A:371:VAL:HG21	1:A:440:PHE:CD1	2.54	0.42
1:A:376:LEU:HD12	1:A:376:LEU:HA	1.80	0.42
1:A:406:TYR:CD1	1:A:454:LEU:CD1	3.02	0.42
1:A:253:ILE:HG23	1:A:257:LEU:HD22	2.01	0.42
1:A:457:LYS:HB2	1:A:458:GLU:H	1.71	0.42
1:B:331:LEU:HB3	1:B:346:TRP:CE2	2.55	0.42
1:A:215:ASN:OD1	1:A:215:ASN:C	2.63	0.42
1:A:546:LEU:HD12	1:A:546:LEU:O	2.19	0.42
1:A:457:LYS:HB2	1:A:458:GLU:OE1	2.20	0.41
1:A:210:LYS:HB3	1:A:210:LYS:HE3	1.28	0.41
1:B:406:TYR:HD1	1:B:454:LEU:HB2	1.85	0.41
1:A:510:PHE:O	1:A:514:GLU:HB3	2.20	0.41
1:A:405:LEU:C	1:A:407:ASP:H	2.27	0.41
1:A:154:HIS:H	1:A:157:ASN:HB2	1.85	0.41
1:A:183:TYR:C	1:A:185:ALA:H	2.29	0.41
1:A:596:ARG:NH1	1:A:598:ASP:OD2	2.53	0.41
1:A:54:GLY:HA2	1:A:76:CYS:HB2	2.02	0.41
1:A:98:GLU:OE2	1:A:156:GLY:O	2.38	0.41
1:A:43:ASP:OD1	1:A:44:PRO:HD2	2.21	0.41
1:A:150:ALA:HB1	1:A:168:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:THR:C	1:A:251:LYS:NZ	2.78	0.41
1:B:609:GLU:HA	1:B:612:GLN:HG2	2.01	0.41
1:B:415:HIS:HD2	1:B:444:ARG:HD3	1.85	0.41
1:B:450:GLY:O	1:B:453:GLN:HB2	2.21	0.41
1:B:577:ASN:OD1	1:B:579:LYS:HG3	2.21	0.41
1:A:145:SER:OG	1:A:168:LYS:HD2	2.21	0.41
1:A:160:VAL:HG12	1:A:161:LEU:O	2.21	0.41
1:A:504:LYS:HE3	1:A:504:LYS:HB3	1.93	0.41
1:A:606:LYS:O	1:A:609:GLU:HG2	2.21	0.41
1:A:339:PHE:O	1:A:343:ILE:HG12	2.21	0.41
1:B:157:ASN:HD22	1:B:157:ASN:HA	1.56	0.41
1:B:337:THR:HG21	1:B:341:GLU:HG2	2.03	0.41
1:B:564:SER:HA	1:B:565:PRO:HD3	1.94	0.41
1:B:454:LEU:N	1:B:454:LEU:HD23	2.35	0.40
1:A:341:GLU:O	1:A:344:ASN:HB2	2.22	0.40
1:B:606:LYS:HE2	1:B:610:TRP:CZ2	2.57	0.40
1:A:343:ILE:HD12	1:A:477:ILE:HD13	2.02	0.40
1:A:436:ASP:HA	1:A:437:PRO:HD3	1.90	0.40
1:A:242:LEU:HD13	1:A:298:GLU:HB2	2.03	0.40
1:A:426:SER:O	1:A:430:ARG:CG	2.69	0.40
1:B:363:ASN:N	1:B:364:PRO:HD2	2.35	0.40
1:B:422:TYR:OH	1:B:545:ALA:HB1	2.21	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	498/626 (80%)	465 (93%)	26 (5%)	7 (1%)	9	34
1	B	293/626 (47%)	267 (91%)	22 (8%)	4 (1%)	9	34
All	All	791/1252 (63%)	732 (92%)	48 (6%)	11 (1%)	9	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	LYS
1	A	187	PRO
1	A	390	VAL
1	B	251	LYS
1	A	211	ASP
1	A	406	TYR
1	A	455	TYR
1	B	252	ASN
1	A	457	LYS
1	B	567	PRO
1	B	254	PRO

