



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:11 PM UTC

PDB ID : 7P2B / pdb_00007p2b
Title : Crystal structure of human gelsolin amyloid mutant A551P
Authors : Bollati, M.; de Rosa, M.
Deposited on : 2021-07-05
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

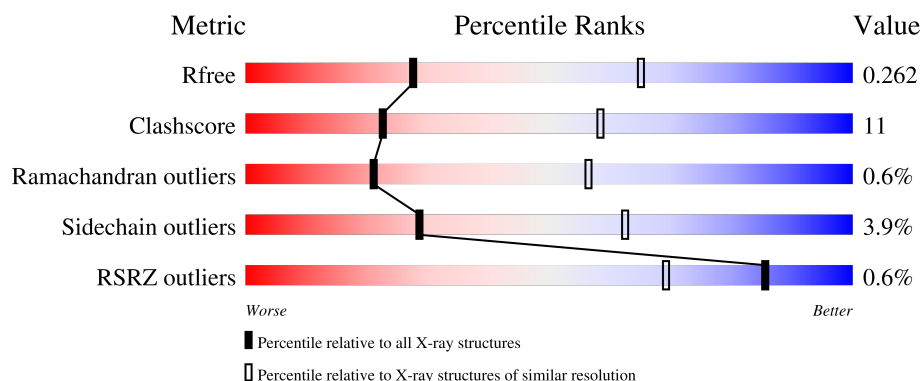
1 Overall quality at a glance

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	778	 69% 21% 8%
1	B	778	 70% 21% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11331 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 Gelsolin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	717	Total	C	N	O	S	9	1	0
			5607	3537	979	1075	16			
1	B	709	Total	C	N	O	S	3	0	0
			5537	3496	970	1055	16			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP P06396
A	-21	GLY	-	expression tag	UNP P06396
A	-20	SER	-	expression tag	UNP P06396
A	-19	SER	-	expression tag	UNP P06396
A	-18	HIS	-	expression tag	UNP P06396
A	-17	HIS	-	expression tag	UNP P06396
A	-16	HIS	-	expression tag	UNP P06396
A	-15	HIS	-	expression tag	UNP P06396
A	-14	HIS	-	expression tag	UNP P06396
A	-13	HIS	-	expression tag	UNP P06396
A	-12	SER	-	expression tag	UNP P06396
A	-11	SER	-	expression tag	UNP P06396
A	-10	GLY	-	expression tag	UNP P06396
A	-9	LEU	-	expression tag	UNP P06396
A	-8	VAL	-	expression tag	UNP P06396
A	-7	PRO	-	expression tag	UNP P06396
A	-6	ARG	-	expression tag	UNP P06396
A	-5	GLY	-	expression tag	UNP P06396
A	-4	SER	-	expression tag	UNP P06396
A	-3	HIS	-	expression tag	UNP P06396
A	-2	MET	-	expression tag	UNP P06396
A	-1	ALA	-	expression tag	UNP P06396
A	0	SER	-	expression tag	UNP P06396
A	551	PRO	ALA	engineered mutation	UNP P06396
B	-22	MET	-	initiating methionine	UNP P06396

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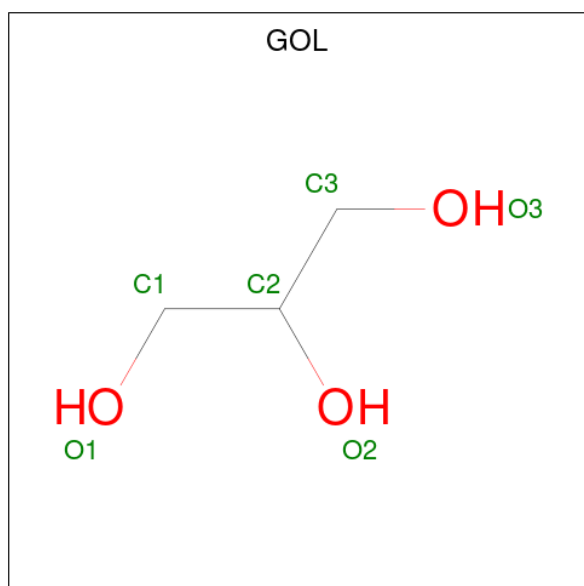
Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	GLY	-	expression tag	UNP P06396
B	-20	SER	-	expression tag	UNP P06396
B	-19	SER	-	expression tag	UNP P06396
B	-18	HIS	-	expression tag	UNP P06396
B	-17	HIS	-	expression tag	UNP P06396
B	-16	HIS	-	expression tag	UNP P06396
B	-15	HIS	-	expression tag	UNP P06396
B	-14	HIS	-	expression tag	UNP P06396
B	-13	HIS	-	expression tag	UNP P06396
B	-12	SER	-	expression tag	UNP P06396
B	-11	SER	-	expression tag	UNP P06396
B	-10	GLY	-	expression tag	UNP P06396
B	-9	LEU	-	expression tag	UNP P06396
B	-8	VAL	-	expression tag	UNP P06396
B	-7	PRO	-	expression tag	UNP P06396
B	-6	ARG	-	expression tag	UNP P06396
B	-5	GLY	-	expression tag	UNP P06396
B	-4	SER	-	expression tag	UNP P06396
B	-3	HIS	-	expression tag	UNP P06396
B	-2	MET	-	expression tag	UNP P06396
B	-1	ALA	-	expression tag	UNP P06396
B	0	SER	-	expression tag	UNP P06396
B	551	PRO	ALA	engineered mutation	UNP P06396

