



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:43 PM GMT

PDB ID : 1KFI
Title : Crystal Structure of the Exocytosis-Sensitive Phosphoprotein, pp63/Parafusin (phosphoglucomutase) from Paramecium
Authors : Mueller, S.; Diederichs, K.; Breed, J.; Kissmehl, R.; Hauser, K.; Plattner, H.; Welte, W.
Deposited on : 2001-11-21
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

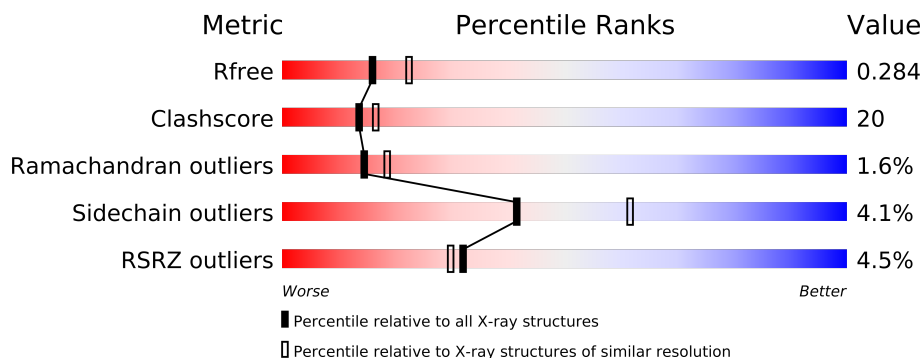
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	572	
1	B	572	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9207 atoms, of which 0 are hydrogen and 0 are deuterium.

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 phosphoglucomutase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	570	Total	C	N	O	S	0	0	0
			4490	2858	769	850	13			
1	B	570	Total	C	N	O	S	0	0	0
			4490	2858	769	850	13			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

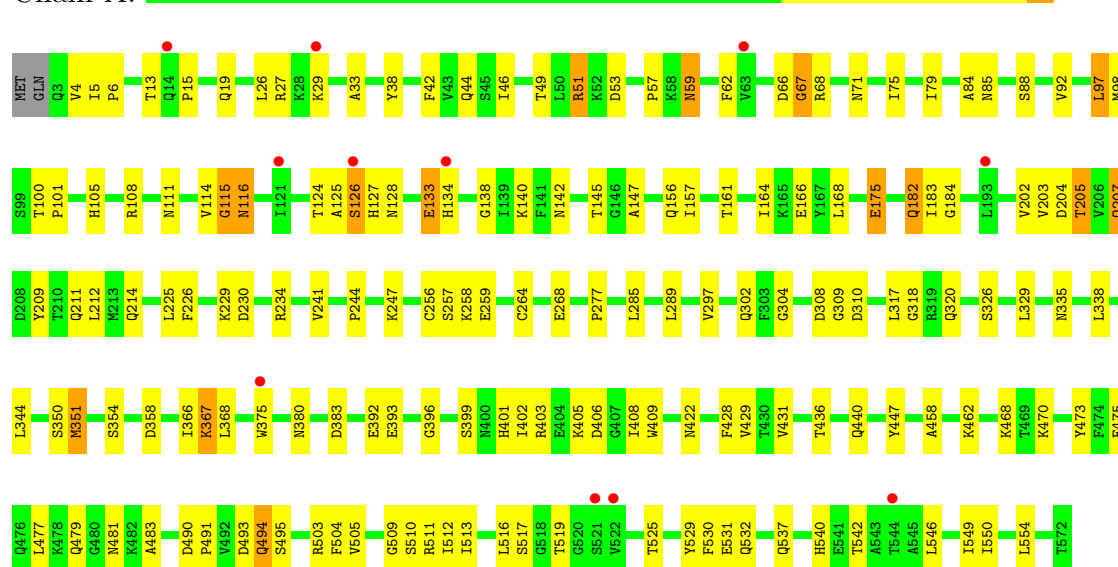
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	126	Total	O	0	0
			126	126		
4	B	79	Total	O	0	0
			79	79		

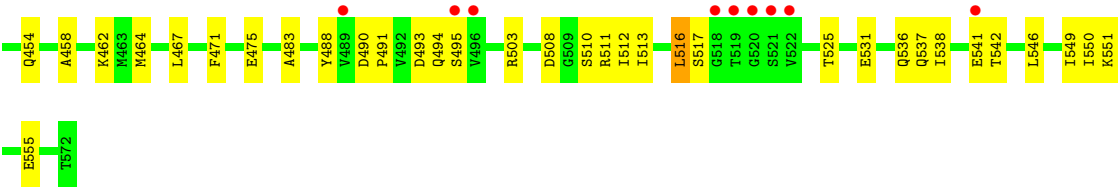
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: phosphoglucumutase 1

Chain A:





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.35Å 133.61Å 150.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 27.96 – 2.42	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.40) 93.8 (27.96-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.89 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.286 0.233 , 0.284	Depositor DCC
R_{free} test set	971 reflections (1.96%)	DCC
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 32.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 49705 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9207	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.37	0/4592	0.62	0/6207
1	B	0.36	0/4592	0.61	1/6207 (0.0%)
All	All	0.37	0/9184	0.61	1/12414 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	541	GLU	N-CA-C	-5.34	96.59	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4490	0	4386	160	0