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	446/526 (85%)	380 (85%)	66 (15%)	3	13
1	B	278/526 (53%)	230 (83%)	48 (17%)	2	9
All	All	724/1052 (69%)	610 (84%)	114 (16%)	2	11

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	31	ASN
1	A	39	LYS
1	A	45	ARG
1	A	46	GLU
1	A	49	THR
1	A	50	GLU
1	A	68	GLU
1	A	83	GLU
1	A	93	LEU
1	A	95	SER
1	A	143	MSE

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Mol	Chain	Res	Type
1	A	152	SER
1	A	164	GLU
1	A	166	LYS
1	A	169	SER
1	A	171	GLN
1	A	174	ARG
1	A	176	ASP
1	A	177	TRP
1	A	182	ARG
1	A	183	TYR
1	A	186	HIS
1	A	190	ASN
1	A	191	ASP
1	A	210	LYS
1	A	226	MSE
1	A	229	LYS
1	A	273	ASP
1	A	282	THR
1	A	283	GLU
1	A	299	ASN
1	A	334	THR
1	A	337	THR
1	A	338	SER
1	A	340	SER
1	A	348	ASP
1	A	354	ASP
1	A	376	LEU
1	A	383	ILE
1	A	388	ASN
1	A	389	ASN
1	A	390	VAL
1	A	412	GLU
1	A	414	ILE
1	A	426	SER
1	A	430	ARG
1	A	431	ARG
1	A	441	ASN
1	A	442	LEU
1	A	458	GLU
1	A	460	LYS
1	A	465	VAL
1	A	467	ILE

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Mol	Chain	Res	Type
1	A	475	ASN
1	A	483	ILE
1	A	504	LYS
1	A	514	GLU
1	A	516	ASP
1	A	517	ILE
1	A	519	GLU
1	A	541	ILE
1	A	543	GLU
1	A	570	LEU
1	A	571	ILE
1	A	579	LYS
1	B	49	THR
1	B	52	PHE
1	B	55	LEU
1	B	153	VAL
1	B	157	ASN
1	B	161	LEU
1	B	166	LYS
1	B	170	LYS
1	B	211	ASP
1	B	217	LYS
1	B	250	LEU
1	B	251	LYS
1	B	253	ILE
1	B	254	PRO
1	B	256	ASP
1	B	329	LEU
1	B	336	SER
1	B	340	SER
1	B	344	ASN
1	B	349	ILE
1	B	361	ASP
1	B	365	ILE
1	B	386	GLU
1	B	390	VAL
1	B	394	GLU
1	B	403	PHE
1	B	408	ASN
1	B	412	GLU
1	B	427	ILE
1	B	434	THR

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Mol	Chain	Res	Type
1	B	458	GLU
1	B	465	VAL
1	B	466	LYS
1	B	467	ILE
1	B	494	GLU
1	B	517	ILE
1	B	518	LYS
1	B	530	LEU
1	B	536	GLU
1	B	542	ASP
1	B	562	LEU
1	B	573	ARG
1	B	579	LYS
1	B	582	LYS
1	B	583	ARG
1	B	586	SER
1	B	588	PHE
1	B	615	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	HIS
1	A	265	GLN
1	A	373	GLN
1	B	157	ASN
1	B	479	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 oligosaccharides in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FLC	A	702	-	12,12,12	3.67	7 (58%)	17,17,17	2.72	6 (35%)
2	GOL	B	703	-	5,5,5	0.37	0	5,5,5	0.31	0
2	GOL	A	701	-	5,5,5	0.38	0	5,5,5	0.27	0
2	GOL	B	704	-	5,5,5	0.37	0	5,5,5	0.30	0
2	GOL	B	701	-	5,5,5	0.35	0	5,5,5	0.38	0
2	GOL	B	702	-	5,5,5	0.36	0	5,5,5	0.25	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
3	FLC	A	702	-	-	8/16/16/16	-
2	GOL	B	703	-	-	2/4/4/4	-
2	GOL	A	701	-	-	4/4/4/4	-
2	GOL	B	704	-	-	3/4/4/4	-
2	GOL	B	701	-	-	1/4/4/4	-
2	GOL	B	702	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FLC	CB-CBC	6.20	1.59	1.53
3	A	702	FLC	CG-CB	-5.99	1.46	1.54
3	A	702	FLC	CA-CB	5.69	1.61	1.54
3	A	702	FLC	OB1-CBC	4.30	1.35	1.22
3	A	702	FLC	OHB-CB	3.62	1.50	1.43
3	A	702	FLC	OB2-CBC	-3.25	1.18	1.30
3	A	702	FLC	CA-CAC	2.85	1.59	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FLC	OHB-CB-CBC	7.79	120.01	108.96
3	A	702	FLC	CG-CB-CBC	-4.52	100.05	110.03
3	A	702	FLC	CB-CG-CGC	-2.80	106.28	113.92
3	A	702	FLC	OG2-CGC-CG	2.74	123.02	114.35
3	A	702	FLC	OG1-CGC-CG	-2.43	116.07	122.95
3	A	702	FLC	CG-CB-CA	2.26	115.11	109.31

