



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:49 PM UTC

PDB ID : 3NV8 / pdb_00003nv8
Title : The structure of 3-deoxy-d-arabino-heptulosonate 7-phosphate synthase in complex with phosphoenol pyruvate and manganese (thesit-free)
Authors : Parker, E.J.; Jameson, G.B.; Jiao, W.; Hutton, R.H.; Webby, C.J.; Baker, E.N.; Baker, H.M.
Deposited on : 2010-07-08
Resolution : 2.25 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

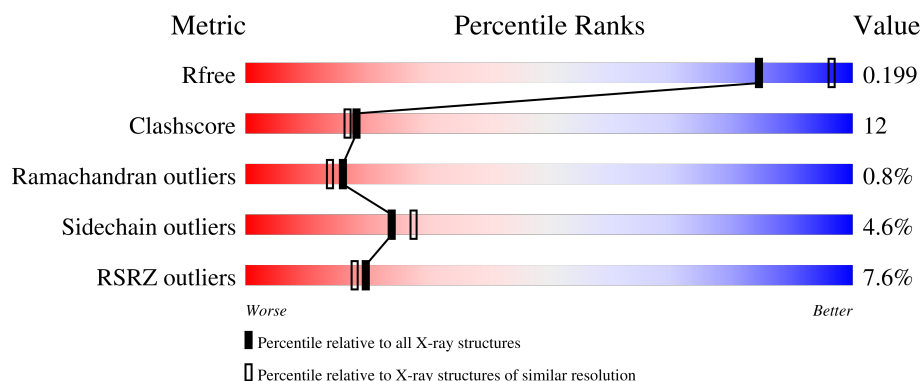
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	464	7% 75% 21% .
1	B	464	8% 77% 20% .

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
2	SO4	A	463	-	-	X	-
4	GOL	B	467	-	X	-	-
4	GOL	B	469	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7534 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.

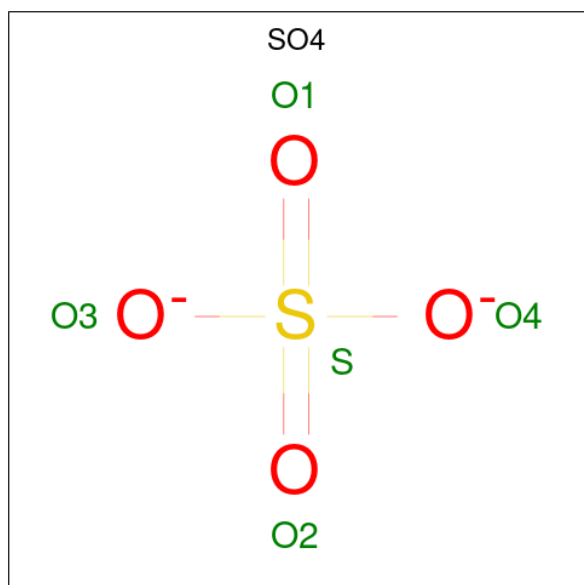
- Molecule 1 is a protein called Probable 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase AroG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	6	0
			3598	2244	661	675	18			
1	B	464	Total	C	N	O	S	0	3	0
			3587	2237	657	675	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O53512
A	0	ALA	-	expression tag	UNP O53512
B	-1	GLY	-	expression tag	UNP O53512
B	0	ALA	-	expression tag	UNP O53512

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

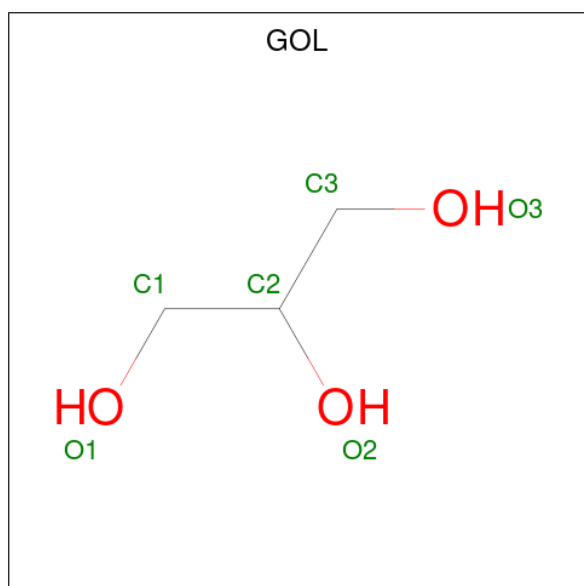


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



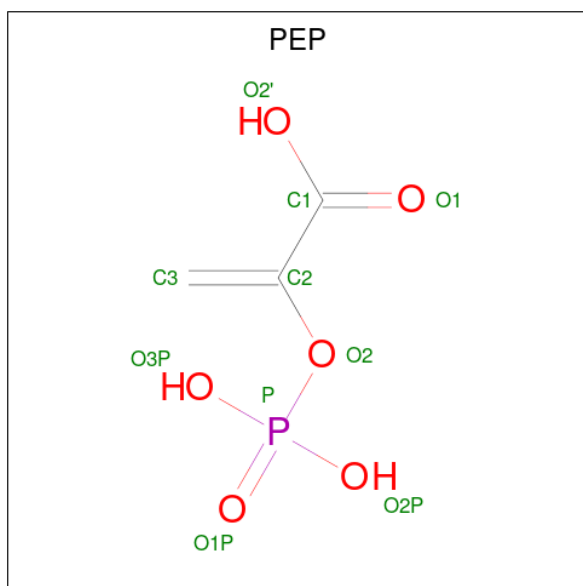
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: $C_3H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	P	0	0
			5	4	1		