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

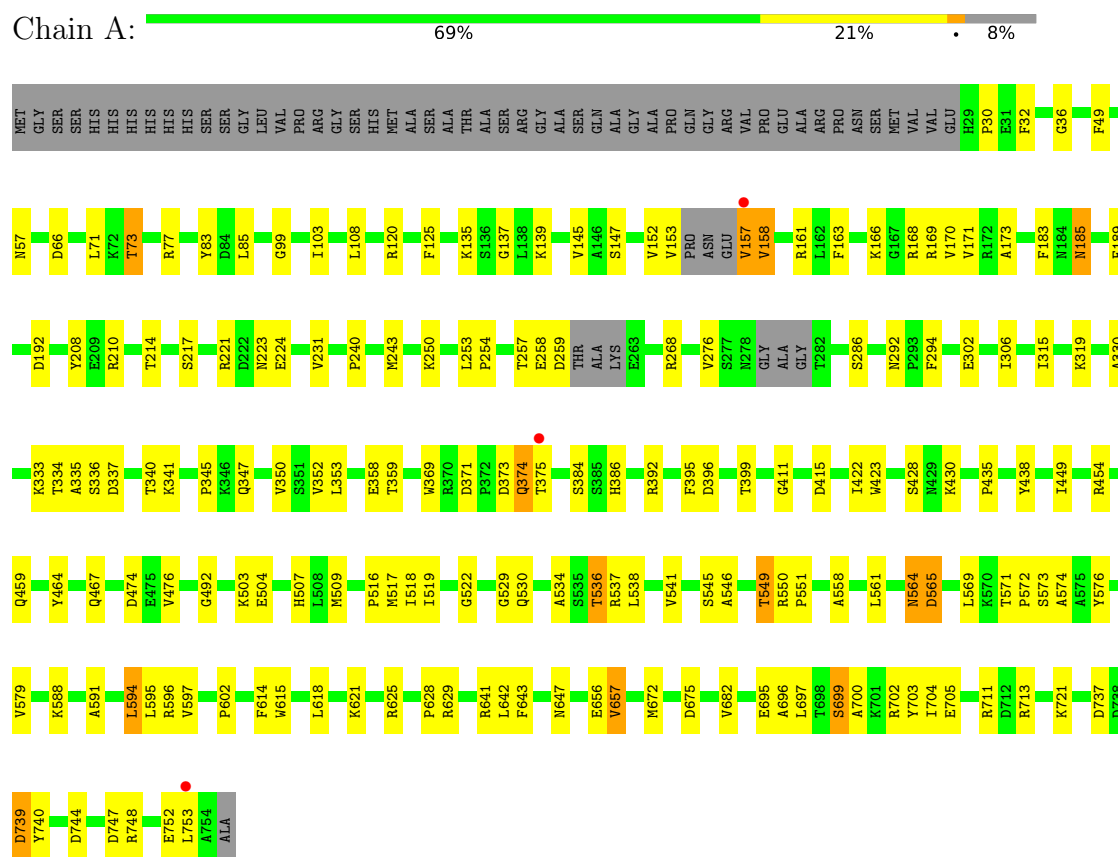
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	48	Total	O	0	0
			48	48		
5	B	55	Total	O	0	0
			55	55		

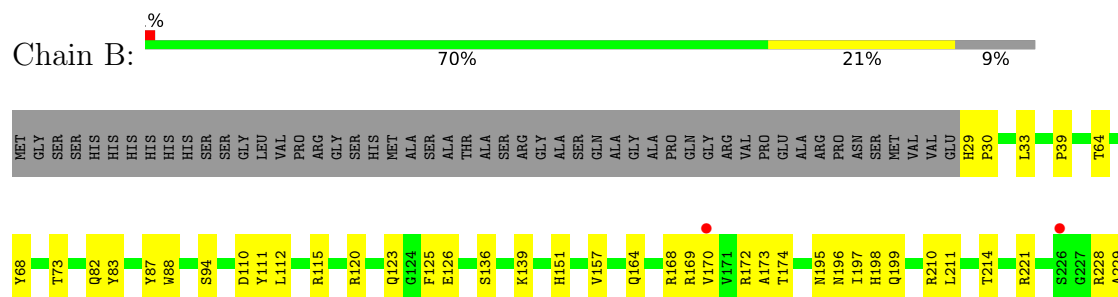
3 Residue-property plots [i](#)

