



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:49 PM UTC

PDB ID : 6Q9R / pdb_00006q9r
Title : Crystal structure of the pathological N184K variant of calcium-free human gelsolin
Authors : Scalone, E.; Boni, F.; Milani, M.; Eloise, M.; de Rosa, M.
Deposited on : 2018-12-18
Resolution : 2.73 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

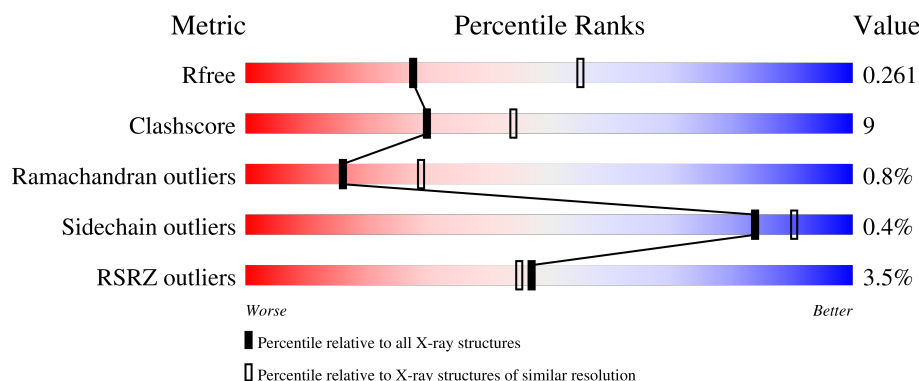
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	4% 74% 17% 8%
1	B	778	3% 74% 18% 8%

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	GOL	A	809	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11503 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	715	Total	C	N	O	S	0	0	0
			5578	3520	975	1067	16			
1	B	713	Total	C	N	O	S	0	0	0
			5564	3512	972	1064	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	184	LYS	ASN	engineered mutation	UNP P06396
B	-22	MET	-	initiating methionine	UNP P06396

Continued on next page...

Continued from previous page...

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	184	LYS	ASN	engineered mutation	UNP P06396

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total Cl 6 6	0	0
2	B	3	Total Cl 3 3	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



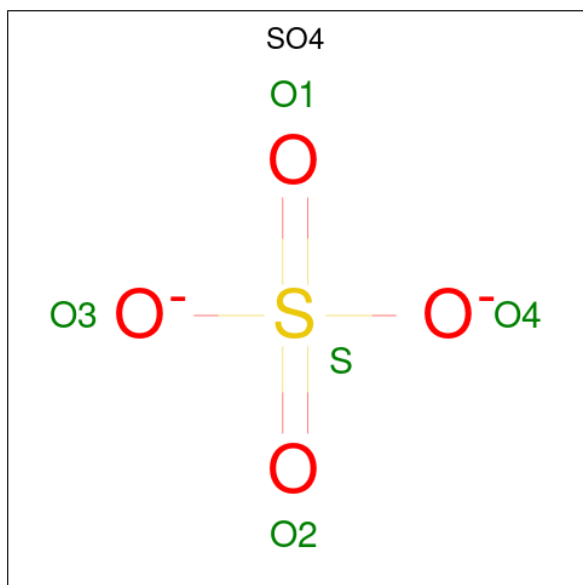
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total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

Continued on next page...

Continued from previous page...

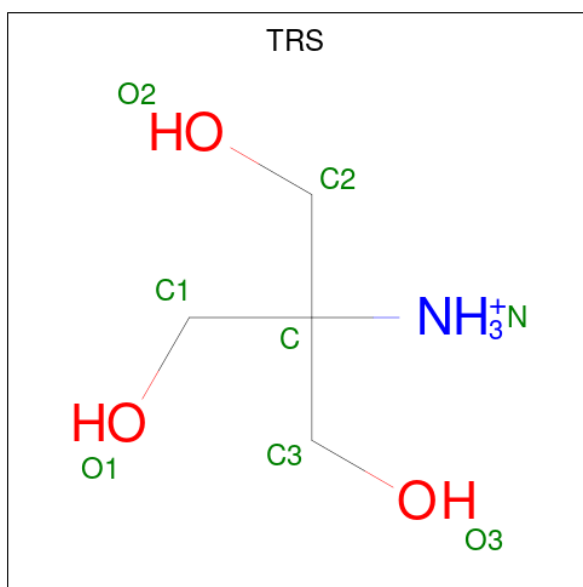
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			8	4	1	3		