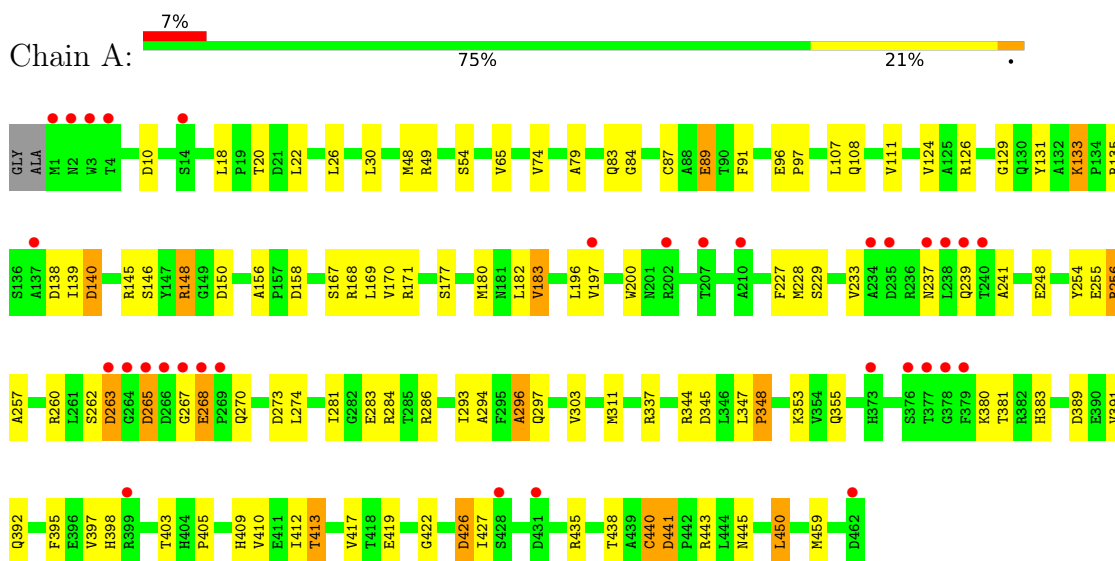
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	134	Total	O	0	0
			134	134		
8	B	146	Total	O	0	0
			146	146		

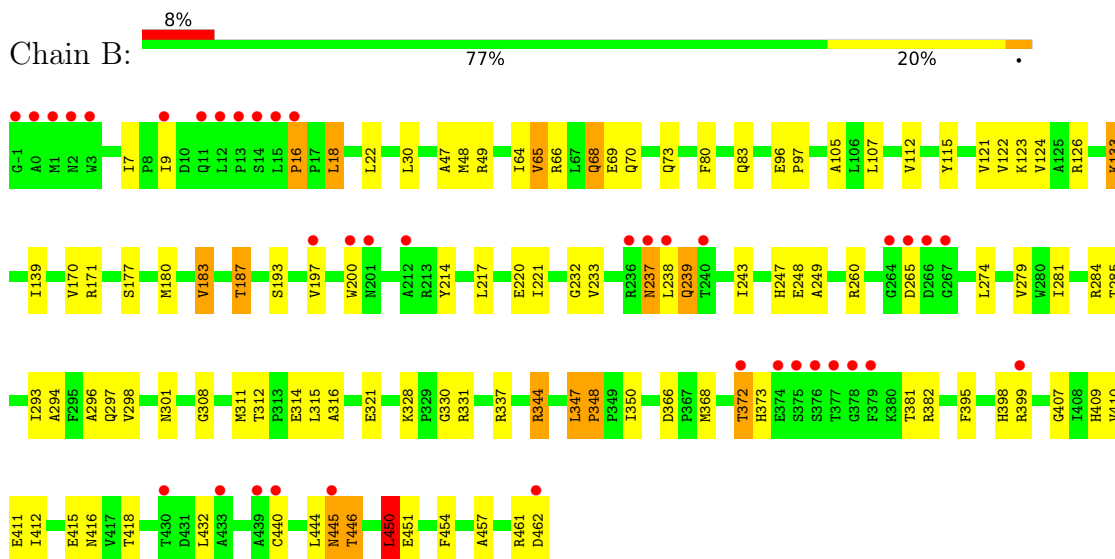
3 Residue-property plots [i](#)

