



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:38 PM UTC

PDB ID : 2CZG / pdb_00002czg
Title : Crystal structure of Probable phosphoribosylglycinamide formyl transferase (PH0318) from *Pyrococcus horikoshii* OT3
Authors : Yoshikawa, S.; Arai, R.; Kamo-Uchikubo, T.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-13
Resolution : 2.35 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

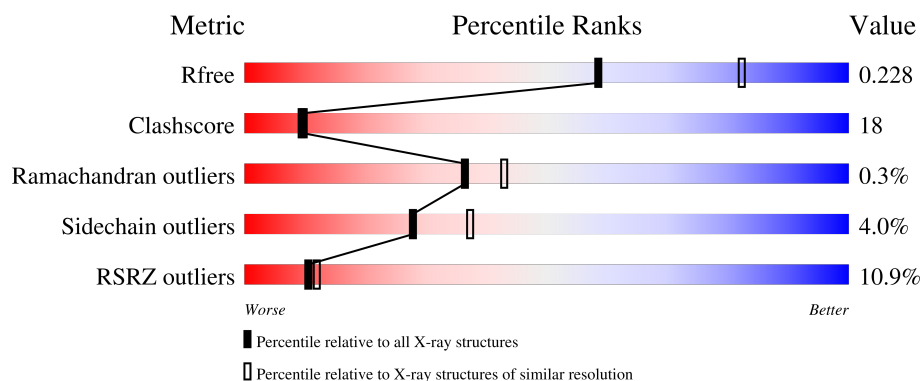
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	433	 10% 65% 26% • 6%
1	B	433	 11% 69% 21% • 7%

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	B	436	-	-	X	-
3	GOL	A	436	-	-	X	-
3	GOL	A	437	-	-	X	-
3	GOL	A	440	-	-	X	-
3	GOL	A	441	-	-	X	-
3	GOL	B	438	-	-	X	-
3	GOL	B	439	-	-	X	-
3	GOL	B	442	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6697 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 phosphoribosylglycinamide formyl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3215	2063	552	586	14			
1	B	403	Total	C	N	O	S	0	0	0
			3198	2053	550	582	13			

- 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	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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	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		

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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		

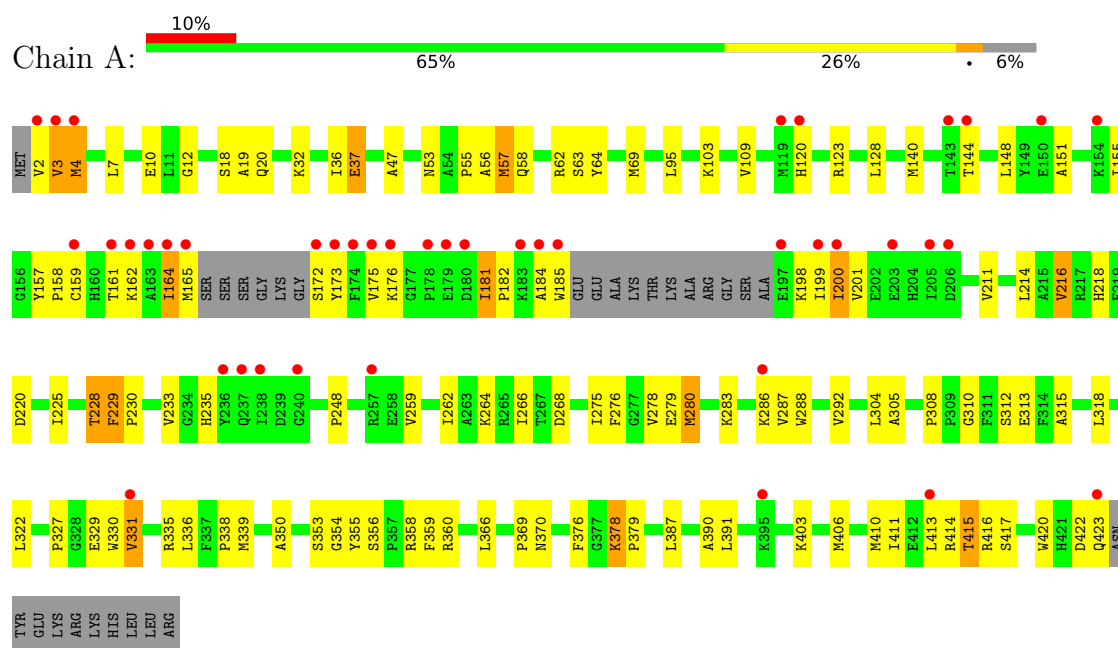
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	104	Total	O	0	0
			104	104		
4	B	84	Total	O	0	0
			84	84		