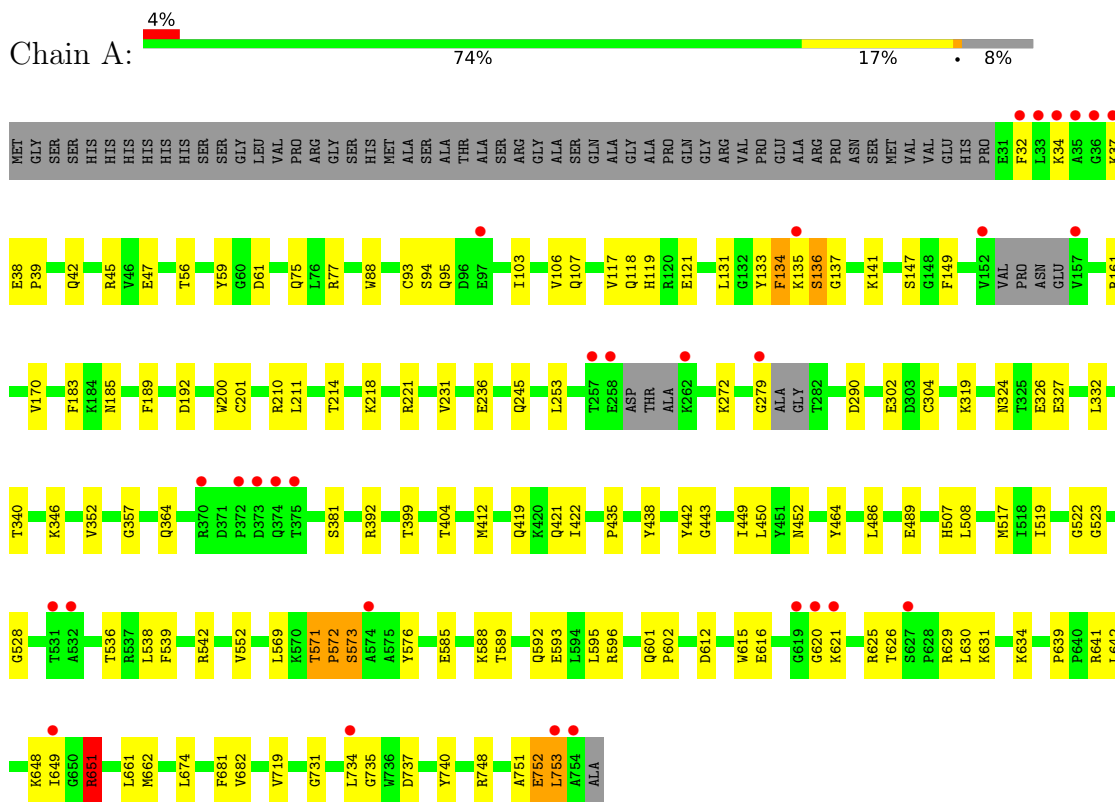
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	110	Total	O	0	0
			110	110		
6	B	122	Total	O	0	0
			122	122		

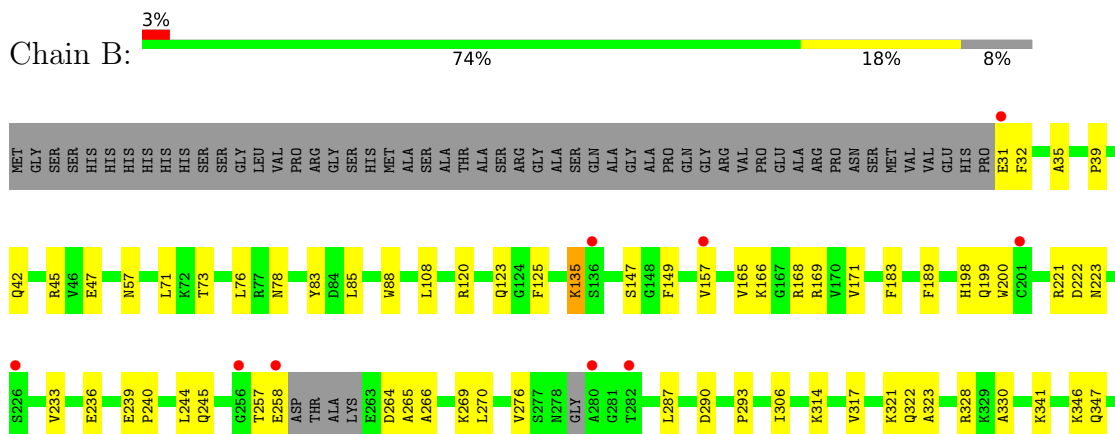
3 Residue-property plots [i](#)

