



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:46 PM UTC

PDB ID : 6Z9L / pdb_00006z9l
Title : Enterococcal PrgA
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Deposited on : 2020-06-04
Resolution : 3.06 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

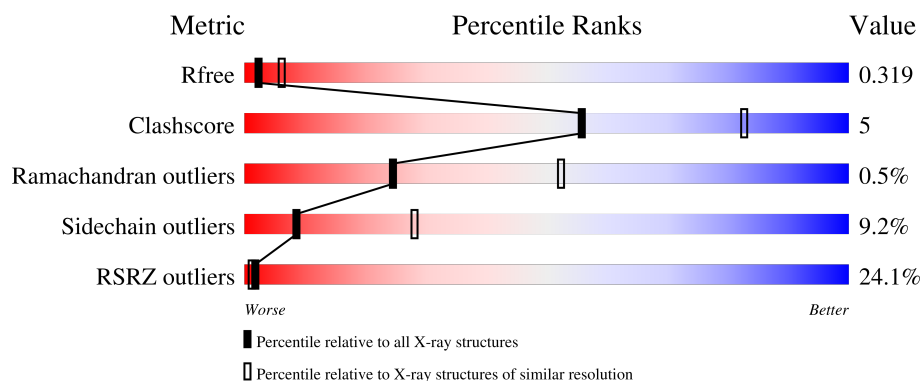
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	787	21% 77% 16% 5%
2	F	9	89% 100%
2	G	9	89% 100%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11803 atoms, of which 5855 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.

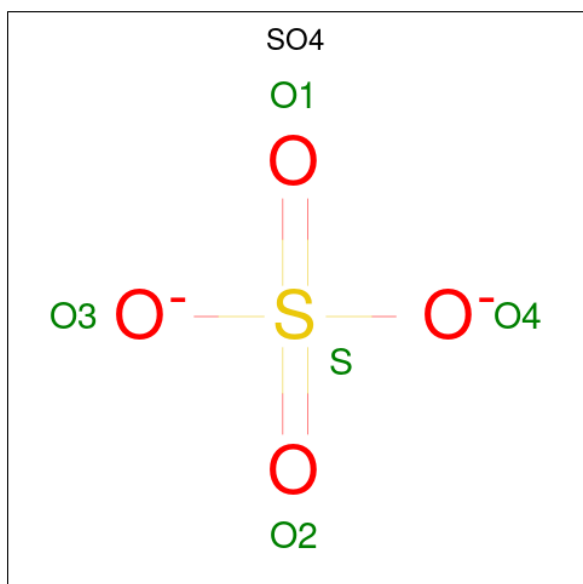
- Molecule 1 is a protein called PrgA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	744	Total	C	H	N	O	S	0	0	0
			11555	3532	5767	1013	1235	8			

- Molecule 2 is a protein called Poly-alanine peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	9	Total	C	H	N	O	0	0	0
			89	27	44	9	9			
2	G	9	Total	C	H	N	O	0	0	0
			89	27	44	9	9			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

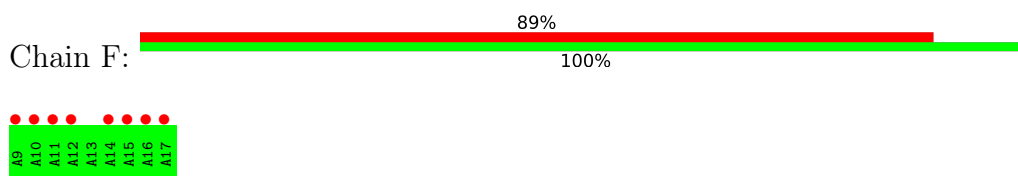
3 Residue-property plots

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: PrgA



• Molecule 2: Poly-alanine peptide



- Molecule 2: Poly-alanine peptide

Chain G:  89%
100%



A10	A11	A12	A13	A14	A15	A16	A17	A18
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4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	126.36Å 126.36Å 293.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.11 – 3.06 49.11 – 3.06	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.11-3.06) 99.5 (49.11-3.06)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.10.1	Depositor
R, R_{free}	0.286 , 0.318 0.293 , 0.319	Depositor DCC
R_{free} test set	2100 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	102.7	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 88.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11803	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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