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	GOL	O1-C1-C2-C3
2	B	702	GOL	O1-C1-C2-C3
2	B	704	GOL	O1-C1-C2-C3
3	A	702	FLC	CAC-CA-CB-CBC
3	A	702	FLC	CBC-CB-CG-CGC
3	A	702	FLC	OHB-CB-CG-CGC
3	A	702	FLC	CA-CB-CG-CGC
2	A	701	GOL	O2-C2-C3-O3
3	A	702	FLC	CAC-CA-CB-OHB
2	A	701	GOL	C1-C2-C3-O3
2	B	701	GOL	C1-C2-C3-O3
2	B	703	GOL	O1-C1-C2-C3
2	B	704	GOL	O1-C1-C2-O2
3	A	702	FLC	CB-CA-CAC-OA2
3	A	702	FLC	CAC-CA-CB-CG
2	A	701	GOL	O1-C1-C2-O2
2	B	702	GOL	O1-C1-C2-O2
3	A	702	FLC	CB-CA-CAC-OA1
2	B	704	GOL	O2-C2-C3-O3
2	B	703	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	FLC	2	0

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	505/626 (80%)	0.31	23 (4%) 37 21	9, 36, 71, 104	1 (0%)
1	B	317/626 (50%)	0.59	20 (6%) 26 15	15, 47, 80, 92	0
All	All	822/1252 (65%)	0.41	43 (5%) 33 19	9, 41, 75, 104	1 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188	ASN	3.8
1	B	392	ALA	3.8
1	A	308	LYS	3.7
1	B	257	LEU	3.5
1	B	391	TRP	3.5
1	B	389	ASN	3.3
1	A	189	ASN	3.3
1	B	202	TRP	3.3
1	A	163	GLY	3.3
1	A	167	GLU	3.1
1	A	186	HIS	2.9
1	B	50	GLU	2.8
1	B	255	ALA	2.8
1	B	251	LYS	2.7
1	A	184	PHE	2.7
1	A	517	ILE	2.6
1	B	394	GLU	2.6
1	A	348	ASP	2.5
1	A	34	GLY	2.5
1	A	211	ASP	2.4
1	B	53	ALA	2.4
1	B	172	PHE	2.4
1	B	54	GLY	2.4
1	B	201	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	551	GLY	2.3
1	A	192	ASN	2.3
1	A	463	ALA	2.3
1	B	512	LEU	2.3
1	A	33	GLY	2.3
1	A	30	ASP	2.3
1	B	475	ASN	2.2
1	B	414	ILE	2.2
1	B	256	ASP	2.2
1	A	37[A]	PHE	2.2
1	A	194	LEU	2.1
1	A	182	ARG	2.1
1	B	254	PRO	2.1
1	B	532	ASN	2.1
1	A	81	GLN	2.1
1	A	278	ALA	2.0
1	A	187	PRO	2.0
1	A	172	PHE	2.0
1	A	83	GLU	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
2	GOL	B	704	6/6	0.73	0.15	49,52,73,78	0
2	GOL	B	702	6/6	0.83	0.12	36,51,55,65	0
2	GOL	B	703	6/6	0.86	0.12	35,58,65,66	0
2	GOL	B	701	6/6	0.86	0.14	21,38,43,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FLC	A	702	13/13	0.88	0.13	28,36,60,67	0
2	GOL	A	701	6/6	0.90	0.15	39,48,56,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.