1	B	4490	0	4386	205	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	126	0	0	4	0
4	B	79	0	0	7	0
All	All	9207	0	8772	358	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (358) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:124:THR:HG22	1:A:126:SER:H	1.12	1.10
1:B:375:TRP:CZ3	1:B:405:LYS:HB2	1.96	1.01
1:A:375:TRP:NE1	1:A:405:LYS:HE3	1.81	0.95
1:A:422:ASN:HD21	1:A:429:VAL:H	1.17	0.91
1:B:91:HIS:HD2	1:B:106:TYR:OH	1.55	0.89
1:A:422:ASN:HD21	1:A:429:VAL:N	1.76	0.83
1:A:59:ASN:ND2	1:A:88:SER:H	1.78	0.81
1:B:422:ASN:HD21	1:B:429:VAL:N	1.78	0.81
1:B:351:MET:CE	1:B:513:ILE:HG12	2.10	0.81
1:A:422:ASN:ND2	1:A:429:VAL:H	1.79	0.81
1:B:19:GLN:HE21	1:B:161:THR:HB	1.46	0.80
1:B:8:PRO:HA	1:B:170:VAL:HG12	1.64	0.78
1:B:169:THR:HG22	1:B:170:VAL:H	1.48	0.78
1:B:133:GLU:HG2	1:B:134:HIS:H	1.49	0.77
1:A:124:THR:HG22	1:A:126:SER:N	1.95	0.77
1:A:396:GLY:HA3	1:A:405:LYS:HE2	1.67	0.77
1:B:302:GLN:HG2	1:B:428:PHE:CE1	2.19	0.76
1:A:285:LEU:CD1	1:A:317:LEU:HD12	2.15	0.76
1:A:302:GLN:HG2	1:A:428:PHE:CE2	2.20	0.76
1:A:399:SER:HB3	1:A:401:HIS:HD2	1.51	0.75
1:B:285:LEU:HD12	1:B:317:LEU:HD12	1.67	0.75
1:B:232:SER:HB2	1:B:302:GLN:H	1.50	0.75
1:A:44:GLN:HE22	1:A:85:ASN:HD21	1.34	0.75
1:B:297:VAL:HG23	1:B:298:GLY:H	1.52	0.75
1:B:422:ASN:HD21	1:B:429:VAL:H	1.34	0.74
1:B:312:ASP:OD1	1:B:375:TRP:HH2	1.70	0.74
1:B:68:ARG:NH1	1:B:125:ALA:H	1.86	0.73
1:A:66:ASP:OD1	1:A:124:THR:HG23	1.87	0.73
1:B:351:MET:HE1	1:B:513:ILE:HG12	1.70	0.73
1:B:236:ASP:HB2	1:B:285:LEU:HD23	1.70	0.73
1:B:62:PHE:CZ	1:B:98:MET:HG2	2.23	0.73
1:B:182:GLN:O	1:B:202:VAL:HG11	1.89	0.73
1:A:140:LYS:HE2	1:A:142:ASN:HD21	1.52	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:62:PHE:HZ	1:B:98:MET:HG2	1.54	0.72
1:B:33:ALA:HA	1:B:38:TYR:CD2	2.25	0.71
1:A:19:GLN:HE21	1:A:161:THR:HB	1.55	0.71
1:A:182:GLN:O	1:A:202:VAL:HG11	1.93	0.69
1:B:295:LYS:NZ	1:B:296:ASP:H	1.91	0.69
1:A:542:THR:HG23	4:A:805:HOH:O	1.93	0.69
1:B:258:LYS:H	1:B:258:LYS:HE2	1.58	0.68
1:B:19:GLN:NE2	1:B:161:THR:HB	2.10	0.67
1:A:436:THR:O	1:A:440:GLN:HG3	1.93	0.67
1:B:133:GLU:CD	1:B:133:GLU:H	1.98	0.67