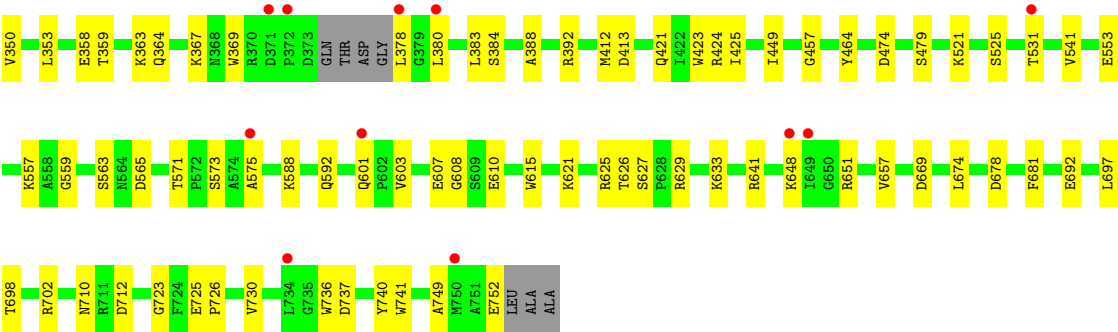
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	169.85Å 169.85Å 150.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.26 – 2.73 75.26 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.9 (75.26-2.73) 99.9 (75.26-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???), REFMAC	Depositor
R, R_{free}	0.213 , 0.260 0.214 , 0.261	Depositor DCC
R_{free} test set	2000 reflections (3.39%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11503	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL, TRS, 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	0.24	2/5702 (0.0%)	0.44	3/7717 (0.0%)
1	B	0.21	1/5689 (0.0%)	0.38	0/7702
All	All	0.22	3/11391 (0.0%)	0.41	3/15419 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	GLY	C-O	-6.55	1.16	1.23
1	B	330	ALA	C-O	-5.39	1.16	1.24
1	A	134	PHE	C-O	-5.25	1.17	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571	THR	CB-CA-C	-8.18	94.06	110.17
1	A	32	PHE	N-CA-C	5.52	115.13	107.73
1	A	136	SER	N-CA-C	-5.16	106.67	113.17

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	651	ARG	Sidechain

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	5578	0	5439	91	2
1	B	5564	0	5421	100	2
2	A	6	0	0	0	0
2	B	3	0	0	1	0
3	A	48	0	64	5	0
3	B	54	0	72	9	0
4	A	10	0	0	1	0
5	B	8	0	12	0	0
6	A	110	0	0	1	1
6	B	122	0	0	4	1
All	All	11503	0	11008	190	3

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 9.