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: Probable 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase AroG



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4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.54Å 203.54Å 66.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.37 – 2.25 39.37 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.4 (39.37-2.25) 97.1 (39.37-2.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	21.89 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.180 , 0.208 (Not available) , 0.199	Depositor DCC
R_{free} test set	3648 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7534	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: SO4, GOL, PO4, PEP, CL, MN

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	0.54	2/3672 (0.1%)	1.35	24/4996 (0.5%)
1	B	0.57	0/3661	1.37	28/4981 (0.6%)
All	All	0.55	2/7333 (0.0%)	1.36	52/9977 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	427	ILE	CA-C	8.57	1.62	1.52
1	A	427	ILE	N-CA	-5.06	1.39	1.46

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ILE	N-CA-C	9.46	121.56	107.75
1	A	427	ILE	CB-CA-C	-7.75	99.60	111.69
1	B	308	GLY	CA-C-N	7.49	127.13	119.56
1	B	308	GLY	C-N-CA	7.49	127.13	119.56
1	B	65	VAL	N-CA-CB	7.45	121.76	110.58
1	B	348	PRO	CA-C-N	-7.37	112.12	119.56
1	B	348	PRO	C-N-CA	-7.37	112.12	119.56
1	A	22	LEU	N-CA-C	-6.81	103.93	111.36
1	B	350	ILE	N-CA-C	-6.66	103.99	110.72
1	B	177	SER	CA-CB-OG	-6.50	98.10	111.10
1	B	233	VAL	N-CA-C	6.37	116.66	108.12
1	A	427	ILE	N-CA-C	-6.29	100.44	108.93
1	B	112	VAL	N-CA-C	-6.19	104.47	110.72
1	A	107	LEU	N-CA-C	-6.17	104.67	111.82
1	B	232	GLY	N-CA-C	6.14	123.52	115.36
1	B	328	LYS	CA-C-N	-5.98	113.78	119.76
1	B	328	LYS	C-N-CA	-5.98	113.78	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	445	ASN	N-CA-C	5.95	117.97	110.24
1	B	461	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	B	16	PRO	N-CA-C	5.85	117.83	110.70
1	A	348	PRO	CA-C-N	-5.79	113.71	119.56
1	A	348	PRO	C-N-CA	-5.79	113.71	119.56
1	A	18	LEU	CA-C-N	-5.78	113.83	119.78
1	A	18	LEU	C-N-CA	-5.78	113.83	119.78
1	A	263	ASP	CB-CA-C	-5.75	98.99	110.42
1	B	133	LYS	N-CA-C	5.63	118.33	108.82
1	A	348	PRO	N-CA-C	5.57	117.50	110.70
1	A	265	ASP	N-CA-C	-5.47	105.41	112.68
1	A	145	ARG	CB-CA-C	-5.46	100.91	109.70
1	B	64	ILE	CA-C-O	-5.43	115.09	120.85
1	B	450	LEU	N-CA-C	5.43	116.88	111.07
1	A	296	ALA	N-CA-C	-5.40	105.56	111.82
1	B	461	ARG	NE-CZ-NH1	-5.40	116.10	121.50
1	B	347	LEU	CA-C-N	-5.35	114.87	120.38
1	B	347	LEU	C-N-CA	-5.35	114.87	120.38
1	B	457	ALA	N-CA-C	-5.34	105.46	111.28
1	A	89	GLU	N-CA-C	-5.33	101.78	110.20
1	B	68	GLN	N-CA-C	5.32	117.77	111.33
1	A	303	VAL	CA-C-N	5.32	125.71	121.61
1	A	303	VAL	C-N-CA	5.32	125.71	121.61
1	B	105	ALA	N-CA-C	-5.31	105.57	111.36
1	B	7	ILE	N-CA-C	5.23	113.69	107.73
1	A	441	ASP	CA-C-N	5.15	125.96	119.98
1	A	441	ASP	C-N-CA	5.15	125.96	119.98
1	A	20	THR	N-CA-C	5.15	116.89	111.28
1	B	233	VAL	CB-CA-C	-5.14	105.74	111.35
1	A	158	ASP	N-CA-C	5.13	116.99	109.24
1	B	18	LEU	N-CA-C	5.13	116.15	109.64
1	A	156	ALA	CA-C-N	-5.07	109.25	120.56
1	A	156	ALA	C-N-CA	-5.07	109.25	120.56
1	A	54	SER	N-CA-C	5.05	119.39	112.88
1	B	187	THR	N-CA-C	-5.05	107.07	113.18

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	3598	0	3544	83	0
1	B	3587	0	3536	88	0
2	A	5	0	0	2	0
2	B	10	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	16	2	0
4	B	24	0	32	13	0
5	A	10	0	2	3	0
6	B	1	0	0	1	0
7	B	5	0	0	0	0
8	A	134	0	0	6	0
8	B	146	0	0	10	0
All	All	7534	0	7130	174	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 12.