1:B:375:TRP:CH2	1:B:405:LYS:HB2	2.29	0.67
1:B:39:LEU:HD21	1:B:74:ALA:HA	1.76	0.66
1:B:183:ILE:HA	1:B:202:VAL:HG13	1.77	0.66
1:B:314:ASN:HD22	1:B:316:ILE:HD13	1.59	0.66
1:B:351:MET:HE3	1:B:513:ILE:HG12	1.77	0.66
1:B:350:SER:HB2	1:B:392:GLU:HG2	1.76	0.66
1:B:83:TYR:CE1	1:B:170:VAL:HG11	2.31	0.66
1:A:97:LEU:O	1:A:205:THR:HB	1.96	0.65
1:A:318:GLY:HA3	1:A:431:VAL:CG2	2.27	0.65
1:B:15:PRO:HG3	1:B:164:ILE:O	1.97	0.65
1:B:66:ASP:OD2	1:B:68:ARG:NH1	2.30	0.64
1:A:71:ASN:O	1:A:75:ILE:HG13	1.97	0.64
1:A:351:MET:HE2	1:A:351:MET:O	1.98	0.64
1:A:358:ASP:HA	1:A:368:LEU:HD22	1.80	0.64
1:A:68:ARG:CZ	1:A:125:ALA:HB3	2.28	0.64
1:A:105:HIS:CD2	1:A:212:LEU:HD22	2.34	0.63
1:A:29:LYS:NZ	1:A:134:HIS:HA	2.14	0.63
1:A:289:LEU:HD22	1:A:317:LEU:HB2	1.79	0.63
1:B:436:THR:O	1:B:440:GLN:HG3	2.00	0.62
1:A:15:PRO:HG3	1:A:164:ILE:O	2.00	0.62
1:B:285:LEU:CD1	1:B:317:LEU:HD12	2.29	0.62
1:A:375:TRP:HE1	1:A:405:LYS:HE3	1.61	0.61
1:B:351:MET:HE2	1:B:511:ARG:HH21	1.65	0.61
1:A:318:GLY:HA3	1:A:431:VAL:HG22	1.81	0.61
1:B:406:ASP:HB3	1:B:409:TRP:HB3	1.83	0.61
1:A:62:PHE:CZ	1:A:98:MET:HG2	2.36	0.60
1:A:351:MET:HE3	1:A:513:ILE:HG12	1.82	0.60
1:A:51:ARG:HH21	1:B:51:ARG:HH21	1.47	0.60
1:A:59:ASN:ND2	1:A:59:ASN:H	2.00	0.60
1:B:285:LEU:HD13	1:B:289:LEU:HD13	1.84	0.60
1:B:422:ASN:ND2	1:B:429:VAL:H	1.99	0.60
1:B:157:ILE:O	1:B:161:THR:HG23	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:286:VAL:HG13	1:B:291:ILE:CG1	2.32	0.60
1:B:406:ASP:OD2	1:B:409:TRP:HB2	2.02	0.60
1:B:83:TYR:CD1	1:B:170:VAL:HG11	2.36	0.59
1:A:358:ASP:CG	1:A:368:LEU:HD21	2.22	0.59
1:B:314:ASN:ND2	1:B:316:ILE:HD13	2.18	0.59
1:A:207:GLN:HE21	1:A:207:GLN:HA	1.68	0.59
1:A:75:ILE:O	1:A:79:ILE:HG13	2.02	0.59
1:B:91:HIS:CD2	1:B:106:TYR:OH	2.46	0.59
1:B:312:ASP:OD1	1:B:375:TRP:CH2	2.53	0.58
1:A:100:THR:HB	1:A:101:PRO:HD3	1.85	0.58
1:B:12:VAL:HA	1:B:166:GLU:HB3	1.85	0.58
1:A:124:THR:HG21	1:A:310:ASP:HB3	1.85	0.58
1:A:68:ARG:HD3	4:A:733:HOH:O	2.03	0.58
1:A:380:ASN:HD21	1:B:52:LYS:CE	2.15	0.58
1:B:511:ARG:NH1	1:B:531:GLU:OE1	2.36	0.58
1:A:375:TRP:CZ2	1:A:405:LYS:HB3	2.39	0.58
1:A:145:THR:HG23	1:B:53:ASP:HB2	1.86	0.58