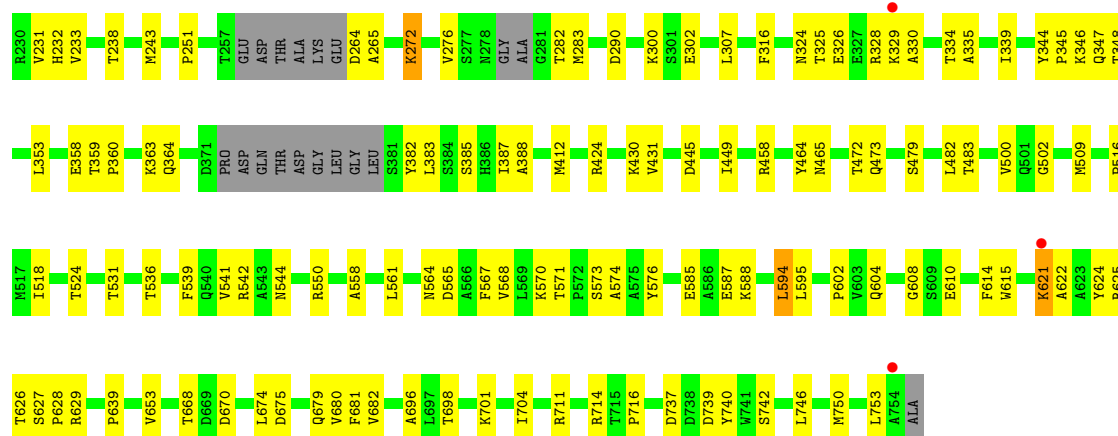
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Gelsolin



• Molecule 1: Gelsolin





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	170.07Å 170.07Å 152.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 3.00 19.91 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.91-3.00) 99.5 (19.91-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.98Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.213 , 0.263 0.213 , 0.262	Depositor DCC
R_{free} test set	2249 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11331	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: GOL, SO4, CL

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	0.13	0/5734	0.33	0/7766
1	B	0.17	0/5664	0.35	0/7671
All	All	0.15	0/11398	0.34	0/15437

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	5607	0	5450	121	0
1	B	5537	0	5395	113	0
2	A	20	0	0	1	0
2	B	15	0	0	1	0
3	A	30	0	40	1	0
3	B	18	0	24	1	0
4	B	1	0	0	0	0
5	A	48	0	0	1	0
5	B	55	0	0	2	0
All	All	11331	0	10909	233	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 11.