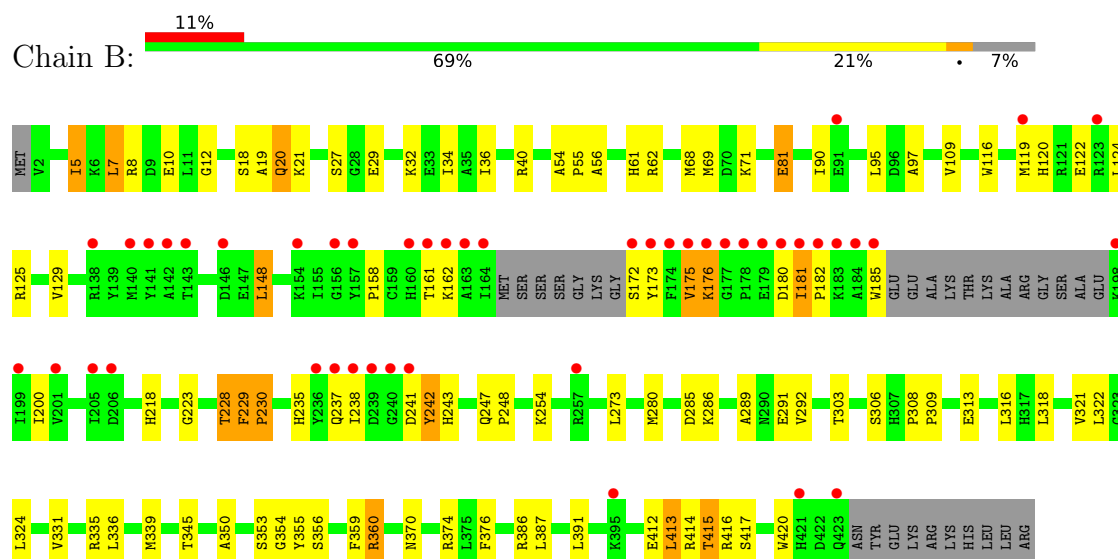
3 Residue-property plots [i](#)

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: phosphoribosylglycinamide formyl transferase



- Molecule 1: phosphoribosylglycinamide formyl transferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	105.47Å 219.28Å 120.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 2.35 49.92 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.92-2.35) 98.8 (49.92-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.07 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.228 0.195 , 0.228	Depositor DCC
R_{free} test set	5817 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6697	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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, 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	0.59	2/3292 (0.1%)	1.00	21/4462 (0.5%)
1	B	0.51	0/3275	0.96	11/4440 (0.2%)
All	All	0.55	2/6567 (0.0%)	0.98	32/8902 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	MET	SD-CE	-14.19	1.44	1.79
1	A	280	MET	SD-CE	-5.41	1.66	1.79

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	PHE	N-CA-C	8.87	123.37	112.54
1	B	20	GLN	N-CA-C	-8.73	96.89	110.42
1	A	109	VAL	N-CA-C	7.82	115.36	108.63
1	A	157	TYR	CA-C-N	6.93	143.62	127.00
1	A	157	TYR	C-N-CA	6.93	143.62	127.00
1	A	376	PHE	N-CA-C	6.89	120.79	112.38
1	A	20	GLN	N-CA-C	-6.89	99.08	110.17
1	A	157	TYR	C-N-CD	-6.65	105.96	120.60
1	A	69	MET	N-CA-C	-6.63	104.81	113.17
1	A	390	ALA	N-CA-C	-6.60	98.97	109.59
1	A	322	LEU	N-CA-C	-6.42	105.45	113.28
1	A	19	ALA	N-CA-C	6.18	119.21	110.50
1	A	411	ILE	N-CA-C	6.02	116.97	108.36
1	A	378	LYS	CA-C-N	5.87	125.49	119.56
1	A	378	LYS	C-N-CA	5.87	125.49	119.56
1	A	229	PHE	N-CA-C	5.75	118.61	109.40
1	A	58	GLN	N-CA-C	-5.74	104.99	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	MET	N-CA-C	-5.74	106.32	113.38
1	B	229	PHE	N-CA-C	5.74	119.64	108.85
1	A	56	ALA	CA-C-N	-5.61	112.23	122.38
1	A	56	ALA	C-N-CA	-5.61	112.23	122.38
1	B	19	ALA	N-CA-C	5.60	118.35	110.23
1	B	129	VAL	N-CA-C	5.58	116.23	110.82
1	B	34	ILE	N-CA-C	-5.46	105.17	110.42
1	B	81	GLU	N-CA-C	5.17	119.67	112.90
1	A	304	LEU	N-CA-C	-5.17	106.24	112.54
1	B	181	ILE	CB-CA-C	-5.13	108.83	113.70
1	A	220	ASP	N-CA-C	-5.13	102.43	110.17
1	A	181	ILE	CB-CA-C	-5.07	108.88	113.70
1	B	230	PRO	N-CA-C	-5.05	103.60	111.13
1	A	292	VAL	N-CA-C	5.05	115.01	108.35
1	B	54	ALA	N-CA-C	-5.04	103.12	110.08

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	3215	0	3209	138	0
1	B	3198	0	3194	96	0
2	A	10	0	0	1	0
2	B	20	0	0	3	0
3	A	36	0	48	27	2
3	B	30	0	40	18	2
4	A	104	0	0	2	0
4	B	84	0	0	2	0
All	All	6697	0	6491	229	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 18.