All (190) 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:557:LYS:HD3	1:B:559:GLY:H	1.27	0.99
1:B:264:ASP:HB2	1:B:651:ARG:HH21	1.39	0.86
1:A:648:LYS:NZ	1:A:651:ARG:HG3	1.98	0.79
1:A:625:ARG:HE	1:A:626:THR:H	1.33	0.76
1:B:293:PRO:HB2	1:B:367:LYS:HG2	1.69	0.75
1:A:648:LYS:HZ3	1:A:651:ARG:HG3	1.52	0.73
1:B:323:ALA:O	1:B:328:ARG:NH1	2.23	0.70
1:A:595:LEU:HD13	1:A:602:PRO:HB3	1.74	0.70
1:A:536:THR:HG22	1:A:571:THR:HA	1.75	0.69
1:A:131:LEU:HD13	1:A:170:VAL:HG11	1.73	0.68
1:B:264:ASP:O	1:B:266:ALA:N	2.27	0.66
1:A:419:GLN:HB2	1:A:452:ASN:HD22	1.60	0.66
1:A:449:ILE:HB	1:A:464:TYR:HB2	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:LEU:HD23	1:A:634:LYS:HA	1.77	0.66
1:B:166:LYS:HE3	1:B:258:GLU:HB2	1.76	0.66
1:A:94:SER:OG	1:A:95:GLN:N	2.27	0.65
1:A:519:ILE:HD12	1:A:552:VAL:HG22	1.78	0.65
1:A:218:LYS:HE2	1:A:221:ARG:HH22	1.62	0.65
1:B:557:LYS:HD3	1:B:559:GLY:N	2.07	0.64
1:B:702:ARG:NH2	6:B:906:HOH:O	2.31	0.64
1:B:169:ARG:HD2	1:B:657:VAL:HG22	1.81	0.62
1:A:751:ALA:O	1:A:753:LEU:N	2.33	0.62
1:B:321:LYS:HG3	1:B:322:GLN:HG2	1.82	0.62
1:B:341:LYS:NZ	6:B:907:HOH:O	2.33	0.62
1:B:741:TRP:HB2	3:B:812:GOL:H32	1.83	0.61
1:A:737:ASP:HB3	1:A:740:TYR:HB2	1.81	0.61
1:B:588:LYS:O	1:B:592:GLN:HG3	2.00	0.61
1:B:120:ARG:HH22	1:B:346:LYS:HE3	1.66	0.61
1:A:625:ARG:HE	1:A:626:THR:N	2.00	0.60
1:B:737:ASP:HB3	1:B:740:TYR:HB2	1.83	0.59
1:A:37:LYS:HG3	1:A:42:GLN:HE22	1.66	0.59
1:A:542:ARG:HG3	1:A:629:ARG:HH21	1.68	0.59
1:B:625:ARG:HE	1:B:627:SER:H	1.50	0.59
1:A:508:LEU:HG	1:A:517:MET:HE1	1.85	0.58
1:A:75:GLN:NE2	6:A:901:HOH:O	2.36	0.58
1:A:682:VAL:HG13	1:A:719:VAL:HA	1.86	0.58
1:B:45:ARG:NH2	1:B:149:PHE:O	2.37	0.58
1:B:35:ALA:HA	1:B:42:GLN:HE22	1.70	0.57
1:A:641:ARG:NH2	4:A:815:SO4:O3	2.31	0.57
1:B:563:SER:OG	1:B:607:GLU:OE2	2.20	0.56
1:B:353:LEU:HD23	1:B:358:GLU:HA	1.86	0.56
1:B:269:LYS:HZ1	1:B:710:ASN:CG	2.13	0.56
1:B:425:ILE:HG13	1:B:479:SER:HB3	1.87	0.56
1:A:641:ARG:HE	3:A:809:GOL:H11	1.71	0.56
1:A:45:ARG:NH1	1:A:47:GLU:OE2	2.39	0.56
1:B:168:ARG:NH2	1:B:669:ASP:OD1	2.38	0.55
1:A:340:THR:HG22	1:A:346:LYS:HE2	1.87	0.55
1:B:565:ASP:OD2	1:B:629:ARG:NH2	2.39	0.55
1:A:200:TRP:CZ2	1:A:236:GLU:HG2	2.42	0.55
1:A:734:LEU:HG	1:A:735:GLY:N	2.22	0.54
1:B:31:GLU:OE2	1:B:32:PHE:N	2.29	0.54
1:A:662:MET:HA	1:A:734:LEU:CD2	2.37	0.54
1:A:629:ARG:NH1	3:A:807:GOL:O2	2.41	0.54
1:B:264:ASP:CG	1:B:651:ARG:HE	2.15	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:LEU:HD23	1:A:734:LEU:N	2.23	0.54
1:B:264:ASP:OD1	1:B:651:ARG:HB3	2.08	0.54
1:B:378:LEU:C	1:B:633:LYS:HE2	2.33	0.53
1:B:521:LYS:HB2	1:B:553:GLU:HG2	1.90	0.53
1:B:424:ARG:NH1	1:B:525:SER:OG	2.41	0.53
1:A:585:GLU:HG2	1:A:588:LYS:HE2	1.91	0.53
1:A:601:GLN:HG3	1:A:602:PRO:HD2	1.90	0.53
1:A:201:CYS:HB3	1:A:210:ARG:HD3	1.91	0.53
1:B:641:ARG:HH21	3:B:807:GOL:H32	1.74	0.52