All (174) 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:311:MET:HE1	1:B:315:LEU:HB3	1.34	1.08
1:B:73:GLN:NE2	8:B:616:HOH:O	1.89	1.04
1:A:48:MET:HE3	1:A:170:VAL:HG23	1.35	1.03
1:A:133:LYS:HE3	1:A:440:CYS:SG	1.99	1.02
1:B:133:LYS:NZ	1:B:440:CYS:SG	2.33	0.99
1:B:311:MET:CE	1:B:315:LEU:HB3	1.93	0.98
1:B:311:MET:HE1	1:B:315:LEU:CB	1.93	0.97
1:B:122:VAL:HA	4:B:467:GOL:H31	1.45	0.97
1:B:48:MET:CE	1:B:170:VAL:HG23	1.94	0.97
1:A:48:MET:HE3	1:A:170:VAL:CG2	1.96	0.95
1:B:48:MET:HE3	1:B:170:VAL:HG23	1.49	0.93
1:A:48:MET:CE	1:A:170:VAL:HG23	1.98	0.91
1:A:48:MET:CE	1:A:170:VAL:CG2	2.52	0.87
1:A:283:GLU:OE2	8:A:487:HOH:O	1.93	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:VAL:HG21	1:A:419:GLU:OE2	1.79	0.82
1:A:392:GLN:HA	1:A:459:MET:CE	2.11	0.81
1:B:180:MET:HE3	1:B:183:VAL:HG22	1.65	0.79
1:A:89:GLU:OE2	8:A:478:HOH:O	2.02	0.76
1:A:48:MET:HE2	1:A:167:SER:HA	1.68	0.74
1:A:392:GLN:HA	1:A:459:MET:HE3	1.69	0.73
1:A:398:HIS:HB3	1:A:405:PRO:HD3	1.70	0.73
1:B:311:MET:HE2	1:B:316:ALA:N	2.05	0.72
1:A:133:LYS:CE	1:A:440:CYS:SG	2.78	0.72
1:B:48:MET:HE1	1:B:170:VAL:CG2	2.21	0.71
1:B:48:MET:CE	1:B:170:VAL:CG2	2.68	0.71
1:B:123:LYS:NZ	4:B:466:GOL:H32	2.05	0.71
1:B:122:VAL:HA	4:B:467:GOL:C3	2.22	0.69
1:B:311:MET:HE3	1:B:312:THR:H	1.57	0.69
1:B:48:MET:HE1	1:B:170:VAL:HG23	1.75	0.67
1:A:108:GLN:NE2	1:A:450:LEU:HD21	2.09	0.67
1:B:311:MET:HE1	1:B:315:LEU:CG	2.24	0.67
1:B:321:GLU:OE1	8:B:586:HOH:O	2.13	0.66
1:A:380:LYS:NZ	1:A:441:ASP:OD1	2.25	0.65
1:A:398:HIS:CB	1:A:405:PRO:HD3	2.26	0.65
1:A:197:VAL:HA	1:A:200:TRP:CE3	2.32	0.64
1:A:48:MET:CE	1:A:170:VAL:HG21	2.27	0.64
1:B:126:ARG:HH11	1:B:409:HIS:CE1	2.15	0.64
1:B:68:GLN:HE22	1:B:331:ARG:N	1.96	0.63
1:B:123:LYS:HZ2	4:B:466:GOL:H32	1.63	0.62
1:A:49:ARG:HG2	1:A:257:ALA:HB2	1.82	0.62
1:A:395:PHE:CD1	1:A:459:MET:HE2	2.35	0.62
1:A:84:GLY:HA2	1:A:410:VAL:O	1.99	0.61
2:A:463:SO4:O2	8:A:549:HOH:O	2.15	0.61
1:B:96:GLU:HB3	1:B:97:PRO:HD3	1.83	0.60
4:B:469:GOL:C1	8:B:613:HOH:O	2.49	0.60
1:A:248:GLU:OE1	5:A:467:PEP:C3	2.49	0.59
1:A:392:GLN:HA	1:A:459:MET:HE1	1.82	0.59
1:A:180:MET:HE3	1:A:183:VAL:HG22	1.84	0.59
1:B:238:LEU:O	1:B:239:GLN:HB3	2.02	0.58
1:B:368:MET:HE2	1:B:411:GLU:HB2	1.84	0.58
1:B:311:MET:HE2	1:B:312:THR:O	2.03	0.58
1:B:372:THR:HG22	1:B:382:ARG:HE	1.68	0.58
1:B:311:MET:CE	1:B:312:THR:O	2.52	0.58
1:A:96:GLU:HB3	1:A:97:PRO:HD3	1.86	0.57
1:B:18:LEU:H	4:B:468:GOL:H2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LEU:O	1:B:239:GLN:CB	2.53	0.57
1:A:417:VAL:HG22	1:A:435:ARG:O	2.05	0.57
1:A:260:ARG:HG3	1:A:274:LEU:HD12	1.87	0.56
1:B:311:MET:HE3	1:B:315:LEU:HB3	1.84	0.56