All (229) 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)
3:A:437:GOL:C3	1:B:308:PRO:HG2	1.74	1.18
1:A:308:PRO:HG3	3:B:439:GOL:H31	1.16	1.14
1:A:308:PRO:HG3	3:B:439:GOL:C3	1.78	1.12
1:B:387:LEU:HD12	1:B:413:LEU:HD21	1.32	1.11
1:A:216:VAL:HG22	1:A:275:ILE:HG13	1.35	1.04
3:A:437:GOL:H31	1:B:308:PRO:HG2	1.30	1.03
1:A:370:ASN:HD22	3:A:437:GOL:H12	1.25	0.99
1:A:330:TRP:HE1	3:A:438:GOL:H32	1.27	0.99
1:A:161:THR:HG22	1:A:173:TYR:O	1.65	0.97
1:B:40:ARG:HH12	3:B:438:GOL:H31	1.31	0.94
1:A:158:PRO:HG3	1:A:176:LYS:HE2	1.48	0.94
3:A:437:GOL:H31	1:B:308:PRO:CG	1.99	0.92
1:A:370:ASN:ND2	3:A:437:GOL:H12	1.87	0.89
1:A:280:MET:HE2	1:A:287:VAL:HG11	1.55	0.88
1:B:354:GLY:HA3	1:B:415:THR:HG21	1.54	0.88
1:B:370:ASN:H	3:B:439:GOL:H12	1.39	0.87
1:A:312:SER:HB3	3:A:436:GOL:H11	1.57	0.84
1:A:312:SER:OG	3:A:436:GOL:H31	1.79	0.82
1:A:330:TRP:NE1	3:A:438:GOL:H32	1.96	0.81
1:A:148:LEU:HD12	1:A:181:ILE:HG23	1.63	0.81
1:A:280:MET:HE2	1:A:287:VAL:CG1	2.12	0.80
1:A:370:ASN:HD22	3:A:437:GOL:C1	1.95	0.79
1:B:61:HIS:HB3	3:B:442:GOL:H12	1.65	0.78
1:B:62:ARG:HD2	3:B:441:GOL:H12	1.64	0.78
1:B:235:HIS:ND1	1:B:237:GLN:NE2	2.32	0.77
1:A:312:SER:CB	3:A:436:GOL:H31	2.14	0.77
1:A:264:LYS:NZ	3:A:439:GOL:H2	2.00	0.77
1:A:218:HIS:NE2	1:A:228:THR:CG2	2.50	0.75
1:A:308:PRO:CG	3:B:439:GOL:H31	2.09	0.75
1:A:358:ARG:HH22	3:A:440:GOL:H12	1.49	0.75
1:B:356:SER:HB2	1:B:416:ARG:HG3	1.68	0.74
1:B:387:LEU:CD1	1:B:413:LEU:HD21	2.16	0.73
1:A:164:ILE:HD12	1:A:198:LYS:HB3	1.71	0.73
3:A:437:GOL:H32	1:B:308:PRO:HG2	1.69	0.72
1:B:248:PRO:HD3	1:B:339:MET:HE1	1.71	0.72
1:B:95:LEU:HD23	1:B:116:TRP:HD1	1.54	0.72
1:A:159:CYS:HB3	1:A:175:VAL:HG23	1.70	0.72
1:A:266:ILE:HD12	1:A:278:VAL:CG1	2.20	0.72
1:B:27:SER:HB3	1:B:56:ALA:HB3	1.71	0.72
1:B:331:VAL:HG11	1:B:336:LEU:HD12	1.73	0.70
1:A:353:SER:O	1:A:415:THR:HG21	1.91	0.70
1:B:414:ARG:HB2	1:B:420:TRP:CE3	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ILE:HD12	1:B:243:HIS:CG	2.28	0.69
1:B:415:THR:HG22	1:B:417:SER:H	1.57	0.69
3:A:437:GOL:C3	1:B:308:PRO:CG	2.61	0.69
1:B:5:ILE:HD11	1:B:273:LEU:HD12	1.74	0.68
1:A:37:GLU:HG3	1:A:315:ALA:HB2	1.74	0.68
1:A:164:ILE:HG21	1:A:198:LYS:HD2	1.75	0.68
1:A:266:ILE:HD12	1:A:278:VAL:HG13	1.75	0.68
1:A:308:PRO:HG3	3:B:439:GOL:H32	1.73	0.68
1:A:37:GLU:HG3	1:A:315:ALA:CB	2.24	0.66
1:B:370:ASN:H	3:B:439:GOL:C1	2.06	0.66
1:B:360:ARG:HG2	1:B:420:TRP:CZ3	2.30	0.66
1:A:262:ILE:HB	1:A:280:MET:CE	2.26	0.66
1:B:354:GLY:HA3	1:B:415:THR:CG2	2.24	0.65
4:A:447:HOH:O	3:B:438:GOL:H32	1.97	0.65