1:A:45:ARG:NH2	1:A:149:PHE:O	2.42	0.52
1:A:218:LYS:HE2	1:A:221:ARG:NH2	2.24	0.52
1:A:399:THR:HG21	1:B:457:GLY:HA3	1.91	0.52
1:A:641:ARG:NE	3:A:809:GOL:H11	2.25	0.52
1:A:279:GLY:H	1:A:327:GLU:CD	2.18	0.52
1:A:571:THR:HB	1:A:572:PRO:HD2	1.92	0.52
1:B:314:LYS:NZ	6:B:917:HOH:O	2.43	0.51
1:A:538:LEU:HD12	1:A:539:PHE:H	1.75	0.51
1:B:629:ARG:NH1	2:B:802:CL:CL	2.81	0.51
1:B:120:ARG:HB3	1:B:350:VAL:HB	1.92	0.50
1:B:200:TRP:CZ2	1:B:236:GLU:HG2	2.46	0.50
1:A:648:LYS:HZ2	1:A:651:ARG:HG3	1.75	0.50
1:B:287:LEU:HD21	1:B:290:ASP:HB3	1.94	0.50
1:B:57:ASN:O	1:B:223:ASN:HB3	2.12	0.49
1:A:734:LEU:HD23	1:A:734:LEU:H	1.75	0.49
1:A:642:LEU:HB2	1:A:661:LEU:HD22	1.94	0.49
1:B:306:ILE:HD12	1:B:317:VAL:HG22	1.95	0.49
1:A:364:GLN:OE1	3:A:809:GOL:O1	2.23	0.48
1:A:593:GLU:HA	1:A:596:ARG:HD3	1.95	0.48
1:B:571:THR:HG23	1:B:573:SER:H	1.78	0.48
1:B:76:LEU:C	1:B:78:ASN:H	2.20	0.48
1:B:147:SER:HB2	1:B:149:PHE:HD1	1.78	0.48
1:A:61:ASP:HB3	1:A:141:LYS:HD2	1.96	0.48
1:B:183:PHE:HA	1:B:189:PHE:CZ	2.48	0.48
1:B:364:GLN:NE2	3:B:808:GOL:O1	2.37	0.48
1:B:723:GLY:HA3	3:B:812:GOL:H2	1.93	0.48
1:B:359:THR:O	1:B:363:LYS:HG3	2.13	0.48
1:B:413:ASP:OD1	1:B:726:PRO:HB2	2.14	0.48
1:B:425:ILE:HG13	1:B:479:SER:CB	2.43	0.48
1:B:346:LYS:NZ	6:B:922:HOH:O	2.47	0.47
1:A:38:GLU:HB2	1:A:39:PRO:HD2	1.96	0.47
1:B:363:LYS:HD2	1:B:369:TRP:CD1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:HG23	1:A:119:HIS:CE1	2.49	0.47
1:B:239:GLU:HG3	1:B:244:LEU:HD21	1.96	0.47
1:A:37:LYS:HG3	1:A:42:GLN:NE2	2.30	0.47
1:A:221:ARG:HD3	1:A:231:VAL:HG23	1.96	0.47
1:A:272:LYS:HG2	1:A:290:ASP:HA	1.97	0.47
1:A:748:ARG:O	1:A:752:GLU:HG2	2.15	0.47
1:B:71:LEU:HD11	1:B:83:TYR:HB3	1.95	0.47
1:B:384:SER:OG	3:B:807:GOL:H31	2.14	0.47
1:B:449:ILE:HB	1:B:464:TYR:HB2	1.96	0.47
1:A:662:MET:HA	1:A:734:LEU:HD21	1.97	0.46
1:B:678:ASP:HB2	3:B:809:GOL:H32	1.97	0.46
1:A:185:ASN:ND2	1:A:253:LEU:O	2.48	0.46
1:B:71:LEU:HD13	1:B:85:LEU:HG	1.97	0.46
1:B:603:VAL:O	1:B:603:VAL:HG23	2.16	0.46
1:A:422:ILE:HG23	1:A:449:ILE:HD13	1.98	0.46
1:B:541:VAL:O	1:B:565:ASP:HB3	2.16	0.45
1:B:674:LEU:HB3	1:B:681:PHE:HB2	1.97	0.45
1:A:585:GLU:O	1:A:589:THR:HG22	2.16	0.45
1:B:625:ARG:HE	1:B:626:THR:N	2.13	0.45
1:A:486:LEU:HA	1:A:489:GLU:HG2	1.99	0.45
1:A:412:MET:HE3	1:A:412:MET:HB3	1.81	0.45
1:A:56:THR:HA	1:A:59:TYR:CD1	2.51	0.45
1:B:575:ALA:O	1:B:603:VAL:HG22	2.17	0.45
1:B:641:ARG:HG3	3:B:808:GOL:H31	1.98	0.45
1:A:571:THR:HB	1:A:572:PRO:CD	2.44	0.45
1:A:118:GLN:HB2	1:A:352:VAL:HB	1.99	0.45
1:B:615:TRP:CD2	1:B:621:LYS:HB3	2.51	0.45
1:B:625:ARG:NE	1:B:627:SER:H	2.15	0.45
1:A:211:LEU:O	1:A:214:THR:OG1	2.35	0.44
1:B:165:VAL:HG13	1:B:171:VAL:HG21	1.99	0.44
1:B:35:ALA:HB1	1:B:71:LEU:HD23	1.99	0.44
1:B:135:LYS:HE3	1:B:135:LYS:HB2	1.53	0.44
1:B:221:ARG:NH1	1:B:222:ASP:OD1	2.48	0.44
1:B:712:ASP:HB2	3:B:806:GOL:H12	1.99	0.44
1:B:749:ALA:O	1:B:752:GLU:HB3	2.17	0.44