1:B:27:ARG:NH1	1:B:128:ASN:ND2	2.52	0.58
1:B:74:ALA:O	1:B:78:ILE:HG13	2.03	0.58
1:A:126:SER:HB2	3:A:601:SO4:O1	2.04	0.57
1:A:209:TYR:OH	1:A:408:ILE:HB	2.05	0.57
1:A:59:ASN:HD21	1:A:88:SER:H	1.53	0.57
1:B:21:PRO:HG3	1:B:42:PHE:CZ	2.40	0.57
1:B:314:ASN:HD22	1:B:316:ILE:CD1	2.18	0.57
1:B:229:LYS:HG3	1:B:230:ASP:OD1	2.05	0.57
1:B:26:LEU:HD23	1:B:139:ILE:HD13	1.87	0.56
1:B:13:THR:HG22	1:B:166:GLU:CA	2.36	0.56
1:B:111:ASN:HA	1:B:115:GLY:HA2	1.87	0.56
1:A:75:ILE:HD13	1:A:92:VAL:HG21	1.86	0.56
1:B:351:MET:CE	1:B:511:ARG:HH21	2.19	0.56
1:B:140:LYS:NZ	1:B:142:ASN:HD21	2.03	0.56
1:B:142:ASN:N	1:B:142:ASN:HD22	2.02	0.56
1:B:256:CYS:SG	1:B:261:LEU:HD21	2.46	0.56
1:A:509:GLY:O	1:A:511:ARG:HG3	2.06	0.56
1:A:257:SER:OG	1:A:259:GLU:HG2	2.05	0.55
1:A:59:ASN:H	1:A:59:ASN:HD22	1.55	0.55
1:A:351:MET:CE	1:A:513:ILE:HD13	2.37	0.55
1:B:185:VAL:HG12	1:B:187:LYS:HD2	1.87	0.55
1:A:108:ARG:NH1	1:A:403:ARG:NH1	2.55	0.55
1:A:399:SER:HB3	1:A:401:HIS:CD2	2.37	0.55
1:A:229:LYS:HG3	1:A:230:ASP:OD1	2.07	0.55
1:B:152:ASP:O	1:B:156:GLN:HG2	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:114:VAL:O	1:B:116:ASN:N	2.40	0.55
1:B:258:LYS:CE	1:B:258:LYS:H	2.19	0.55
1:B:290:ASP:O	1:B:320:GLN:HG2	2.06	0.55
1:B:375:TRP:N	1:B:375:TRP:CD1	2.73	0.55
1:A:68:ARG:NH2	1:A:125:ALA:HB3	2.22	0.54
1:B:297:VAL:HG23	1:B:298:GLY:N	2.21	0.54
1:B:219:PHE:O	1:B:223:LYS:HB2	2.07	0.54
1:A:66:ASP:OD2	1:A:68:ARG:HD2	2.07	0.54
1:B:75:ILE:HD13	1:B:92:VAL:HG21	1.89	0.54
1:B:183:ILE:HG22	1:B:184:GLY:N	2.23	0.53
1:B:374:GLY:O	1:B:377:PHE:HD1	1.91	0.53
1:B:246:ALA:O	1:B:250:PHE:HB2	2.08	0.53
1:B:13:THR:HG22	1:B:166:GLU:N	2.23	0.53
1:A:380:ASN:HD21	1:B:52:LYS:HE2	1.72	0.53
1:A:493:ASP:OD2	1:A:495:SER:HB2	2.08	0.53
1:A:51:ARG:HH21	1:B:51:ARG:NH2	2.05	0.53
1:B:26:LEU:HD11	1:B:28:LYS:HE2	1.89	0.53
1:A:62:PHE:HZ	1:A:98:MET:HG2	1.73	0.53
1:A:473:TYR:CZ	1:A:477:LEU:HD21	2.44	0.53
1:B:21:PRO:HG3	1:B:42:PHE:HZ	1.75	0.52
1:A:517:SER:HB3	1:A:525:THR:HB	1.91	0.52
1:B:359:LYS:O	1:B:363:LYS:HG2	2.09	0.52
1:B:68:ARG:CZ	1:B:125:ALA:HB3	2.40	0.52
1:A:133:GLU:CD	1:A:133:GLU:H	2.12	0.52