1:B:12:GLY:HA3	1:B:18:SER:O	1.97	0.65
1:A:3:VAL:HG11	1:A:225:ILE:HD11	1.78	0.65
1:B:353:SER:O	1:B:415:THR:HG21	1.97	0.64
1:A:161:THR:OG1	1:A:199:ILE:HG21	1.98	0.64
1:A:422:ASP:OD1	1:A:423:GLN:HG3	1.98	0.64
1:A:120:HIS:HB3	1:A:123:ARG:HB2	1.80	0.64
1:B:291:GLU:HG3	1:B:292:VAL:N	2.13	0.63
1:B:122:GLU:HB2	2:B:436:SO4:O4	1.98	0.63
1:A:64:TYR:CZ	3:A:441:GOL:H2	2.33	0.63
1:B:5:ILE:HD11	1:B:273:LEU:CD1	2.28	0.63
1:B:158:PRO:HB3	1:B:176:LYS:HA	1.81	0.62
1:A:259:VAL:HA	1:A:280:MET:HE1	1.80	0.62
1:B:162:LYS:HB3	1:B:172:SER:HB3	1.81	0.62
1:A:350:ALA:HA	1:A:413:LEU:HD12	1.82	0.62
1:B:228:THR:HG21	1:B:335:ARG:NH1	2.14	0.62
1:B:173:TYR:HE2	1:B:180:ASP:HB3	1.65	0.61
1:B:291:GLU:HG3	1:B:292:VAL:H	1.65	0.61
1:B:350:ALA:HA	1:B:413:LEU:HD22	1.82	0.61
1:A:262:ILE:HB	1:A:280:MET:HE3	1.81	0.61
1:A:264:LYS:HZ2	3:A:439:GOL:H2	1.63	0.61
1:A:62:ARG:HD2	3:A:441:GOL:H12	1.83	0.61
1:A:358:ARG:NH2	3:A:440:GOL:H12	2.15	0.60
1:A:414:ARG:HB2	1:A:420:TRP:CE3	2.36	0.60
1:A:275:ILE:HD13	1:A:313:GLU:HB2	1.84	0.59
1:B:387:LEU:HD12	1:B:413:LEU:CD2	2.21	0.59
1:A:199:ILE:N	1:A:199:ILE:HD12	2.18	0.59
1:A:148:LEU:CD1	1:A:181:ILE:HG23	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LYS:HG3	1:B:97:ALA:HB2	1.85	0.58
1:B:370:ASN:ND2	3:B:439:GOL:O3	2.36	0.58
1:A:359:PHE:CD2	1:A:413:LEU:HD22	2.37	0.58
1:A:360:ARG:HG2	1:A:420:TRP:CZ3	2.39	0.58
1:B:120:HIS:HB3	2:B:436:SO4:O2	2.03	0.58
1:B:218:HIS:NE2	1:B:228:THR:CG2	2.66	0.58
1:B:228:THR:HG21	1:B:335:ARG:HH11	1.69	0.58
1:A:327:PRO:HB2	3:B:439:GOL:O1	2.04	0.57
1:A:57:MET:HB2	1:A:63:SER:HB3	1.87	0.57
1:A:370:ASN:HA	3:A:437:GOL:H11	1.87	0.57
1:A:62:ARG:HG3	1:A:62:ARG:HH11	1.69	0.57
1:A:140:MET:HG2	1:A:155:ILE:HD11	1.87	0.56
1:A:159:CYS:HB3	1:A:175:VAL:CG2	2.34	0.56
1:A:159:CYS:SG	1:A:201:VAL:HG13	2.45	0.56
1:A:53:ASN:HD21	3:B:442:GOL:H31	1.71	0.56
1:B:331:VAL:HG11	1:B:336:LEU:CD1	2.36	0.56
1:A:312:SER:HB3	3:A:436:GOL:H31	1.86	0.56
1:A:4:MET:HE3	4:A:453:HOH:O	2.04	0.56
1:B:254:LYS:HD3	1:B:285:ASP:OD1	2.05	0.55
1:B:29:GLU:OE2	1:B:386:ARG:HD2	2.06	0.55
1:A:164:ILE:HG21	1:A:198:LYS:CD	2.37	0.55
1:B:218:HIS:NE2	1:B:228:THR:HG23	2.22	0.54
1:B:40:ARG:HH12	3:B:438:GOL:C3	2.11	0.54
1:A:218:HIS:NE2	1:A:228:THR:HG21	2.22	0.54
1:A:264:LYS:HE2	1:A:268:ASP:OD2	2.08	0.53
1:A:415:THR:HG23	1:A:417:SER:H	1.73	0.53
1:A:262:ILE:CB	1:A:280:MET:HE3	2.39	0.53
1:B:360:ARG:HG2	1:B:420:TRP:CE3	2.44	0.53
1:A:12:GLY:HA3	1:A:18:SER:O	2.09	0.53
1:A:181:ILE:N	1:A:182:PRO:HD2	2.24	0.53
1:A:354:GLY:HA3	1:A:415:THR:HG21	1.90	0.53
1:A:218:HIS:NE2	1:A:228:THR:HG23	2.24	0.52