1:A:413:THR:HG23	1:A:443:ARG:HD2	1.88	0.56
1:A:413:THR:HG21	1:A:443:ARG:NH1	2.21	0.56
1:B:126:ARG:HH11	1:B:409:HIS:HE1	1.52	0.56
1:A:48:MET:HE1	1:A:170:VAL:HG21	1.88	0.55
1:B:311:MET:HE2	1:B:316:ALA:H	1.70	0.55
1:A:410:VAL:HG23	1:A:412:ILE:HG23	1.87	0.55
1:B:197:VAL:HA	1:B:200:TRP:CE3	2.41	0.55
1:B:133:LYS:HD2	1:B:440:CYS:SG	2.47	0.55
1:A:48:MET:HE1	1:A:170:VAL:CG2	2.37	0.55
1:B:187:THR:CG2	1:B:243:ILE:HD12	2.37	0.54
1:B:418:THR:O	1:B:432:LEU:HD23	2.07	0.54
1:B:123:LYS:CE	4:B:466:GOL:H32	2.37	0.54
1:B:311:MET:HE3	1:B:312:THR:N	2.22	0.54
1:A:91:PHE:CE2	1:A:150:ASP:HB3	2.42	0.54
1:B:9:ILE:HD11	1:B:47:ALA:HB1	1.89	0.54
1:B:395:PHE:O	1:B:399[A]:ARG:HG2	2.08	0.53
1:A:83:GLN:HA	1:A:124:VAL:O	2.08	0.53
1:B:126:ARG:HD2	1:B:409:HIS:HE1	1.73	0.53
1:B:344:ARG:HH11	1:B:344:ARG:HG3	1.74	0.52
1:B:344:ARG:HH11	1:B:344:ARG:CG	2.22	0.51
1:A:417:VAL:CG2	1:A:435:ARG:O	2.57	0.51
1:A:108:GLN:HB3	1:A:450:LEU:HD11	1.93	0.51
1:A:30:LEU:HD13	1:A:256:ARG:NH1	2.27	0.50
1:A:417:VAL:HG12	1:A:445:ASN:HB3	1.93	0.50
4:B:469:GOL:H11	8:B:613:HOH:O	2.10	0.50
1:B:311:MET:CE	1:B:316:ALA:N	2.74	0.50
1:A:347:LEU:N	1:A:348:PRO:CD	2.75	0.50
1:B:18:LEU:N	4:B:468:GOL:H2	2.27	0.50
1:B:249:ALA:HB2	1:B:279:VAL:HB	1.94	0.50
1:A:237:ASN:HD22	1:A:237:ASN:N	2.09	0.49
1:A:281:ILE:HD13	1:A:293:ILE:HD13	1.94	0.49
1:B:180:MET:HE3	1:B:183:VAL:CG2	2.40	0.49
1:A:10:ASP:OD1	1:B:171:ARG:NH2	2.45	0.49
1:A:263:ASP:HB2	1:A:265:ASP:H	1.78	0.49
1:B:297:GLN:HB2	4:B:469:GOL:H31	1.93	0.49
1:A:169:LEU:HD22	1:A:254:TYR:HB2	1.95	0.49
1:A:395:PHE:CD1	1:A:459:MET:CE	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:GLN:HA	1:B:124:VAL:O	2.13	0.48
1:A:135:ARG:HG3	1:A:146:SER:HB3	1.95	0.48
1:B:237:ASN:HD22	1:B:237:ASN:N	2.12	0.48
1:B:281:ILE:HD11	1:B:296:ALA:HB2	1.94	0.48
1:A:197:VAL:HA	1:A:200:TRP:CZ3	2.49	0.48
1:B:247:HIS:HD2	1:B:248:GLU:O	1.97	0.48
1:A:422:GLY:HA2	1:A:426:ASP:HA	1.96	0.47
1:B:298:VAL:HG23	4:B:469:GOL:H31	1.96	0.47
1:A:262:SER:O	1:A:263:ASP:C	2.58	0.47
1:B:415:GLU:C	1:B:446:THR:HG22	2.39	0.47
1:B:70:GLN:OE1	4:B:467:GOL:H2	2.14	0.47
1:B:297:GLN:HB2	4:B:469:GOL:C3	2.44	0.47
6:B:470:CL:CL	8:B:612:HOH:O	2.58	0.47
1:A:148[A]:ARG:NH2	8:A:597:HOH:O	2.48	0.47
1:A:395:PHE:CG	1:A:459:MET:HE2	2.50	0.47
1:B:260:ARG:HG3	1:B:274:LEU:HD12	1.97	0.47
1:B:366:ASP:OD1	1:B:366:ASP:C	2.57	0.47
1:A:126:ARG:HH11	1:A:409:HIS:HE1	1.62	0.46
1:A:268[B]:GLU:O	1:A:270:GLN:NE2	2.48	0.46
1:B:68:GLN:HE22	1:B:330:GLY:C	2.23	0.46
1:A:355:GLN:HG3	1:A:403:THR:HG21	1.97	0.46
1:A:438:THR:OG1	1:A:441:ASP:O	2.31	0.46
1:B:48:MET:HE3	1:B:170:VAL:CG2	2.32	0.46
1:B:294:ALA:HA	1:B:297:GLN:HE21	1.80	0.46
1:B:115:TYR:OH	1:B:220:GLU:HG2	2.17	0.45