1:B:42:PHE:CE2	1:B:139:ILE:HB	2.46	0.51
1:B:203:VAL:HG22	1:B:204:ASP:N	2.26	0.51
1:A:13:THR:HG22	1:A:166:GLU:HA	1.92	0.51
1:B:51:ARG:N	1:B:51:ARG:HD2	2.25	0.51
1:A:326:SER:HB3	1:A:354:SER:OG	2.11	0.51
1:B:239:HIS:NE2	1:B:263:ASN:ND2	2.59	0.51
1:A:447:TYR:HA	1:A:530:PHE:O	2.11	0.51
1:B:58:LYS:HE3	4:B:751:HOH:O	2.11	0.51
1:A:124:THR:CG2	1:A:126:SER:H	2.02	0.51
1:A:396:GLY:CA	1:A:405:LYS:HE2	2.38	0.51
1:B:286:VAL:HG13	1:B:291:ILE:HG13	1.92	0.51
1:B:13:THR:HG22	1:B:166:GLU:HA	1.91	0.51
1:B:42:PHE:HE2	1:B:139:ILE:HB	1.76	0.50
1:B:546:LEU:O	1:B:549:ILE:HG22	2.11	0.50
1:A:396:GLY:HA3	1:A:405:LYS:CE	2.40	0.50
1:B:291:ILE:HD11	1:B:317:LEU:HD13	1.92	0.50
1:B:66:ASP:CG	1:B:68:ARG:NH1	2.65	0.50
1:A:114:VAL:O	1:A:116:ASN:N	2.42	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:289:LEU:HD22	1:A:317:LEU:CB	2.41	0.50
1:B:165:LYS:O	1:B:166:GLU:HB3	2.12	0.50
1:A:350:SER:HB3	1:A:392:GLU:HG2	1.92	0.50
1:A:277:PRO:CD	1:A:308:ASP:HB3	2.42	0.50
1:A:66:ASP:OD2	1:A:66:ASP:O	2.29	0.50
1:B:295:LYS:HZ2	1:B:296:ASP:H	1.58	0.50
1:B:193:LEU:O	1:B:194:GLU:HB2	2.11	0.50
1:A:211:GLN:HA	1:A:214:GLN:HE21	1.76	0.50
1:A:511:ARG:O	1:A:549:ILE:HD11	2.12	0.49
1:A:183:ILE:HA	1:A:202:VAL:HG13	1.95	0.49
1:A:126:SER:O	1:A:128:ASN:N	2.45	0.49
1:B:513:ILE:HD12	1:B:513:ILE:N	2.27	0.49
1:A:403:ARG:HG3	1:A:403:ARG:HH11	1.77	0.49
1:B:517:SER:HB3	1:B:525:THR:HB	1.94	0.49
1:B:39:LEU:CD2	1:B:74:ALA:HA	2.41	0.49
1:B:265:ASP:HB2	4:B:772:HOH:O	2.12	0.49
1:B:139:ILE:H	1:B:139:ILE:HD12	1.77	0.49
1:A:108:ARG:HH12	1:A:403:ARG:HH12	1.61	0.49
1:A:27:ARG:NH1	1:A:27:ARG:HB3	2.28	0.49
1:B:238:MET:HE1	1:B:276:ASP:N	2.28	0.48
1:A:44:GLN:HE22	1:A:85:ASN:ND2	2.07	0.48
1:B:517:SER:CB	1:B:525:THR:HB	2.43	0.48
1:B:100:THR:HB	1:B:101:PRO:HD3	1.96	0.48
1:A:483:ALA:HA	1:A:503:ARG:O	2.13	0.48
1:A:258:LYS:HE2	1:A:258:LYS:H	1.78	0.48
1:A:335:ASN:HD22	1:A:338:LEU:HD12	1.78	0.48
1:B:183:ILE:CG2	1:B:184:GLY:N	2.75	0.48
1:A:27:ARG:HB3	1:A:27:ARG:HH11	1.78	0.48
1:A:513:ILE:HB	1:A:529:TYR:HB2	1.96	0.48
1:A:108:ARG:HH12	1:A:403:ARG:NH1	2.11	0.48
1:B:4:VAL:HA	1:B:189:GLU:O	2.14	0.48