3:A:437:GOL:C2	1:B:308:PRO:HG2	2.38	0.52
1:B:148:LEU:HD12	1:B:185:TRP:HB2	1.91	0.52
1:A:161:THR:HG22	1:A:173:TYR:C	2.34	0.52
1:A:64:TYR:CE2	3:A:441:GOL:H32	2.45	0.52
1:B:181:ILE:N	1:B:182:PRO:HD2	2.25	0.51
1:A:161:THR:HG23	1:A:173:TYR:H	1.75	0.51
1:B:68:MET:HE3	1:B:90:ILE:HD11	1.91	0.51
1:A:164:ILE:HD13	1:A:164:ILE:H	1.75	0.51
1:A:161:THR:HG21	1:A:184:ALA:HB1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:HIS:NE2	1:A:279:GLU:OE2	2.32	0.51
1:B:40:ARG:NH1	3:B:438:GOL:H31	2.14	0.51
1:A:248:PRO:HD3	1:A:339:MET:HE1	1.92	0.50
1:A:406:MET:O	1:A:410:MET:HG3	2.11	0.50
1:A:266:ILE:HD12	1:A:278:VAL:HG11	1.94	0.50
1:B:62:ARG:HH11	1:B:62:ARG:HG3	1.77	0.50
1:B:32:LYS:HD2	1:B:55:PRO:HB3	1.94	0.50
1:A:358:ARG:HH22	3:A:440:GOL:C1	2.23	0.50
1:B:27:SER:CB	1:B:56:ALA:HB3	2.41	0.50
1:B:61:HIS:CB	3:B:442:GOL:H12	2.38	0.50
1:B:370:ASN:N	3:B:439:GOL:H12	2.18	0.50
1:A:164:ILE:HD13	1:A:165:MET:H	1.76	0.49
1:B:8:ARG:NH2	4:B:473:HOH:O	2.45	0.49
1:B:158:PRO:HG3	1:B:176:LYS:HE3	1.95	0.49
1:A:305:ALA:HA	1:B:309:PRO:HG3	1.94	0.49
1:A:415:THR:HG23	1:A:416:ARG:N	2.28	0.48
1:B:345:THR:HG22	1:B:391:LEU:HD23	1.95	0.48
1:B:173:TYR:CE2	1:B:180:ASP:HB3	2.45	0.48
1:B:360:ARG:HD2	1:B:412:GLU:OE1	2.14	0.48
1:A:414:ARG:HD2	1:A:415:THR:O	2.14	0.48
1:B:414:ARG:HB2	1:B:420:TRP:CZ3	2.47	0.48
1:A:176:LYS:O	1:A:176:LYS:HD3	2.13	0.48
1:A:359:PHE:O	1:B:10:GLU:HG2	2.14	0.48
1:A:228:THR:HG21	1:A:335:ARG:NH1	2.28	0.48
1:B:158:PRO:HB3	1:B:176:LYS:HD3	1.96	0.48
1:A:32:LYS:HD2	1:A:55:PRO:HB3	1.96	0.47
3:A:440:GOL:H32	4:B:510:HOH:O	2.13	0.47
1:A:360:ARG:HG2	1:A:420:TRP:CE3	2.49	0.47
1:A:2:VAL:O	1:A:3:VAL:C	2.58	0.47
1:A:331:VAL:HG13	1:A:331:VAL:O	2.14	0.47
1:A:366:LEU:HD12	1:B:324:LEU:HD22	1.97	0.47
1:B:161:THR:HA	1:B:200:ILE:O	2.15	0.47
1:A:331:VAL:CG1	1:A:336:LEU:HG	2.45	0.47
1:A:10:GLU:HG2	1:B:359:PHE:O	2.15	0.46
1:A:262:ILE:HB	1:A:280:MET:HE1	1.97	0.46
1:B:7:LEU:HG	1:B:223:GLY:HA2	1.97	0.46
1:A:312:SER:CB	3:A:436:GOL:H11	2.37	0.46
1:A:120:HIS:CD2	1:A:123:ARG:HD3	2.51	0.46
1:A:164:ILE:H	1:A:164:ILE:CD1	2.29	0.46
1:A:415:THR:CG2	1:A:417:SER:H	2.28	0.46
1:B:122:GLU:CD	1:B:125:ARG:HH21	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ILE:HG22	1:A:200:ILE:N	2.29	0.46
1:A:378:LYS:HA	1:A:379:PRO:HD3	1.79	0.46
1:A:420:TRP:HZ2	2:A:435:SO4:O3	1.98	0.46
1:B:228:THR:HA	1:B:335:ARG:O	2.16	0.46
1:B:360:ARG:HG3	1:B:412:GLU:HB2	1.98	0.46
1:A:62:ARG:HG3	1:A:62:ARG:NH1	2.32	0.45
1:B:313:GLU:HA	1:B:316:LEU:HD12	1.98	0.45
1:A:158:PRO:HA	1:A:176:LYS:HA	1.97	0.45