All (233) 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:325:THR:CG2	1:B:329:LYS:HE3	1.56	1.33
1:B:325:THR:CG2	1:B:329:LYS:CE	2.25	1.15
1:B:325:THR:HG23	1:B:329:LYS:HE3	1.21	1.14
1:B:325:THR:HG22	1:B:329:LYS:CE	1.83	1.08
1:B:325:THR:HG22	1:B:329:LYS:HE3	1.43	0.95
1:A:579:VAL:HG11	1:A:588:LYS:HE3	1.57	0.87
1:A:509:MET:HE3	1:A:550:ARG:HG2	1.60	0.82
1:B:325:THR:CG2	1:B:329:LYS:NZ	2.43	0.82
1:A:221:ARG:HH22	1:A:753:LEU:HB3	1.45	0.80
1:B:595:LEU:HD13	1:B:602:PRO:HB3	1.62	0.80
1:A:541:VAL:HG11	1:A:591:ALA:HB2	1.64	0.78
1:B:614:PHE:HD1	1:B:615:TRP:CD1	2.02	0.77
1:B:518:ILE:HD12	1:B:594:LEU:HD23	1.66	0.77
1:A:152:VAL:O	1:A:153:VAL:HG22	1.88	0.73
1:B:300:LYS:HE3	1:B:300:LYS:HA	1.69	0.73
1:A:737:ASP:HB3	1:A:740:TYR:HB2	1.71	0.72
1:A:169:ARG:HG2	1:A:657:VAL:HB	1.71	0.72
1:B:585:GLU:HA	1:B:588:LYS:HE2	1.72	0.71
1:A:161:ARG:HH11	1:A:163:PHE:HE2	1.36	0.71
1:B:325:THR:HG22	1:B:329:LYS:NZ	2.04	0.70
1:B:465:ASN:HB2	1:B:483:THR:HG21	1.72	0.69
1:A:713:ARG:H	1:A:713:ARG:HD2	1.57	0.69
1:A:152:VAL:O	1:A:153:VAL:CG2	2.42	0.68
1:B:558:ALA:HB3	1:B:622:ALA:HB3	1.75	0.68
1:B:614:PHE:HD1	1:B:615:TRP:HD1	1.40	0.68
1:A:319:LYS:HD2	1:A:352:VAL:HG12	1.77	0.67
1:B:604:GLN:CD	1:B:604:GLN:H	2.04	0.65
1:B:307:LEU:HB3	1:B:316:PHE:HB2	1.79	0.65
1:A:518:ILE:HG12	1:A:594:LEU:HD23	1.79	0.63
1:B:325:THR:HG21	1:B:329:LYS:NZ	2.13	0.63
1:B:272:LYS:NZ	1:B:290:ASP:OD1	2.31	0.62
1:A:516:PRO:HB3	1:A:549:THR:HG23	1.81	0.62
1:B:325:THR:HG22	1:B:329:LYS:CD	2.30	0.61
1:A:571:THR:HG23	1:A:573:SER:H	1.64	0.61
1:B:737:ASP:HB3	1:B:740:TYR:HB2	1.82	0.61
1:B:198:HIS:HB3	1:B:243:MET:HE3	1.82	0.61
1:B:126:GLU:OE1	1:B:172:ARG:NH1	2.33	0.61
1:B:221:ARG:HG3	1:B:229:ALA:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ASP:OD1	1:A:374:GLN:N	2.32	0.60
1:B:449:ILE:HB	1:B:464:TYR:HB2	1.84	0.60
1:B:196:ASN:HD22	1:B:232:HIS:HE1	1.49	0.60
1:B:570:LYS:NZ	1:B:571:THR:O	2.29	0.59
1:B:585:GLU:CD	1:B:585:GLU:H	2.09	0.59
1:A:369:TRP:NE1	1:A:371:ASP:OD1	2.35	0.59
1:B:625:ARG:NH2	1:B:627:SER:OG	2.36	0.59
1:B:568:VAL:HG11	1:B:594:LEU:HD12	1.84	0.58
1:A:595:LEU:HD13	1:A:602:PRO:HB3	1.85	0.58
1:A:504:GLU:HG2	1:A:517:MET:HE1	1.86	0.58
1:A:695:GLU:O	1:A:699:SER:OG	2.21	0.58
1:B:169:ARG:NH2	1:B:670:ASP:OD2	2.36	0.57
1:A:454:ARG:NH2	1:A:459:GLN:HE22	2.02	0.57
1:B:82:GLN:NE2	1:B:383:LEU:O	2.38	0.57
1:B:199:GLN:HE22	1:B:214:THR:HG22	1.70	0.57
1:A:152:VAL:C	1:A:153:VAL:HG22	2.29	0.57
1:A:517:MET:HE2	1:A:519:ILE:HD11	1.86	0.56
1:A:99:GLY:O	1:A:103:ILE:HG13	2.04	0.56
1:B:325:THR:HG22	1:B:329:LYS:HZ2	1.71	0.56
1:B:564:ASN:ND2	1:B:627:SER:O	2.39	0.55
1:A:530:GLN:H	1:A:530:GLN:CD	2.14	0.55
1:A:534:ALA:HB3	1:A:537:ARG:HG2	1.89	0.55
1:B:360:PRO:HD3	1:B:382:TYR:CD1	2.42	0.55
1:A:682:VAL:HG11	1:A:696:ALA:HB1	1.87	0.55
1:A:396:ASP:OD2	1:A:399:THR:HG22	2.06	0.55
1:A:335:ALA:HB1	1:A:350:VAL:HG21	1.89	0.55
1:A:330:ALA:O	1:A:334:THR:HG23	2.08	0.54
1:B:39:PRO:HA	1:B:73:THR:HB	1.90	0.54
1:B:502:GLY:O	1:B:550:ARG:NH1	2.41	0.54
1:A:516:PRO:HB2	1:A:551:PRO:HD3	1.90	0.53
1:B:211:LEU:HD13	1:B:746:LEU:HA	1.90	0.53
1:A:558:ALA:HA	1:A:618:LEU:HD13	1.89	0.53
1:A:166:LYS:NZ	1:A:259:ASP:H	2.07	0.53
1:A:739:ASP:OD1	1:A:739:ASP:N	2.40	0.53
1:A:139:LYS:NZ	1:A:224:GLU:OE2	2.42	0.52
1:A:503:LYS:NZ	5:A:901:HOH:O	2.41	0.52
1:B:110:ASP:OD1	1:B:111:TYR:N	2.42	0.52
1:A:395:PHE:CE2	1:A:546:ALA:HA	2.44	0.52
1:A:700:ALA:O	1:A:704:ILE:HG13	2.10	0.52
1:A:240:PRO:HD2	1:A:243:MET:HE3	1.91	0.52
1:B:509:MET:HE3	1:B:550:ARG:HE	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ARG:HD3	1:B:169:ARG:NH2	2.25	0.51