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	0.14	0/5828	0.33	0/7840
2	F	0.10	0/44	0.25	0/60
2	G	0.05	0/44	0.19	0/60
All	All	0.14	0/5916	0.33	0/7960

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 [i](#)

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	5788	5767	5767	55	2
2	F	45	44	44	0	0
2	G	45	44	44	0	0
3	A	70	0	0	1	0
All	All	5948	5855	5855	55	2

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 5.

All (55) 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:A:341:PHE:HB3	1:A:342:PRO:CD	2.16	0.76
1:A:771:VAL:O	1:A:774:ASP:N	2.27	0.67
1:A:311:PRO:HB2	1:A:312:PRO:HD2	1.83	0.61
1:A:358:GLN:NE2	1:A:495:GLY:O	2.35	0.59
1:A:451:SER:O	1:A:454:THR:OG1	2.21	0.58
1:A:311:PRO:HB2	1:A:312:PRO:CD	2.36	0.55
1:A:475:TYR:O	1:A:479:HIS:ND1	2.39	0.53
1:A:367:GLU:OE1	1:A:452:LYS:NZ	2.29	0.52
1:A:501:SER:N	1:A:502:PRO:HD3	2.25	0.52
1:A:341:PHE:HB3	1:A:342:PRO:HD3	1.91	0.52
1:A:309:ASN:O	1:A:338:ASN:ND2	2.43	0.51
1:A:754:ALA:O	1:A:758:LEU:HD23	2.11	0.50
1:A:594:ALA:O	1:A:598:THR:HG23	2.11	0.50
1:A:94:GLN:O	1:A:98:VAL:HG23	2.12	0.50
1:A:95:GLN:O	1:A:98:VAL:HB	2.11	0.49
1:A:341:PHE:HB3	1:A:342:PRO:HD2	1.94	0.47
1:A:122:ALA:HA	1:A:125:VAL:HG12	1.95	0.47
1:A:401:ILE:HD12	1:A:507:ILE:HD12	1.96	0.47
1:A:87:ILE:HD11	1:A:747:ALA:HB1	1.96	0.46
1:A:489:LEU:HD13	1:A:490:GLY:N	2.31	0.46
1:A:463:LEU:O	1:A:467:LEU:HD22	2.16	0.46
1:A:118:VAL:O	1:A:121:GLU:HB3	2.17	0.45
1:A:310:LEU:HD21	1:A:382:LYS:HD3	1.98	0.45
1:A:290:GLN:O	1:A:294:THR:HG23	2.16	0.45
1:A:113:THR:O	1:A:116:GLN:HB3	2.17	0.44
1:A:73:LYS:HA	1:A:76:VAL:HG22	1.99	0.44
1:A:462:MET:HE2	1:A:504:ILE:HB	2.00	0.44
1:A:355:TRP:HA	1:A:355:TRP:CE3	2.53	0.44
1:A:221:LYS:HZ2	1:A:618:THR:CG2	2.31	0.44
1:A:500:ILE:C	1:A:502:PRO:HD3	2.44	0.43
1:A:307:GLY:O	1:A:460:ARG:NH2	2.51	0.43
1:A:661:GLN:O	1:A:665:LYS:HG2	2.18	0.43
1:A:80:ALA:HB2	1:A:758:LEU:HD21	2.01	0.43
1:A:706:GLN:HB2	1:A:707:PRO:HD3	2.01	0.43
1:A:768:TYR:CD1	1:A:768:TYR:N	2.85	0.43
1:A:402:ALA:HB2	1:A:492:SER:CB	2.49	0.43
1:A:83:GLU:OE1	1:A:83:GLU:N	2.52	0.42
1:A:162:VAL:O	1:A:166:GLN:HB2	2.20	0.42
1:A:698:SER:O	1:A:701:ARG:HB3	2.18	0.42
1:A:624:THR:O	1:A:627:GLU:HB3	2.20	0.42
1:A:83:GLU:O	1:A:87:ILE:HD13	2.19	0.42
1:A:302:LEU:O	1:A:305:HIS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ALA:O	1:A:670:THR:HG23	2.20	0.42
1:A:436:GLU:HB2	1:A:507:ILE:HD13	2.02	0.42
1:A:567:ASN:ND2	3:A:908:SO4:O3	2.52	0.41
1:A:91:VAL:HG13	1:A:92:LYS:N	2.36	0.41
1:A:134:ILE:O	1:A:138:LYS:HG3	2.20	0.41
1:A:748:THR:O	1:A:751:TYR:HB3	2.20	0.41
1:A:402:ALA:HB2	1:A:492:SER:HB2	2.02	0.41
1:A:768:TYR:N	1:A:768:TYR:HD1	2.18	0.41
1:A:311:PRO:HG2	1:A:330:LEU:CD1	2.50	0.41
1:A:366:LYS:O	1:A:370:VAL:HG23	2.20	0.41
1:A:398:ALA:HB1	1:A:492:SER:OG	2.21	0.41
1:A:778:GLN:HA	1:A:781:GLU:HB2	2.02	0.41
1:A:380:ARG:NH2	1:A:483:GLN:O	2.40	0.40