1:A:171:ARG:HH12	4:A:465:GOL:C3	2.29	0.45
1:B:123:LYS:NZ	8:B:573:HOH:O	2.45	0.45
1:A:87:CYS:SG	1:A:441:ASP:HB2	2.56	0.45
1:A:392:GLN:CA	1:A:459:MET:HE1	2.47	0.45
1:B:66[A]:ARG:NH1	1:B:69:GLU:OE1	2.47	0.45
1:A:138:ASP:CB	2:A:463:SO4:O3	2.66	0.44
1:B:214:TYR:CZ	1:B:451:GLU:HG3	2.52	0.44
1:B:344:ARG:HG3	8:B:484:HOH:O	2.16	0.44
1:A:49:ARG:CG	1:A:257:ALA:HB2	2.44	0.44
1:A:140:ASP:OD1	1:A:140:ASP:C	2.60	0.44
1:A:131:TYR:OH	8:A:478:HOH:O	2.18	0.44
1:A:391:VAL:C	1:A:459:MET:HE1	2.43	0.44
1:B:107:LEU:HD22	8:B:490:HOH:O	2.17	0.44
1:A:135:ARG:HD2	1:A:135:ARG:HA	1.79	0.44
1:B:301:ASN:O	1:B:331:ARG:NH1	2.51	0.44
1:B:49:ARG:NH1	8:B:502:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ILE:HG22	1:B:444:LEU:HD12	2.00	0.43
1:B:30:LEU:HA	1:B:30:LEU:HD23	1.79	0.43
1:B:314:GLU:N	1:B:314:GLU:OE1	2.49	0.43
1:A:286:ARG:NH1	1:A:311:MET:HE1	2.33	0.43
1:A:74:VAL:HA	1:A:79:ALA:O	2.18	0.43
1:A:228:MET:HE2	1:A:233:VAL:HG11	2.00	0.43
1:A:294:ALA:HA	1:A:297:GLN:HE21	1.84	0.43
1:B:80:PHE:O	1:B:121:VAL:HA	2.19	0.43
1:B:311:MET:HE3	1:B:312:THR:O	2.19	0.43
1:B:133:LYS:CD	1:B:440:CYS:SG	3.06	0.43
1:B:450:LEU:HD12	1:B:450:LEU:HA	1.79	0.42
1:A:248:GLU:OE1	5:A:467:PEP:H32	2.19	0.42
1:A:294:ALA:HA	1:A:297:GLN:NE2	2.33	0.42
1:A:126:ARG:HH11	1:A:409:HIS:CE1	2.36	0.42
1:B:197:VAL:HA	1:B:200:TRP:CZ3	2.54	0.42
1:B:416:ASN:HA	1:B:445:ASN:OD1	2.19	0.42
1:B:293:ILE:O	1:B:297:GLN:HG3	2.20	0.42
1:A:248:GLU:OE1	5:A:467:PEP:H31	2.17	0.42
1:A:96:GLU:HA	1:A:182:LEU:HD21	2.00	0.42
1:A:241:ALA:HA	8:A:485:HOH:O	2.20	0.42
1:A:255:GLU:OE1	1:A:273:ASP:OD2	2.38	0.42
1:B:66[A]:ARG:HA	1:B:66[A]:ARG:HD2	1.70	0.41
1:A:227:PHE:O	1:A:228:MET:C	2.62	0.41
1:A:237:ASN:N	1:A:237:ASN:ND2	2.68	0.41
1:B:398:HIS:O	1:B:399[A]:ARG:C	2.62	0.41
1:B:80:PHE:CZ	1:B:407:GLY:HA2	2.54	0.41
1:B:373:HIS:CE1	1:B:381:THR:HG23	2.56	0.41
1:B:217:LEU:O	1:B:221:ILE:HG13	2.20	0.41
1:A:96:GLU:HG3	8:B:602:HOH:O	2.20	0.41
1:B:217:LEU:HD23	1:B:454:PHE:CD1	2.56	0.41
1:A:267:GLY:C	1:A:268[A]:GLU:HG3	2.45	0.40
1:A:168:ARG:HH22	4:A:465:GOL:H31	1.86	0.40
1:A:281:ILE:HD11	1:A:296:ALA:HB2	2.02	0.40
1:A:348:PRO:HG3	1:A:397:VAL:HG22	2.04	0.40
1:B:347:LEU:O	1:B:348:PRO:C	2.62	0.40
1:A:344:ARG:NH2	1:A:389:ASP:OD1	2.55	0.40
1:B:410:VAL:HG23	1:B:412:ILE:HG23	2.03	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	466/464 (100%)	449 (96%)	11 (2%)	6 (1%)	9	6
1	B	465/464 (100%)	438 (94%)	25 (5%)	2 (0%)	30	31
All	All	931/928 (100%)	887 (95%)	36 (4%)	8 (1%)	16	12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	265	ASP
1	A	239	GLN
1	A	268[A]	GLU
1	A	268[B]	GLU
1	A	426	ASP
1	B	239	GLN
1	A	440	CYS
1	A	129	GLY