1:B:625:ARG:NH1	1:B:626:THR:H	2.09	0.51
1:A:454:ARG:HH21	1:A:459:GLN:HE22	1.58	0.51
1:A:641:ARG:NH2	2:A:802:SO4:O2	2.43	0.51
1:B:509:MET:SD	1:B:544:ASN:HB3	2.51	0.51
1:A:66:ASP:OD1	1:A:145:VAL:HG12	2.11	0.50
1:B:231:VAL:HB	1:B:753:LEU:HD12	1.93	0.50
1:B:542:ARG:HH21	1:B:629:ARG:HH11	1.58	0.50
1:A:641:ARG:NH1	1:A:656:GLU:OE2	2.44	0.50
1:B:68:TYR:CE2	1:B:151:HIS:HE1	2.29	0.50
1:B:680:VAL:HG21	1:B:704:ILE:HD11	1.94	0.50
1:B:516:PRO:HG2	1:B:518:ILE:HD11	1.92	0.50
1:A:36:GLY:HA2	1:A:73:THR:HG21	1.94	0.50
1:A:161:ARG:HD2	1:A:163:PHE:CE2	2.47	0.49
1:A:210:ARG:O	1:A:214:THR:HG23	2.12	0.49
1:B:360:PRO:O	1:B:364:GLN:HG3	2.12	0.49
1:B:675:ASP:OD2	1:B:711:ARG:NH1	2.36	0.49
1:A:415:ASP:OD1	1:A:415:ASP:N	2.39	0.49
1:A:641:ARG:NH1	1:A:641:ARG:HG2	2.27	0.49
1:B:68:TYR:HE2	1:B:151:HIS:HE1	1.59	0.49
1:A:221:ARG:HD3	1:A:231:VAL:HG23	1.94	0.49
1:A:596:ARG:HG2	1:A:596:ARG:HH11	1.78	0.49
1:A:641:ARG:HG2	1:A:641:ARG:HH11	1.76	0.49
1:B:387:ILE:HD13	1:B:639:PRO:HB3	1.95	0.48
1:A:422:ILE:HD12	1:A:449:ILE:HG12	1.95	0.48
1:A:337:ASP:HB3	1:A:341:LYS:HE2	1.95	0.48
1:A:449:ILE:HB	1:A:464:TYR:HB2	1.95	0.48
1:A:615:TRP:CD1	1:A:621:LYS:HD2	2.48	0.48
1:A:647:ASN:HD22	1:A:702:ARG:NH2	2.12	0.48
1:A:170:VAL:O	1:A:170:VAL:HG23	2.14	0.48
1:A:319:LYS:HD2	1:A:352:VAL:CG1	2.44	0.48
1:A:435:PRO:HA	1:A:438:TYR:CD1	2.48	0.48
1:A:642:LEU:HD23	1:A:657:VAL:HG11	1.95	0.48
1:B:87:TYR:CZ	1:B:120:ARG:HG3	2.49	0.48
1:B:29:HIS:N	1:B:30:PRO:HD2	2.29	0.47
1:A:675:ASP:OD1	1:A:711:ARG:NH2	2.43	0.47
1:B:561:LEU:HA	1:B:567:PHE:CZ	2.50	0.47
1:A:615:TRP:CG	1:A:621:LYS:HD2	2.49	0.47
1:A:675:ASP:CG	1:A:711:ARG:HH22	2.22	0.47
1:B:674:LEU:HB3	1:B:681:PHE:HB2	1.96	0.47
1:B:564:ASN:HB3	1:B:629:ARG:HE	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:GLY:O	1:A:721:LYS:HG3	2.15	0.47
1:B:330:ALA:O	1:B:334:THR:HG23	2.15	0.47
1:B:570:LYS:HD3	1:B:570:LYS:C	2.40	0.47
1:B:711:ARG:HE	3:B:805:GOL:H2	1.78	0.47
1:A:336:SER:O	1:A:340:THR:HG23	2.15	0.47
1:B:445:ASP:OD1	1:B:524:THR:OG1	2.23	0.47
1:A:77:ARG:CZ	1:A:392:ARG:HG3	2.45	0.47
1:A:564:ASN:OD1	1:A:628:PRO:HA	2.15	0.47
1:A:625:ARG:HE	1:A:625:ARG:HA	1.80	0.47
1:A:330:ALA:O	1:A:333:LYS:HB3	2.15	0.46
1:B:325:THR:CG2	1:B:329:LYS:HZ2	2.25	0.46
1:B:479:SER:O	1:B:483:THR:HG23	2.15	0.46
1:B:539:PHE:HB2	1:B:568:VAL:HG13	1.98	0.46
1:B:324:ASN:O	1:B:328:ARG:HG3	2.16	0.46
1:A:36:GLY:HA3	1:A:83:TYR:CE1	2.51	0.46
1:A:474:ASP:OD1	1:A:474:ASP:N	2.47	0.46
1:A:125:PHE:CD2	1:A:347:GLN:HG3	2.50	0.46
1:A:744:ASP:HB3	1:A:747:ASP:HB2	1.98	0.46
1:B:264:ASP:OD1	1:B:265:ALA:N	2.48	0.46
1:B:335:ALA:O	1:B:339:ILE:HG12	2.16	0.46
1:A:139:LYS:HG2	1:A:173:ALA:HB3	1.98	0.46
1:A:157:VAL:HB	1:A:158:VAL:H	1.64	0.46
1:B:197:ILE:HB	1:B:231:VAL:HG22	1.98	0.46
1:B:565:ASP:OD2	1:B:629:ARG:NH2	2.49	0.46
1:A:550:ARG:O	1:A:550:ARG:HG3	2.16	0.45
1:A:571:THR:HG22	1:A:574:ALA:O	2.17	0.45
1:B:325:THR:HG22	1:B:329:LYS:HD2	1.97	0.45
1:A:353:LEU:HD13	1:A:358:GLU:HA	1.98	0.45
1:B:500:VAL:HB	1:B:714:ARG:HB3	1.99	0.45
1:B:750:MET:HE3	1:B:750:MET:HB3	1.76	0.45
1:A:183:PHE:HA	1:A:189:PHE:CZ	2.52	0.44
1:A:268:ARG:NH2	1:A:703:TYR:O	2.50	0.44
1:A:423:TRP:HB3	1:A:430:LYS:HB3	2.00	0.44
1:B:325:THR:HG21	1:B:329:LYS:HZ1	1.82	0.44
1:B:458:ARG:NH1	5:B:905:HOH:O	2.50	0.44
1:A:85:LEU:HD21	1:A:108:LEU:HD23	1.99	0.44
1:A:430:LYS:HB2	1:A:430:LYS:HE2	1.84	0.44
1:A:185:ASN:HD22	1:A:253:LEU:HB2	1.83	0.44
1:B:324:ASN:HD21	1:B:326:GLU:HB2	1.82	0.44
1:A:569:LEU:HB3	1:A:576:TYR:HB2	2.00	0.44
1:B:112:LEU:O	1:B:115:ARG:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:LEU:HD21	1:B:388:ALA:HA	1.99	0.44