1:A:147:SER:HB2	1:A:149:PHE:HD2	1.83	0.43
1:A:625:ARG:NE	1:A:625:ARG:HA	2.32	0.43
1:A:37:LYS:CG	1:A:42:GLN:HE22	2.31	0.43
1:B:198:HIS:CE1	1:B:240:PRO:HG2	2.53	0.43
1:A:88:TRP:HA	1:A:121:GLU:O	2.19	0.43
1:A:304:CYS:HB3	1:A:319:LYS:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ASN:OD1	1:A:326:GLU:HB2	2.19	0.43
1:A:674:LEU:HB3	1:A:681:PHE:HB2	2.00	0.43
1:B:648:LYS:HD3	1:B:648:LYS:HA	1.73	0.43
1:A:616:GLU:HA	1:A:620:GLY:H	1.83	0.43
1:B:45:ARG:O	1:B:47:GLU:HG3	2.18	0.43
1:B:108:LEU:HD23	1:B:108:LEU:HA	1.86	0.43
1:B:276:VAL:CG1	1:B:306:ILE:HG12	2.49	0.43
1:A:183:PHE:HA	1:A:189:PHE:CZ	2.54	0.43
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.90	0.43
1:B:608:GLY:N	1:B:610:GLU:OE2	2.52	0.42
1:A:404:THR:O	1:A:731:GLY:HA3	2.19	0.42
1:B:730:VAL:HG13	1:B:736:TRP:CG	2.55	0.42
1:A:615:TRP:CE3	1:A:621:LYS:HB3	2.54	0.42
1:B:383:LEU:HD11	1:B:392:ARG:HH22	1.84	0.42
1:B:697:LEU:HD23	1:B:697:LEU:HA	1.86	0.42
1:A:625:ARG:NE	1:A:626:THR:H	2.10	0.42
1:A:106:VAL:HG23	1:A:332:LEU:HD12	2.01	0.42
1:B:648:LYS:NZ	1:B:692:GLU:OE2	2.52	0.42
1:A:357:GLY:HA2	1:A:381:SER:HB2	2.02	0.42
1:B:412:MET:HE3	1:B:412:MET:HB3	1.95	0.42
1:A:442:TYR:HD1	1:A:523:GLY:HA3	1.84	0.42
1:B:625:ARG:HE	1:B:626:THR:H	1.66	0.42
1:B:725:GLU:OE2	3:B:804:GOL:H12	2.20	0.41
1:A:103:ILE:O	1:A:107:GLN:HG3	2.21	0.41
1:B:169:ARG:HA	1:B:169:ARG:HD3	1.99	0.41
1:B:269:LYS:NZ	1:B:710:ASN:OD1	2.53	0.41
1:A:161:ARG:NH2	1:A:192:ASP:OD2	2.53	0.41
1:A:435:PRO:HA	1:A:438:TYR:CD1	2.55	0.41
1:A:34:LYS:HE2	1:A:34:LYS:H	1.85	0.41
1:A:569:LEU:HB3	1:A:576:TYR:HB2	2.03	0.41
1:B:76:LEU:HD23	1:B:76:LEU:HA	1.91	0.41
1:A:639:PRO:O	3:A:809:GOL:H12	2.20	0.41
1:B:125:PHE:CE2	1:B:347:GLN:HG2	2.55	0.41
1:B:199:GLN:HG2	1:B:233:VAL:HG13	2.01	0.41
1:B:601:GLN:H	1:B:601:GLN:HG3	1.67	0.41
1:A:464:TYR:OH	1:A:507:HIS:ND1	2.53	0.41
1:B:270:LEU:HD13	1:B:270:LEU:HA	1.93	0.41
1:A:443:GLY:HA3	1:A:522:GLY:H	1.86	0.41
1:A:592:GLN:O	1:A:596:ARG:HG3	2.20	0.41
1:B:76:LEU:O	1:B:78:ASN:N	2.48	0.41
1:B:421:GLN:HG2	1:B:423:TRP:CZ2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:698:THR:HG22	1:B:702:ARG:HD2	2.02	0.41
1:A:93:CYS:SG	1:A:94:SER:N	2.95	0.41
1:A:133:TYR:HB2	1:A:134:PHE:CE2	2.56	0.40
1:A:612:ASP:HA	1:A:615:TRP:HB2	2.02	0.40
1:A:302:GLU:H	1:A:302:GLU:CD	2.28	0.40
1:B:474:ASP:OD1	1:B:474:ASP:N	2.50	0.40
1:B:290:ASP:OD1	1:B:290:ASP:N	2.53	0.40
1:B:383:LEU:HD21	1:B:388:ALA:HA	2.03	0.40
1:B:565:ASP:CG	1:B:629:ARG:HH21	2.28	0.40
1:A:77:ARG:CZ	1:A:392:ARG:HG3	2.51	0.40
1:A:421:GLN:NE2	1:A:450:LEU:HD23	2.36	0.40
1:B:39:PRO:HA	1:B:73:THR:HB	2.03	0.40
1:B:88:TRP:CZ2	1:B:123:GLN:HB2	2.56	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:SER:OG	1:B:245:GLN:OE1[5_555]	2.18	0.02
6:A:921:HOH:O	6:B:937:HOH:O[5_555]	2.18	0.02
1:A:245:GLN:OE1	1:B:147:SER:OG[5_555]	2.19	0.01