All (2) 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:404:TYR:O	1:A:419:LYS:NZ[8_665]	2.06	0.14
1:A:404:TYR:O	1:A:419:LYS:HZ1[8_665]	1.57	0.03

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	742/787 (94%)	711 (96%)	27 (4%)	4 (0%)	24	52
2	F	7/9 (78%)	7 (100%)	0	0	100	100
2	G	7/9 (78%)	7 (100%)	0	0	100	100
All	All	756/805 (94%)	725 (96%)	27 (4%)	4 (0%)	24	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	PRO
1	A	341	PHE
1	A	498	ASN
1	A	311	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	622/659 (94%)	565 (91%)	57 (9%)	8	28

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	69	ILE
1	A	72	GLN
1	A	83	GLU
1	A	107	GLN
1	A	123	LYS
1	A	128	GLU
1	A	141	VAL
1	A	150	GLU
1	A	155	VAL
1	A	161	ASP
1	A	200	LEU
1	A	274	LEU
1	A	281	LEU
1	A	292	GLN
1	A	302	LEU
1	A	303	LYS
1	A	308	ILE
1	A	335	LEU
1	A	341	PHE
1	A	355	TRP
1	A	368	LEU
1	A	375	LEU

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Mol	Chain	Res	Type
1	A	385	LEU
1	A	414	VAL
1	A	438	LEU
1	A	463	LEU
1	A	467	LEU
1	A	481	LEU
1	A	489	LEU
1	A	492	SER
1	A	493	LEU
1	A	500	ILE
1	A	514	LEU
1	A	534	LEU
1	A	556	GLN
1	A	559	ARG
1	A	580	LEU
1	A	605	VAL
1	A	615	LEU
1	A	622	LEU
1	A	625	ILE
1	A	629	ILE
1	A	636	LEU
1	A	643	VAL
1	A	649	ILE
1	A	659	GLU
1	A	670	THR
1	A	671	LEU
1	A	673	SER
1	A	690	VAL
1	A	692	LEU
1	A	746	VAL
1	A	749	LEU
1	A	763	LEU
1	A	773	ARG
1	A	789	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	766	GLN
1	A	797	GLN

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](#)