1:A:353:LEU:HD13	1:A:359:THR:H	1.83	0.44
1:A:315:ILE:HG13	1:A:350:VAL:HG23	1.99	0.44
1:A:168:ARG:HG3	1:A:208:TYR:HD2	1.82	0.44
1:B:571:THR:HG23	1:B:574:ALA:H	1.81	0.44
1:B:679:GLN:HB3	1:B:716:PRO:HG2	2.00	0.44
1:B:345:PRO:O	1:B:348:THR:OG1	2.31	0.43
1:B:412:MET:HB3	1:B:412:MET:HE3	1.76	0.43
1:A:135:LYS:HB3	1:A:135:LYS:HE3	1.80	0.43
1:A:384:SER:HB3	1:A:386:HIS:CD2	2.53	0.43
1:B:300:LYS:HB3	1:B:302:GLU:OE1	2.18	0.43
1:A:565:ASP:OD1	1:A:629:ARG:NH2	2.51	0.43
1:B:536:THR:HA	1:B:570:LYS:O	2.17	0.43
1:B:541:VAL:O	1:B:565:ASP:HB3	2.19	0.43
1:B:561:LEU:O	1:B:624:TYR:HB2	2.17	0.43
1:B:739:ASP:O	1:B:742:SER:OG	2.25	0.43
1:A:345:PRO:HB3	1:A:347:GLN:HE21	1.83	0.43
1:A:561:LEU:HD11	1:A:614:PHE:HZ	1.84	0.43
1:A:643:PHE:CE2	1:A:656:GLU:HB2	2.54	0.43
1:A:672:MET:HE3	1:A:672:MET:HB3	1.85	0.43
1:B:594:LEU:O	1:B:594:LEU:HD22	2.19	0.43
1:A:518:ILE:HA	1:A:551:PRO:HD2	2.01	0.42
1:B:344:TYR:O	1:B:346:LYS:NZ	2.50	0.42
1:A:250:LYS:HE3	1:A:250:LYS:HB3	1.78	0.42
1:A:257:THR:O	1:A:258:GLU:HG3	2.18	0.42
1:A:399:THR:O	1:A:399:THR:OG1	2.31	0.42
1:B:238:THR:O	1:B:238:THR:OG1	2.29	0.42
1:B:608:GLY:N	1:B:610:GLU:OE2	2.51	0.42
1:A:166:LYS:HZ3	1:A:259:ASP:H	1.66	0.42
1:B:614:PHE:CD1	1:B:615:TRP:CD1	2.93	0.42
1:A:71:LEU:HD13	1:A:85:LEU:HG	2.00	0.42
1:B:588:LYS:H	1:B:588:LYS:HG2	1.65	0.42
1:A:538:LEU:HD22	1:A:618:LEU:HD21	2.01	0.42
1:A:697:LEU:HD23	1:A:697:LEU:HA	1.82	0.42
1:B:164:GLN:NE2	2:B:801:SO4:O1	2.44	0.42
1:B:283:MET:HE3	1:B:283:MET:HB3	1.84	0.42
1:B:353:LEU:HD13	1:B:358:GLU:HA	2.00	0.42
1:A:503:LYS:HE2	3:A:807:GOL:H32	2.02	0.42
1:A:137:GLY:HA3	1:A:171:VAL:HG13	2.00	0.42
1:B:88:TRP:CZ2	1:B:123:GLN:HB2	2.55	0.42
1:A:292:ASN:HB3	1:A:294:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:PRO:HA	1:B:363:LYS:HE3	2.02	0.41
1:A:57:ASN:O	1:A:223:ASN:HB3	2.20	0.41
1:B:210:ARG:O	1:B:214:THR:HG23	2.20	0.41
1:B:682:VAL:HG11	1:B:696:ALA:HB1	2.02	0.41
1:A:32:PHE:CE1	1:A:108:LEU:HD13	2.55	0.41
1:A:536:THR:HG22	1:A:572:PRO:HD2	2.02	0.41
1:B:621:LYS:H	1:B:621:LYS:HG2	1.42	0.41
1:A:467:GLN:HB3	1:A:476:VAL:HG22	2.03	0.41
1:B:125:PHE:CD2	1:B:347:GLN:HB2	2.55	0.41
1:B:701:LYS:NZ	5:B:904:HOH:O	2.49	0.41
1:A:120:ARG:HB3	1:A:350:VAL:HG12	2.03	0.41
1:A:625:ARG:HA	1:A:625:ARG:NE	2.36	0.41
1:B:564:ASN:HD21	1:B:628:PRO:HA	1.85	0.41
1:A:152:VAL:C	1:A:153:VAL:CG2	2.92	0.41
1:B:139:LYS:HG2	1:B:173:ALA:HB3	2.03	0.41
1:B:430:LYS:HG2	1:B:482:LEU:HD13	2.03	0.41
1:A:541:VAL:HA	1:A:551:PRO:HA	2.02	0.41
1:B:424:ARG:O	1:B:431:VAL:HG22	2.21	0.40
1:B:73:THR:HG23	1:B:83:TYR:CE1	2.56	0.40
1:A:161:ARG:HG3	1:A:192:ASP:HB3	2.04	0.40
1:A:169:ARG:HE	1:A:169:ARG:HB2	1.78	0.40
1:A:748:ARG:HE	1:A:748:ARG:HB3	1.71	0.40
1:B:324:ASN:ND2	1:B:326:GLU:HB2	2.36	0.40
1:B:482:LEU:HD23	1:B:482:LEU:HA	1.91	0.40
1:A:158:VAL:HG13	1:B:157:VAL:HG21	2.03	0.40
1:A:340:THR:OG1	1:A:341:LYS:HD3	2.21	0.40
1:A:411:GLY:O	1:A:507:HIS:HB2	2.20	0.40
1:A:435:PRO:HA	1:A:438:TYR:CE1	2.57	0.40
1:A:594:LEU:O	1:A:597:VAL:HG22	2.21	0.40
1:B:359:THR:O	1:B:363:LYS:HG3	2.20	0.40
1:B:576:TYR:N	1:B:576:TYR:CD1	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	710/778 (91%)	664 (94%)	40 (6%)	6 (1%)	16	50
1	B	701/778 (90%)	669 (95%)	30 (4%)	2 (0%)	36	70
All	All	1411/1556 (91%)	1333 (94%)	70 (5%)	8 (1%)	21	56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	752	GLU
1	A	374	GLN
1	A	529	GLY
1	A	254	PRO
1	B	531	THR
1	B	251	PRO
1	A	522	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	588/630 (93%)	564 (96%)	24 (4%)	27	61
1	B	580/630 (92%)	558 (96%)	22 (4%)	29	63
All	All	1168/1260 (93%)	1122 (96%)	46 (4%)	28	62