1:B:351:MET:HB3	1:B:352:PRO:HD3	1.96	0.48
1:B:150:PRO:HG3	4:B:775:HOH:O	2.13	0.48
1:A:289:LEU:HD21	1:A:304:GLY:N	2.29	0.47
1:B:131:GLY:HA3	1:B:133:GLU:OE2	2.14	0.47
1:B:186:TYR:HE1	1:B:202:VAL:HG12	1.79	0.47
1:A:458:ALA:O	1:A:462:LYS:HG3	2.14	0.47
1:B:139:ILE:HD12	1:B:139:ILE:N	2.30	0.47
1:B:458:ALA:O	1:B:462:LYS:HG3	2.14	0.47
1:B:464:MET:HA	1:B:467:LEU:HD12	1.97	0.47
1:B:234:ARG:CD	1:B:288:LEU:HD13	2.45	0.47
1:B:399:SER:HB3	1:B:401:HIS:ND1	2.30	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:378:PHE:O	1:B:382:MET:HG3	2.14	0.47
1:A:203:VAL:HG22	1:A:204:ASP:N	2.29	0.47
1:A:318:GLY:HA3	1:A:431:VAL:HG21	1.95	0.47
1:A:351:MET:HE2	1:A:511:ARG:NH2	2.30	0.47
1:A:403:ARG:CG	1:A:403:ARG:HH11	2.28	0.47
1:B:551:LYS:O	1:B:555:GLU:HG3	2.15	0.47
1:B:351:MET:HE3	1:B:513:ILE:CG1	2.43	0.47
1:A:19:GLN:NE2	1:A:161:THR:HB	2.27	0.47
1:A:277:PRO:HD2	1:A:308:ASP:HB3	1.97	0.47
1:B:471:PHE:O	1:B:475:GLU:HG3	2.14	0.47
1:A:285:LEU:HD13	1:A:317:LEU:HD12	1.92	0.47
1:A:205:THR:HG23	4:A:812:HOH:O	2.15	0.46
1:A:546:LEU:O	1:A:549:ILE:HG22	2.15	0.46
1:B:239:HIS:H	1:B:263:ASN:HB3	1.80	0.46
1:B:232:SER:HB2	1:B:302:GLN:N	2.27	0.46
1:A:510:SER:C	1:A:511:ARG:HG3	2.35	0.46
1:B:147:ALA:HB2	1:B:403:ARG:HB3	1.97	0.46
1:B:295:LYS:HZ2	1:B:295:LYS:HB3	1.81	0.46
1:A:351:MET:HE1	1:A:513:ILE:HD13	1.96	0.46
1:B:185:VAL:CG1	1:B:187:LYS:HD2	2.45	0.46
1:B:209:TYR:OH	1:B:408:ILE:HB	2.15	0.46
1:B:351:MET:O	1:B:511:ARG:NH2	2.48	0.46
1:A:519:THR:HG22	1:A:519:THR:O	2.15	0.46
1:A:383:ASP:OD2	1:A:403:ARG:NH1	2.48	0.46
1:A:111:ASN:HB3	1:B:57:PRO:HB3	1.98	0.46
1:A:84:ALA:HB1	1:A:168:LEU:HB3	1.97	0.46
1:A:66:ASP:O	1:A:71:ASN:ND2	2.49	0.46
1:A:67:GLY:O	1:A:268:GLU:HA	2.16	0.46
1:A:124:THR:HG21	1:A:310:ASP:CB	2.46	0.45
1:A:59:ASN:HD22	1:A:59:ASN:N	2.14	0.45
1:B:510:SER:C	1:B:511:ARG:HG3	2.36	0.45
1:B:327:ASP:O	1:B:331:VAL:HG23	2.16	0.45
1:B:109:LYS:O	1:B:113:GLU:HG3	2.16	0.45
1:B:210:THR:HG23	1:B:249:ILE:HG12	1.97	0.45
1:A:258:LYS:CE	1:A:258:LYS:H	2.29	0.45
1:A:247:LYS:HE3	1:A:264:CYS:O	2.17	0.45
1:B:288:LEU:O	1:B:301:PRO:HD2	2.17	0.45
1:B:429:VAL:HG13	1:B:433:GLU:OE2	2.17	0.45