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	707/778 (91%)	673 (95%)	28 (4%)	6 (1%)	16	29
1	B	705/778 (91%)	669 (95%)	31 (4%)	5 (1%)	18	32
All	All	1412/1556 (91%)	1342 (95%)	59 (4%)	11 (1%)	16	29

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	752	GLU
1	B	531	THR
1	A	573	SER
1	A	649	ILE
1	B	135	LYS
1	B	257	THR
1	B	265	ALA
1	A	631	LYS
1	A	528	GLY
1	A	753	LEU
1	B	157	VAL

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	583/629 (93%)	578 (99%)	5 (1%)	70	82
1	B	582/629 (92%)	582 (100%)	0	100	100
All	All	1165/1258 (93%)	1160 (100%)	5 (0%)	84	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LYS
1	A	136	SER
1	A	572	PRO
1	A	573	SER
1	A	651	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	75	GLN
1	A	118	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	206	ASN
1	A	368	ASN
1	A	421	GLN
1	A	452	ASN
1	A	455	HIS
1	A	465	ASN
1	A	467	GLN
1	A	592	GLN
1	A	647	ASN
1	B	118	GLN
1	B	195	ASN
1	B	204	ASN
1	B	349	GLN
1	B	364	GLN
1	B	429	ASN
1	B	459	GLN
1	B	461	GLN
1	B	467	GLN
1	B	638	HIS
1	B	647	ASN

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 29 ligands modelled in this entry, 9 are monoatomic - leaving 20 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	$\# Z > 2$
3	GOL	B	808	-	5,5,5	0.96	0	5,5,5	1.03	0
3	GOL	B	806	-	5,5,5	0.88	0	5,5,5	1.10	0
3	GOL	B	812	-	5,5,5	0.91	0	5,5,5	1.03	0
5	TRS	B	813	-	7,7,7	0.33	0	9,9,9	0.27	0
3	GOL	A	811	-	5,5,5	0.99	0	5,5,5	1.02	0
3	GOL	A	812	-	5,5,5	0.96	0	5,5,5	1.06	0
4	SO4	A	816	-	4,4,4	0.24	0	6,6,6	0.08	0
3	GOL	A	810	-	5,5,5	0.94	0	5,5,5	1.13	1 (20%)
3	GOL	B	807	-	5,5,5	0.93	0	5,5,5	1.02	0
3	GOL	B	804	-	5,5,5	0.93	0	5,5,5	1.08	0
4	SO4	A	815	-	4,4,4	0.23	0	6,6,6	0.10	0
3	GOL	A	809	-	5,5,5	0.91	0	5,5,5	1.08	0
3	GOL	A	813	-	5,5,5	0.93	0	5,5,5	1.05	0
3	GOL	B	810	-	5,5,5	0.93	0	5,5,5	1.06	0
3	GOL	A	807	-	5,5,5	0.91	0	5,5,5	1.05	0
3	GOL	A	814	-	5,5,5	0.91	0	5,5,5	1.07	0
3	GOL	A	808	-	5,5,5	0.92	0	5,5,5	1.15	0
3	GOL	B	811	-	5,5,5	0.95	0	5,5,5	1.07	0
3	GOL	B	809	-	5,5,5	0.93	0	5,5,5	1.04	0
3	GOL	B	805	-	5,5,5	0.92	0	5,5,5	1.09	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	808	-	-	0/4/4/4	-
3	GOL	A	809	-	-	2/4/4/4	-
3	GOL	B	806	-	-	2/4/4/4	-
3	GOL	B	812	-	-	1/4/4/4	-
5	TRS	B	813	-	-	2/9/9/9	-
3	GOL	A	811	-	-	2/4/4/4	-
3	GOL	A	812	-	-	0/4/4/4	-
3	GOL	A	810	-	-	1/4/4/4	-
3	GOL	A	813	-	-	0/4/4/4	-
3	GOL	B	807	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	807	-	-	2/4/4/4	-
3	GOL	A	814	-	-	4/4/4/4	-
3	GOL	B	804	-	-	1/4/4/4	-
3	GOL	B	810	-	-	2/4/4/4	-
3	GOL	A	808	-	-	2/4/4/4	-
3	GOL	B	809	-	-	0/4/4/4	-
3	GOL	B	805	-	-	2/4/4/4	-
3	GOL	B	811	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	810	GOL	C3-C2-C1	-2.07	104.21	111.80

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	807	GOL	O1-C1-C2-O2
3	A	807	GOL	O1-C1-C2-C3
3	A	808	GOL	C1-C2-C3-O3
3	A	809	GOL	O1-C1-C2-C3
3	A	814	GOL	O1-C1-C2-C3
3	A	814	GOL	C1-C2-C3-O3
3	B	805	GOL	C1-C2-C3-O3
3	B	807	GOL	O1-C1-C2-C3
3	B	807	GOL	C1-C2-C3-O3
3	B	810	GOL	C1-C2-C3-O3
3	B	810	GOL	O2-C2-C3-O3
3	A	811	GOL	C1-C2-C3-O3
3	B	806	GOL	C1-C2-C3-O3
3	A	811	GOL	O2-C2-C3-O3
3	A	814	GOL	O1-C1-C2-O2
3	A	814	GOL	O2-C2-C3-O3
3	A	808	GOL	O2-C2-C3-O3
3	B	807	GOL	O1-C1-C2-O2
3	A	809	GOL	O1-C1-C2-O2
3	B	805	GOL	O2-C2-C3-O3
3	B	806	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	812	GOL	O1-C1-C2-O2
3	B	804	GOL	O1-C1-C2-O2
3	B	807	GOL	O2-C2-C3-O3
5	B	813	TRS	C2-C-C1-O1
3	A	810	GOL	O2-C2-C3-O3
5	B	813	TRS	N-C-C1-O1