14 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	SO4	A	906	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	905	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	A	911	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	A	914	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	902	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	A	909	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	A	908	-	4,4,4	0.23	0	6,6,6	0.05	0
3	SO4	A	913	-	4,4,4	0.23	0	6,6,6	0.06	0
3	SO4	A	901	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	907	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	A	912	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	A	903	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	A	904	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	910	-	4,4,4	0.23	0	6,6,6	0.08	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	908	SO4	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	744/787 (94%)	1.31	168 (22%) 2 1	54, 106, 266, 514	0
2	F	9/9 (100%)	2.92	8 (88%) 0 0	188, 213, 227, 231	0
2	G	9/9 (100%)	2.59	8 (88%) 0 0	183, 219, 242, 250	0
All	All	762/805 (94%)	1.35	184 (24%) 2 1	54, 107, 265, 514	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	788	LEU	6.8
1	A	97	VAL	6.7
1	A	516	ASP	6.1
1	A	135	GLU	5.7
1	A	101	ASN	5.6
1	A	118	VAL	5.4
1	A	712	ALA	5.4
1	A	105	LEU	5.2
1	A	746	VAL	5.2
1	A	99	ASP	4.9
1	A	705	ALA	4.8
1	A	793	ALA	4.8
1	A	100	GLN	4.7
1	A	63	VAL	4.5
1	A	122	ALA	4.5
1	A	792	VAL	4.5
1	A	795	GLU	4.4
1	A	772	LEU	4.4
1	A	74	GLN	4.4
2	F	16	ALA	4.4
2	G	10	ALA	4.3
1	A	70	VAL	4.3
1	A	740	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	341	PHE	4.2
1	A	730	TYR	4.2
1	A	119	VAL	4.1
1	A	96	ALA	4.1
1	A	721	ALA	4.1
1	A	125	VAL	4.1
1	A	741	LYS	4.1
1	A	786	GLU	4.1
1	A	91	VAL	4.0
1	A	410	TYR	3.9
1	A	794	LYS	3.9
1	A	749	LEU	3.9
1	A	55	ALA	3.9
1	A	80	ALA	3.9
1	A	117	ALA	3.8
1	A	359	HIS	3.8
1	A	94	GLN	3.7
1	A	752	ALA	3.7
1	A	165	GLN	3.7
1	A	128	GLU	3.7
1	A	498	ASN	3.7
1	A	745	ALA	3.7
1	A	104	ALA	3.6
2	F	17	ALA	3.6
1	A	71	ASP	3.6
2	F	14	ALA	3.6
1	A	737	LEU	3.6
1	A	112	VAL	3.5
1	A	108	SER	3.4
1	A	73	LYS	3.4
1	A	747	ALA	3.4
1	A	771	VAL	3.4
1	A	709	TYR	3.3
1	A	743	GLN	3.3
1	A	518	SER	3.2
1	A	758	LEU	3.2
1	A	75	GLN	3.2
1	A	57	THR	3.2
1	A	729	ALA	3.2
1	A	780	ALA	3.2
1	A	748	THR	3.2
1	A	595	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	734	MET	3.2
1	A	129	ALA	3.2
2	F	9	ALA	3.2
1	A	791	GLN	3.1
1	A	779	GLN	3.1
1	A	751	TYR	3.1
1	A	777	ALA	3.0
1	A	56	ILE	3.0
1	A	86	ALA	3.0
1	A	98	VAL	3.0
1	A	775	LEU	2.9
1	A	342	PRO	2.9
1	A	785	GLN	2.9
1	A	627	GLU	2.9