1:A:162:LYS:HG2	1:A:172:SER:HB2	1.97	0.45
1:B:21:LYS:HE3	1:B:81:GLU:O	2.17	0.45
1:A:37:GLU:CG	1:A:315:ALA:HB2	2.45	0.45
1:A:308:PRO:CG	3:B:439:GOL:C3	2.72	0.45
1:A:148:LEU:HD12	1:A:181:ILE:CG2	2.42	0.45
1:B:247:GLN:HG2	1:B:339:MET:SD	2.57	0.45
1:B:331:VAL:HG13	1:B:331:VAL:O	2.17	0.44
1:A:47:ALA:O	1:A:63:SER:HA	2.17	0.44
1:A:198:LYS:C	1:A:199:ILE:HD12	2.42	0.44
1:A:331:VAL:HG12	1:A:336:LEU:HG	2.00	0.44
1:A:228:THR:HA	1:A:335:ARG:O	2.18	0.44
1:B:109:VAL:HG11	1:B:321:VAL:HG11	2.00	0.43
1:B:280:MET:HG2	1:B:289:ALA:HA	1.99	0.43
1:A:283:LYS:HB2	1:A:288:TRP:HZ3	1.84	0.43
1:B:120:HIS:CB	2:B:436:SO4:O2	2.66	0.43
1:A:161:THR:OG1	1:A:199:ILE:CG2	2.64	0.43
1:A:354:GLY:HA3	1:A:415:THR:CG2	2.47	0.43
1:A:10:GLU:HA	1:B:359:PHE:O	2.19	0.43
1:B:228:THR:CG2	1:B:335:ARG:HH11	2.30	0.43
1:A:144:THR:HA	1:A:185:TRP:CH2	2.53	0.43
1:A:310:GLY:CA	1:B:374:ARG:HH22	2.32	0.43
1:B:119:MET:HE2	1:B:120:HIS:CE1	2.54	0.43
1:A:162:LYS:HG2	1:A:172:SER:CB	2.48	0.43
1:A:262:ILE:O	1:A:266:ILE:HG13	2.18	0.43
1:A:103:LYS:HE3	1:A:103:LYS:HB2	1.77	0.42
1:A:214:LEU:HA	1:A:276:PHE:O	2.19	0.42
1:B:175:VAL:HG22	1:B:175:VAL:O	2.19	0.42
1:A:199:ILE:CG2	1:A:200:ILE:N	2.83	0.42
1:B:229:PHE:HA	1:B:230:PRO:HD3	1.77	0.42
1:B:303:THR:HA	1:B:306:SER:OG	2.19	0.42
1:B:8:ARG:NH2	1:B:20:GLN:NE2	2.66	0.42
1:A:305:ALA:HB2	1:A:391:LEU:HD22	2.00	0.42
1:A:359:PHE:CD1	1:A:359:PHE:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLU:OE2	1:A:338:PRO:HG3	2.20	0.42
1:A:200:ILE:HG23	1:A:200:ILE:O	2.20	0.42
1:A:161:THR:O	1:A:172:SER:HB2	2.19	0.42
1:B:359:PHE:CD1	1:B:359:PHE:N	2.88	0.42
1:A:228:THR:HG21	1:A:335:ARG:HH11	1.83	0.41
1:A:151:ALA:O	1:A:155:ILE:HD13	2.20	0.41
1:A:262:ILE:HD12	1:A:280:MET:HE3	2.02	0.41
1:A:286:LYS:HA	1:A:286:LYS:HD3	1.87	0.41
1:A:36:ILE:HG23	1:B:36:ILE:HD13	2.03	0.41
1:A:211:VAL:HA	1:A:233:VAL:O	2.19	0.41
1:B:241:ASP:OD1	1:B:242:TYR:O	2.38	0.41
1:A:164:ILE:HD13	1:A:164:ILE:N	2.34	0.41
1:A:330:TRP:CD1	3:A:438:GOL:H32	2.53	0.41
1:A:369:PRO:O	1:A:403:LYS:HD3	2.21	0.41
1:A:161:THR:CG2	1:A:173:TYR:HB3	2.51	0.41
1:B:415:THR:CG2	1:B:416:ARG:N	2.84	0.41
1:A:120:HIS:CD2	1:A:123:ARG:H	2.39	0.40
1:A:229:PHE:HA	1:A:230:PRO:HD3	1.80	0.40
1:A:159:CYS:N	1:A:175:VAL:O	2.54	0.40
1:A:175:VAL:HG23	1:A:175:VAL:O	2.22	0.40
1:B:124:LEU:HD23	1:B:291:GLU:OE2	2.21	0.40
1:B:8:ARG:HD2	1:B:322:LEU:O	2.20	0.40
1:B:95:LEU:HD23	1:B:116:TRP:CD1	2.44	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)
3:A:441:GOL:O3	3:B:442:GOL:O2[3_555]	2.12	0.08
3:A:441:GOL:C3	3:B:442:GOL:O3[3_555]	2.12	0.08