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	808	GOL	2	0
3	B	806	GOL	1	0
3	B	812	GOL	2	0
3	B	807	GOL	2	0
3	B	804	GOL	1	0
4	A	815	SO4	1	0
3	A	809	GOL	4	0
3	A	807	GOL	1	0
3	B	809	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

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	715/778 (91%)	0.17	30 (4%) 40 39	40, 57, 103, 134	0
1	B	713/778 (91%)	0.07	20 (2%) 55 52	36, 55, 97, 140	0
All	All	1428/1556 (91%)	0.12	50 (3%) 47 45	36, 56, 101, 140	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	VAL	4.7
1	A	753	LEU	4.4
1	B	258	GLU	4.1
1	A	36	GLY	3.9
1	A	620	GLY	3.8
1	A	754	ALA	3.7
1	B	734	LEU	3.6
1	B	136	SER	3.6
1	A	649	ILE	3.4
1	A	373	ASP	3.4
1	A	32	PHE	3.4
1	B	575	ALA	3.3
1	A	279	GLY	3.2
1	A	157	VAL	3.1
1	A	372	PRO	3.0
1	A	531	THR	2.9
1	A	258	GLU	2.9
1	B	280	ALA	2.9
1	B	649	ILE	2.8
1	B	372	PRO	2.7
1	B	226	SER	2.7
1	B	157	VAL	2.7
1	B	371	ASP	2.7
1	B	750	MET	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	380	LEU	2.7
1	A	375	THR	2.6
1	B	601	GLN	2.6
1	A	734	LEU	2.5
1	B	201	CYS	2.5
1	A	627	SER	2.4
1	A	374	GLN	2.4
1	B	648	LYS	2.4
1	B	31	GLU	2.4
1	B	531	THR	2.4
1	A	37	LYS	2.4
1	A	619	GLY	2.4
1	A	532	ALA	2.4
1	A	574	ALA	2.4
1	A	33	LEU	2.3
1	B	256	GLY	2.3
1	A	135	LYS	2.3
1	B	378	LEU	2.3
1	A	34	LYS	2.3
1	A	262	LYS	2.2
1	A	257	THR	2.2
1	B	282	THR	2.2
1	A	97	GLU	2.2
1	A	35	ALA	2.1
1	A	370	ARG	2.0
1	A	621	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	TRS	B	813	8/8	0.66	0.22	111,115,118,120	0
3	GOL	B	810	6/6	0.67	0.25	79,88,89,90	0
3	GOL	A	814	6/6	0.74	0.27	84,86,87,89	0
3	GOL	B	807	6/6	0.74	0.19	61,62,66,67	0
3	GOL	A	808	6/6	0.75	0.18	79,81,81,83	0
3	GOL	A	811	6/6	0.76	0.24	77,85,86,88	0
3	GOL	A	807	6/6	0.80	0.16	60,62,71,72	0
2	CL	B	803	1/1	0.82	0.27	104,104,104,104	0
4	SO4	A	815	5/5	0.85	0.17	71,73,78,83	0
3	GOL	B	812	6/6	0.85	0.21	91,95,99,105	0
3	GOL	B	811	6/6	0.86	0.20	78,81,83,85	0
2	CL	B	802	1/1	0.86	0.18	85,85,85,85	0
3	GOL	A	813	6/6	0.87	0.15	52,56,59,60	0
2	CL	A	805	1/1	0.89	0.10	82,82,82,82	0
3	GOL	B	809	6/6	0.91	0.22	74,75,79,80	0
3	GOL	B	804	6/6	0.91	0.13	66,68,70,70	0
3	GOL	B	808	6/6	0.91	0.14	62,67,76,79	0
4	SO4	A	816	5/5	0.93	0.09	76,76,77,80	0
2	CL	A	802	1/1	0.93	0.12	74,74,74,74	0
2	CL	B	801	1/1	0.94	0.16	72,72,72,72	0
3	GOL	A	809	6/6	0.94	0.10	56,62,70,74	0
2	CL	A	806	1/1	0.94	0.11	81,81,81,81	0
3	GOL	A	812	6/6	0.94	0.10	70,72,76,77	0
2	CL	A	801	1/1	0.95	0.09	72,72,72,72	0
2	CL	A	804	1/1	0.95	0.07	71,71,71,71	0
3	GOL	B	806	6/6	0.95	0.08	38,42,46,48	0
3	GOL	A	810	6/6	0.95	0.08	50,50,51,53	0
2	CL	A	803	1/1	0.96	0.11	79,79,79,79	0
3	GOL	B	805	6/6	0.97	0.07	43,44,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.