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	PHE
1	A	73	THR
1	A	147	SER
1	A	157	VAL
1	A	158	VAL

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Mol	Chain	Res	Type
1	A	185	ASN
1	A	217	SER
1	A	276	VAL
1	A	286	SER
1	A	302	GLU
1	A	306	ILE
1	A	375	THR
1	A	428	SER
1	A	536	THR
1	A	545	SER
1	A	549	THR
1	A	564	ASN
1	A	565	ASP
1	A	594	LEU
1	A	657	VAL
1	A	699	SER
1	A	705[A]	GLU
1	A	705[B]	GLU
1	A	739	ASP
1	B	33	LEU
1	B	64	THR
1	B	94	SER
1	B	136	SER
1	B	170	VAL
1	B	174	THR
1	B	195	ASN
1	B	228	ARG
1	B	233	VAL
1	B	272	LYS
1	B	276	VAL
1	B	282	THR
1	B	385	SER
1	B	472	THR
1	B	473	GLN
1	B	573	SER
1	B	587	GLU
1	B	594	LEU
1	B	621	LYS
1	B	653	VAL
1	B	668	THR
1	B	698	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	196	ASN
1	A	386	HIS
1	A	419	GLN
1	A	455	HIS
1	A	459	GLN
1	A	485	GLN
1	A	689	GLN
1	B	29	HIS
1	B	75	GLN
1	B	151	HIS
1	B	196	ASN
1	B	198	HIS
1	B	232	HIS
1	B	364	GLN
1	B	461	GLN
1	B	638	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	801	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	B	802	-	4,4,4	0.24	0	6,6,6	0.08	0
3	GOL	A	806	-	5,5,5	0.87	0	5,5,5	1.14	0
3	GOL	B	805	-	5,5,5	0.96	0	5,5,5	1.00	0
2	SO4	B	803	-	4,4,4	0.24	0	6,6,6	0.07	0
3	GOL	B	807	-	5,5,5	0.94	0	5,5,5	1.07	0
3	GOL	B	806	-	5,5,5	0.91	0	5,5,5	1.14	1 (20%)
2	SO4	A	802	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	A	803	-	4,4,4	0.23	0	6,6,6	0.09	0
3	GOL	A	805	-	5,5,5	0.89	0	5,5,5	1.12	0
3	GOL	A	809	-	5,5,5	0.93	0	5,5,5	1.12	0
3	GOL	A	808	-	5,5,5	0.90	0	5,5,5	1.15	1 (20%)
2	SO4	B	801	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	A	804	-	4,4,4	0.24	0	6,6,6	0.07	0
3	GOL	A	807	-	5,5,5	0.88	0	5,5,5	1.08	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	GOL	B	805	-	-	4/4/4/4	-
3	GOL	B	807	-	-	0/4/4/4	-
3	GOL	B	806	-	-	2/4/4/4	-
3	GOL	A	805	-	-	0/4/4/4	-
3	GOL	A	809	-	-	0/4/4/4	-
3	GOL	A	808	-	-	2/4/4/4	-
3	GOL	A	806	-	-	2/4/4/4	-
3	GOL	A	807	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	808	GOL	C3-C2-C1	-2.04	104.30	111.80
3	B	806	GOL	C3-C2-C1	-2.04	104.33	111.80