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	399/433 (92%)	388 (97%)	9 (2%)	2 (0%)	24	27
1	B	397/433 (92%)	388 (98%)	9 (2%)	0	100	100
All	All	796/866 (92%)	776 (98%)	18 (2%)	2 (0%)	36	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	331	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	338/360 (94%)	324 (96%)	14 (4%)	27	36
1	B	336/360 (93%)	323 (96%)	13 (4%)	28	39
All	All	674/720 (94%)	647 (96%)	27 (4%)	28	37

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	7	LEU
1	A	37	GLU
1	A	95	LEU
1	A	128	LEU
1	A	164	ILE
1	A	200	ILE
1	A	216	VAL
1	A	228	THR
1	A	318	LEU
1	A	355	TYR
1	A	356	SER

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Mol	Chain	Res	Type
1	A	387	LEU
1	A	415	THR
1	B	5	ILE
1	B	7	LEU
1	B	148	LEU
1	B	175	VAL
1	B	176	LYS
1	B	228	THR
1	B	242	TYR
1	B	286	LYS
1	B	318	LEU
1	B	355	TYR
1	B	360	ARG
1	B	413	LEU
1	B	415	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	120	HIS
1	A	297	HIS
1	A	370	ASN
1	B	53	ASN
1	B	160	HIS
1	B	204	HIS
1	B	222	ASN
1	B	237	GLN
1	B	243	HIS
1	B	297	HIS
1	B	346	HIS
1	B	370	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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	$\# Z > 2$
2	SO4	B	435	-	4,4,4	0.33	0	6,6,6	0.15	0
3	GOL	A	440	-	5,5,5	0.33	0	5,5,5	0.28	0
3	GOL	A	437	-	5,5,5	0.32	0	5,5,5	0.26	0
3	GOL	A	438	-	5,5,5	0.31	0	5,5,5	0.26	0
3	GOL	A	439	-	5,5,5	0.29	0	5,5,5	0.39	0
3	GOL	B	439	-	5,5,5	0.32	0	5,5,5	0.37	0
3	GOL	B	441	-	5,5,5	0.36	0	5,5,5	0.39	0
2	SO4	B	437	-	4,4,4	0.38	0	6,6,6	0.06	0
2	SO4	B	434	-	4,4,4	0.32	0	6,6,6	0.09	0
3	GOL	A	441	3	5,5,5	0.36	0	5,5,5	0.31	0
3	GOL	B	440	-	5,5,5	0.31	0	5,5,5	0.36	0
3	GOL	A	436	-	5,5,5	0.33	0	5,5,5	0.36	0
3	GOL	B	438	-	5,5,5	0.29	0	5,5,5	0.42	0
3	GOL	B	442	3	5,5,5	0.33	0	5,5,5	0.84	0
2	SO4	A	434	-	4,4,4	0.32	0	6,6,6	0.06	0
2	SO4	B	436	-	4,4,4	0.26	0	6,6,6	0.24	0
2	SO4	A	435	-	4,4,4	0.35	0	6,6,6	0.12	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	A	440	-	-	0/4/4/4	-
3	GOL	A	438	-	-	0/4/4/4	-
3	GOL	A	437	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	439	-	-	0/4/4/4	-
3	GOL	B	439	-	-	0/4/4/4	-
3	GOL	B	441	-	-	2/4/4/4	-
3	GOL	A	441	3	-	4/4/4/4	-
3	GOL	B	440	-	-	0/4/4/4	-
3	GOL	B	442	3	-	4/4/4/4	-
3	GOL	A	436	-	-	0/4/4/4	-
3	GOL	B	438	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	441	GOL	C1-C2-C3-O3
3	A	441	GOL	O2-C2-C3-O3
3	B	442	GOL	C1-C2-C3-O3
3	B	442	GOL	O2-C2-C3-O3
3	A	441	GOL	O1-C1-C2-C3
3	B	441	GOL	O1-C1-C2-C3
3	B	442	GOL	O1-C1-C2-C3
3	A	441	GOL	O1-C1-C2-O2
3	B	441	GOL	O1-C1-C2-O2
3	B	442	GOL	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	440	GOL	4	0
3	A	437	GOL	10	0
3	A	438	GOL	3	0
3	A	439	GOL	2	0
3	B	439	GOL	10	0
3	B	441	GOL	1	0
3	A	441	GOL	3	2
3	A	436	GOL	5	0
3	B	438	GOL	4	0
3	B	442	GOL	3	2