5.3.2 Protein sidechains [i](#)

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	377/376 (100%)	357 (95%)	20 (5%)	20	22
1	B	376/376 (100%)	361 (96%)	15 (4%)	28	34
All	All	753/752 (100%)	718 (95%)	35 (5%)	24	28

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	65	VAL
1	A	111	VAL
1	A	133	LYS
1	A	140	ASP
1	A	148[A]	ARG
1	A	148[B]	ARG
1	A	177	SER
1	A	183	VAL
1	A	196	LEU
1	A	229	SER
1	A	256	ARG
1	A	284	ARG
1	A	337	ARG
1	A	345	ASP
1	A	353	LYS
1	A	381	THR
1	A	383	HIS
1	A	413	THR
1	A	450	LEU
1	B	16	PRO
1	B	22	LEU
1	B	65	VAL
1	B	139	ILE
1	B	183	VAL
1	B	193	SER
1	B	237	ASN
1	B	284	ARG
1	B	285	THR
1	B	337	ARG
1	B	344	ARG
1	B	372	THR
1	B	446	THR
1	B	450	LEU
1	B	462	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	11	GLN
1	A	44	GLN
1	A	195	HIS

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Mol	Chain	Res	Type
1	A	237	ASN
1	A	297	GLN
1	A	359	HIS
1	A	373	HIS
1	A	409	HIS
1	B	2	ASN
1	B	68	GLN
1	B	108	GLN
1	B	237	ASN
1	B	297	GLN
1	B	326	HIS
1	B	327	ASN
1	B	369	HIS
1	B	373	HIS
1	B	404	HIS
1	B	409	HIS
1	B	447	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](#)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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
4	GOL	B	466	-	5,5,5	0.44	0	5,5,5	1.16	1 (20%)
4	GOL	A	466	-	5,5,5	0.38	0	5,5,5	0.35	0
2	SO4	B	464	-	4,4,4	0.25	0	6,6,6	0.61	0
4	GOL	B	469	-	5,5,5	0.45	0	5,5,5	0.94	0
7	PO4	B	471	-	4,4,4	1.14	0	6,6,6	0.98	0
4	GOL	A	465	-	5,5,5	0.31	0	5,5,5	0.98	0
4	GOL	B	468	-	5,5,5	0.48	0	5,5,5	1.81	1 (20%)
4	GOL	B	467	-	5,5,5	0.35	0	5,5,5	1.67	2 (40%)
2	SO4	B	463	-	4,4,4	0.24	0	6,6,6	0.76	0
2	SO4	A	463	-	4,4,4	0.22	0	6,6,6	0.53	0
5	PEP	A	467	-	9,9,9	3.03	3 (33%)	11,13,13	3.73	3 (27%)

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
4	GOL	B	466	-	-	2/4/4/4	-
4	GOL	A	466	-	-	2/4/4/4	-
4	GOL	B	469	-	-	2/4/4/4	-
4	GOL	A	465	-	-	4/4/4/4	-
4	GOL	B	468	-	-	4/4/4/4	-
4	GOL	B	467	-	-	4/4/4/4	-
5	PEP	A	467	-	-	4/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	467	PEP	C3-C2	8.03	1.53	1.31
5	A	467	PEP	C2-C1	2.16	1.51	1.49
5	A	467	PEP	O2-C2	2.05	1.44	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	467	PEP	C3-C2-C1	-10.43	103.44	122.73
5	A	467	PEP	O2-C2-C3	-5.07	115.16	124.85
4	B	467	GOL	O3-C3-C2	3.05	124.10	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	467	PEP	O2'-C1-C2	3.01	119.04	113.91
4	B	468	GOL	O2-C2-C3	-2.97	96.88	109.18
4	B	466	GOL	O2-C2-C3	-2.30	99.64	109.18
4	B	467	GOL	O2-C2-C3	2.02	117.54	109.18