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	806	GOL	C1-C2-C3-O3
3	A	808	GOL	C1-C2-C3-O3
3	B	805	GOL	C1-C2-C3-O3
3	B	805	GOL	O2-C2-C3-O3
3	A	808	GOL	O2-C2-C3-O3
3	B	805	GOL	O1-C1-C2-C3
3	B	806	GOL	C1-C2-C3-O3
3	A	806	GOL	O2-C2-C3-O3
3	B	806	GOL	O2-C2-C3-O3
3	B	805	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	805	GOL	1	0
2	A	802	SO4	1	0
2	B	801	SO4	1	0
3	A	807	GOL	1	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 [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	717/778 (92%)	-0.13	3 (0%)	88 76	43, 79, 130, 167	11 (1%)
1	B	709/778 (91%)	-0.17	5 (0%)	84 66	55, 79, 127, 184	3 (0%)
All	All	1426/1556 (91%)	-0.15	8 (0%)	85 69	43, 79, 129, 184	14 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	754	ALA	3.0
1	A	375	THR	2.5
1	A	157	VAL	2.5
1	B	329	LYS	2.5
1	B	621	LYS	2.5
1	B	170	VAL	2.1
1	B	226	SER	2.1
1	A	753	LEU	2.1

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
3	GOL	A	806	6/6	0.53	0.37	69,79,82,85	0
3	GOL	B	805	6/6	0.56	0.24	69,73,76,80	0
3	GOL	A	809	6/6	0.62	0.28	87,89,91,92	0
2	SO4	B	801	5/5	0.65	0.17	103,105,114,119	0
2	SO4	A	804	5/5	0.67	0.17	107,107,117,128	0
3	GOL	B	807	6/6	0.73	0.23	76,80,82,82	0
2	SO4	B	803	5/5	0.74	0.17	86,90,92,98	5
2	SO4	A	803	5/5	0.75	0.11	118,121,126,137	0
3	GOL	A	808	6/6	0.77	0.17	82,87,92,96	0
3	GOL	A	807	6/6	0.77	0.27	75,76,76,81	6
2	SO4	A	802	5/5	0.81	0.16	74,79,81,84	5
3	GOL	A	805	6/6	0.81	0.23	65,70,76,83	0
2	SO4	B	802	5/5	0.83	0.14	102,103,113,122	0
4	CL	B	804	1/1	0.87	0.07	95,95,95,95	0
3	GOL	B	806	6/6	0.91	0.15	57,61,67,68	0
2	SO4	A	801	5/5	0.93	0.14	77,79,88,89	5

6.5 Other polymers [i](#)

There are no such residues in this entry.