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	436	SO4	3	0
2	A	435	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	405/433 (93%)	0.31	42 (10%) 11 13	16, 32, 79, 97	0
1	B	403/433 (93%)	0.23	46 (11%) 10 11	16, 32, 80, 96	0
All	All	808/866 (93%)	0.27	88 (10%) 10 12	16, 32, 79, 97	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	165	MET	6.7
1	A	159	CYS	6.1
1	A	2	VAL	5.9
1	B	164	ILE	5.8
1	A	423	GLN	5.6
1	A	164	ILE	5.3
1	A	176	LYS	5.2
1	A	185	TRP	4.5
1	B	160	HIS	4.4
1	A	174	PHE	4.4
1	A	3	VAL	4.1
1	B	178	PRO	4.1
1	B	176	LYS	3.9
1	A	163	ALA	3.9
1	B	162	LYS	3.9
1	A	200	ILE	3.8
1	B	238	ILE	3.8
1	A	183	LYS	3.7
1	B	174	PHE	3.6
1	A	237	GLN	3.5
1	A	238	ILE	3.5
1	A	172	SER	3.5
1	A	119	MET	3.4
1	A	197	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	181	ILE	3.3
1	A	173	TYR	3.3
1	B	173	TYR	3.3
1	A	175	VAL	3.3
1	B	141	TYR	3.2
1	B	157	TYR	3.1
1	B	163	ALA	3.1
1	B	140	MET	3.1
1	A	240	GLY	3.1
1	B	236	TYR	3.0
1	B	172	SER	3.0
1	B	180	ASP	3.0
1	A	184	ALA	2.9
1	B	237	GLN	2.9
1	A	180	ASP	2.9
1	B	177	GLY	2.9
1	B	185	TRP	2.9
1	A	205	ILE	2.9
1	B	161	THR	2.8
1	B	240	GLY	2.8
1	B	156	GLY	2.8
1	B	142	ALA	2.7
1	B	201	VAL	2.7
1	A	162	LYS	2.7
1	B	138	ARG	2.7
1	A	236	TYR	2.7
1	A	206	ASP	2.7
1	A	331	VAL	2.6
1	A	161	THR	2.6
1	A	143	THR	2.6
1	B	198	LYS	2.6
1	B	175	VAL	2.5
1	A	257	ARG	2.5
1	A	4	MET	2.5
1	B	241	ASP	2.5
1	A	179	GLU	2.5
1	A	203	GLU	2.5
1	B	205	ILE	2.5
1	A	154	LYS	2.5
1	B	395	LYS	2.5
1	A	120	HIS	2.5
1	B	182	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	423	GLN	2.5
1	B	119	MET	2.4
1	B	123	ARG	2.4
1	B	199	ILE	2.4
1	B	184	ALA	2.4
1	B	179	GLU	2.4
1	A	199	ILE	2.3
1	B	206	ASP	2.3
1	A	144	THR	2.3
1	B	421	HIS	2.3
1	A	395	LYS	2.3
1	A	286	LYS	2.2
1	B	183	LYS	2.2
1	B	91	GLU	2.2
1	A	413	LEU	2.1
1	B	143	THR	2.1
1	A	178	PRO	2.1
1	B	154	LYS	2.1
1	B	239	ASP	2.1
1	A	150	GLU	2.0
1	B	146	ASP	2.0
1	B	257	ARG	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
3	GOL	A	440	6/6	0.65	0.25	55,57,61,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	439	6/6	0.67	0.31	50,56,60,69	0
3	GOL	A	437	6/6	0.68	0.37	43,60,72,84	0
2	SO4	B	437	5/5	0.76	0.24	60,61,64,65	5
3	GOL	B	441	6/6	0.76	0.28	55,64,66,71	0
3	GOL	A	436	6/6	0.77	0.27	54,59,60,61	6
3	GOL	A	438	6/6	0.79	0.22	46,51,53,63	0
3	GOL	B	438	6/6	0.82	0.22	41,50,56,59	0
3	GOL	A	441	6/6	0.85	0.21	44,50,55,55	6
3	GOL	B	442	6/6	0.85	0.24	47,57,68,75	0
2	SO4	B	436	5/5	0.86	0.16	62,64,66,67	5
3	GOL	B	440	6/6	0.86	0.18	37,51,59,61	0
3	GOL	B	439	6/6	0.88	0.18	44,55,59,64	0
2	SO4	A	435	5/5	0.91	0.14	56,57,69,69	0
2	SO4	B	435	5/5	0.93	0.14	56,57,62,66	0
2	SO4	A	434	5/5	0.96	0.09	38,44,48,54	0
2	SO4	B	434	5/5	0.98	0.08	36,41,48,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.