1	A	744	GLN	2.9
1	A	66	LYS	2.9
1	A	300	GLU	2.9
1	A	306	LYS	2.9
1	A	72	GLN	2.9
1	A	109	GLN	2.9
2	G	18	ALA	2.9
1	A	81	LYS	2.8
1	A	617	GLN	2.8
1	A	754	ALA	2.8
1	A	121	GLU	2.8
1	A	638	LYS	2.8
1	A	120	ASP	2.8
2	G	13	ALA	2.7
1	A	87	ILE	2.7
1	A	665	LYS	2.7
1	A	724	VAL	2.7
1	A	67	GLN	2.7
1	A	111	ALA	2.7
1	A	787	ALA	2.7
1	A	716	LEU	2.7
1	A	624	THR	2.6
1	A	90	SER	2.6
1	A	713	LEU	2.6
2	F	15	ALA	2.6
2	G	16	ALA	2.6
1	A	139	GLU	2.6
1	A	62	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	796	GLN	2.6
1	A	293	ASN	2.6
1	A	64	THR	2.6
1	A	77	ALA	2.6
1	A	313	LYS	2.6
1	A	719	ALA	2.6
1	A	727	GLN	2.5
1	A	628	LEU	2.5
1	A	763	LEU	2.5
1	A	76	VAL	2.5
2	F	10	ALA	2.5
1	A	116	GLN	2.5
1	A	340	ASN	2.5
1	A	767	GLN	2.5
1	A	476	SER	2.4
1	A	637	GLU	2.4
1	A	708	THR	2.4
1	A	706	GLN	2.4
2	F	11	ALA	2.4
1	A	774	ASP	2.4
1	A	113	THR	2.4
1	A	472	ARG	2.4
1	A	222	GLU	2.4
1	A	78	ASP	2.4
1	A	106	ASP	2.4
1	A	343	THR	2.3
1	A	501	SER	2.3
1	A	92	LYS	2.3
1	A	407	THR	2.3
1	A	693	LYS	2.3
1	A	114	ASP	2.3
1	A	715	GLU	2.3
2	G	14	ALA	2.3
1	A	208	GLU	2.3
1	A	783	ARG	2.3
1	A	632	ARG	2.3
2	G	11	ALA	2.3
1	A	344	SER	2.3
1	A	768	TYR	2.3
1	A	352	ASP	2.3
1	A	131	PRO	2.2
1	A	79	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	82	LYS	2.2
1	A	511	LYS	2.2
1	A	672	ASN	2.2
1	A	782	GLN	2.2
1	A	302	LEU	2.2
1	A	301	GLU	2.2
1	A	765	LEU	2.2
1	A	468	PHE	2.2
1	A	126	VAL	2.2
1	A	68	ALA	2.2
1	A	707	PRO	2.2
1	A	168	VAL	2.1
1	A	755	GLN	2.1
1	A	346	GLU	2.1
2	G	12	ALA	2.1
1	A	145	THR	2.1
1	A	718	LYS	2.1
2	G	15	ALA	2.1
1	A	738	GLU	2.1
1	A	733	SER	2.1
1	A	59	LYS	2.1
1	A	136	LYS	2.1
1	A	596	LYS	2.1
1	A	670	THR	2.1
1	A	784	ARG	2.1
1	A	722	ALA	2.1
1	A	355	TRP	2.1
1	A	528	MET	2.1
1	A	710	GLU	2.1
1	A	759	SER	2.0
1	A	310	LEU	2.0
1	A	93	ASP	2.0
2	F	12	ALA	2.0
1	A	541	ASN	2.0
1	A	303	LYS	2.0

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

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
3	SO4	A	914	5/5	0.33	0.23	176,233,261,263	0
3	SO4	A	907	5/5	0.43	0.13	185,188,218,222	0
3	SO4	A	911	5/5	0.55	0.19	137,147,176,193	0
3	SO4	A	901	5/5	0.63	0.17	169,175,181,182	0
3	SO4	A	910	5/5	0.72	0.14	174,178,189,217	0
3	SO4	A	904	5/5	0.76	0.11	168,186,196,207	0
3	SO4	A	905	5/5	0.76	0.22	132,134,138,158	0
3	SO4	A	909	5/5	0.77	0.12	143,146,155,175	0
3	SO4	A	913	5/5	0.77	0.29	107,134,158,174	0
3	SO4	A	906	5/5	0.77	0.17	102,120,147,200	0
3	SO4	A	902	5/5	0.81	0.13	126,135,138,162	0
3	SO4	A	912	5/5	0.82	0.21	143,148,151,156	0
3	SO4	A	903	5/5	0.85	0.13	165,172,182,183	0
3	SO4	A	908	5/5	0.86	0.30	117,119,131,153	0

6.5 Other polymers [i](#)

There are no such residues in this entry.