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	465	GOL	O1-C1-C2-C3
4	A	465	GOL	C1-C2-C3-O3
4	A	466	GOL	O1-C1-C2-C3
4	B	467	GOL	C1-C2-C3-O3
4	B	468	GOL	O1-C1-C2-O2
4	B	468	GOL	O1-C1-C2-C3
4	B	468	GOL	C1-C2-C3-O3
5	A	467	PEP	O1-C1-C2-C3
5	A	467	PEP	O1-C1-C2-O2
5	A	467	PEP	O2'-C1-C2-C3
5	A	467	PEP	O2'-C1-C2-O2
4	A	465	GOL	O2-C2-C3-O3
4	B	467	GOL	O2-C2-C3-O3
4	B	466	GOL	C1-C2-C3-O3
4	B	467	GOL	O1-C1-C2-C3
4	B	469	GOL	C1-C2-C3-O3
4	A	465	GOL	O1-C1-C2-O2
4	B	467	GOL	O1-C1-C2-O2
4	B	468	GOL	O2-C2-C3-O3
4	B	466	GOL	O2-C2-C3-O3
4	B	469	GOL	O2-C2-C3-O3
4	A	466	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	466	GOL	3	0
4	B	469	GOL	5	0
4	A	465	GOL	2	0
4	B	468	GOL	2	0
4	B	467	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	463	SO4	2	0
5	A	467	PEP	3	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	462/464 (99%)	0.18	32 (6%)	23 21	15, 32, 67, 83	6 (1%)
1	B	464/464 (100%)	0.19	38 (8%)	17 16	14, 29, 70, 89	3 (0%)
All	All	926/928 (99%)	0.18	70 (7%)	20 18	14, 31, 68, 89	9 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	TRP	6.6
1	A	266	ASP	5.8
1	B	12	LEU	5.3
1	A	264	GLY	5.1
1	B	13	PRO	4.8
1	B	11	GLN	4.6
1	B	1	MET	4.6
1	B	265	ASP	4.5
1	B	378	GLY	4.2
1	A	238	LEU	4.0
1	B	372	THR	3.9
1	A	265	ASP	3.7
1	B	-1	GLY	3.6
1	A	234	ALA	3.4
1	B	376	SER	3.4
1	A	268[A]	GLU	3.4
1	A	240	THR	3.4
1	B	375	SER	3.3
1	B	240	THR	3.2
1	A	376	SER	3.2
1	B	267	GLY	3.2
1	A	137	ALA	3.1
1	B	197	VAL	3.1
1	A	237	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.1
1	A	239	GLN	3.0
1	B	377	THR	3.0
1	A	462	ASP	3.0
1	B	430	THR	3.0
1	A	2	ASN	2.9
1	B	0	ALA	2.8
1	B	2	ASN	2.7
1	B	433	ALA	2.7
1	B	3	TRP	2.7
1	B	379	PHE	2.7
1	B	462	ASP	2.6
1	B	200	TRP	2.6
1	A	207	THR	2.6
1	B	440	CYS	2.5
1	B	237	ASN	2.5
1	B	9	ILE	2.5
1	A	235	ASP	2.5
1	A	378	GLY	2.4
1	B	15	LEU	2.4
1	B	238	LEU	2.4
1	B	266	ASP	2.3
1	A	377	THR	2.3
1	B	236	ARG	2.3
1	A	263	ASP	2.3
1	A	399[A]	ARG	2.3
1	B	445	ASN	2.3
1	A	210	ALA	2.2
1	B	212	ALA	2.2
1	A	197	VAL	2.2
1	A	373	HIS	2.2
1	B	264	GLY	2.2
1	A	14[A]	SER	2.2
1	B	14	SER	2.2
1	B	201	ASN	2.2
1	A	379	PHE	2.1
1	B	399[A]	ARG	2.1
1	A	269	PRO	2.1
1	B	16	PRO	2.1
1	A	202	ARG	2.1
1	A	267	GLY	2.1
1	A	4	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	428	SER	2.1
1	B	439	ALA	2.0
1	B	374	GLU	2.0
1	A	431	ASP	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
4	GOL	A	465	6/6	0.80	0.19	56,59,60,60	0
4	GOL	B	466	6/6	0.82	0.24	50,55,57,58	0
4	GOL	A	466	6/6	0.84	0.24	60,66,69,70	0
2	SO4	A	463	5/5	0.87	0.17	42,45,47,48	5
4	GOL	B	467	6/6	0.87	0.21	54,55,57,58	0
4	GOL	B	468	6/6	0.87	0.17	44,49,49,51	0
4	GOL	B	469	6/6	0.87	0.17	49,53,53,54	0
2	SO4	B	464	5/5	0.91	0.18	59,62,64,65	0
3	MN	B	465	1/1	0.92	0.06	42,42,42,42	1
5	PEP	A	467	10/10	0.92	0.14	43,51,64,65	0
6	CL	B	470	1/1	0.95	0.08	71,71,71,71	0
3	MN	A	464	1/1	0.97	0.04	49,49,49,49	1
2	SO4	B	463	5/5	0.97	0.06	39,40,43,46	0
7	PO4	B	471	5/5	0.98	0.06	35,36,38,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.