1:A:511:ARG:CZ	1:A:513:ILE:HD11	2.47	0.45
1:B:122:ILE:HB	1:B:140:LYS:HG2	1.98	0.45
1:A:42:PHE:O	1:A:46:ILE:HG13	2.15	0.45
1:A:126:SER:C	1:A:128:ASN:H	2.20	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:234:ARG:HD3	1:B:288:LEU:HD13	1.98	0.45
1:A:157:ILE:O	1:A:161:THR:HG23	2.17	0.45
1:A:532:GLN:HB3	1:A:546:LEU:HD23	1.99	0.45
1:A:101:PRO:HG3	1:A:405:LYS:O	2.17	0.45
1:A:302:GLN:HG3	4:A:775:HOH:O	2.17	0.45
1:B:71:ASN:O	1:B:75:ILE:HG13	2.16	0.45
1:B:33:ALA:O	1:B:38:TYR:HB3	2.17	0.45
1:A:530:PHE:CE1	1:A:550:ILE:HA	2.51	0.45
1:B:393:GLU:HG3	1:B:447:TYR:OH	2.17	0.45
1:B:375:TRP:N	1:B:375:TRP:HD1	2.15	0.44
1:B:236:ASP:OD1	1:B:238:MET:N	2.44	0.44
1:B:92:VAL:O	1:B:202:VAL:HA	2.17	0.44
1:A:59:ASN:ND2	1:A:88:SER:N	2.58	0.44
1:B:202:VAL:O	1:B:202:VAL:HG13	2.17	0.44
1:B:290:ASP:OD1	1:B:293:LYS:HA	2.17	0.44
1:A:125:ALA:O	1:A:126:SER:O	2.35	0.44
1:B:285:LEU:HD12	1:B:317:LEU:CD1	2.43	0.44
1:B:11:GLN:O	1:B:166:GLU:HA	2.18	0.44
1:A:490:ASP:HA	1:A:491:PRO:HD3	1.87	0.44
1:A:504:PHE:HB2	1:A:512:ILE:HB	1.99	0.44
1:B:312:ASP:OD1	1:B:312:ASP:C	2.56	0.44
1:A:111:ASN:HA	1:A:115:GLY:HA2	1.99	0.44
1:A:490:ASP:O	1:A:494:GLN:HA	2.17	0.44
1:A:537:GLN:HB3	1:A:540:HIS:NE2	2.32	0.44
1:B:69:TYR:O	1:B:70:PHE:HB3	2.17	0.44
1:B:68:ARG:NH2	1:B:128:ASN:O	2.51	0.44
1:A:59:ASN:HD21	1:A:88:SER:N	2.14	0.44
1:B:368:LEU:HD13	1:B:369:PHE:N	2.33	0.44
1:B:375:TRP:CD2	1:B:405:LYS:HD3	2.53	0.43
1:B:295:LYS:HZ3	1:B:296:ASP:H	1.64	0.43
1:B:37:ASN:HA	1:B:40:GLU:OE2	2.18	0.43
1:A:26:LEU:O	1:A:138:GLY:HA2	2.17	0.43
1:B:66:ASP:OD1	1:B:68:ARG:HG2	2.18	0.43
1:A:297:VAL:HG12	1:A:320:GLN:NE2	2.33	0.43
1:A:241:VAL:HG12	1:A:309:GLY:O	2.18	0.43
1:B:351:MET:CE	1:B:511:ARG:NH2	2.82	0.43
1:A:380:ASN:HD21	1:B:52:LYS:HE3	1.83	0.43
1:B:284:ASP:HB2	4:B:731:HOH:O	2.17	0.43
1:B:302:GLN:HG3	4:B:750:HOH:O	2.18	0.43
1:A:13:THR:HG22	1:A:166:GLU:CA	2.48	0.43
1:B:42:PHE:O	1:B:46:ILE:HG13	2.19	0.43
1:B:488:TYR:OH	1:B:491:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:66:ASP:OD1	1:B:68:ARG:NH1	2.51	0.43
1:B:27:ARG:NH1	1:B:128:ASN:HD21	2.17	0.43
1:B:49:THR:HG23	1:B:156:GLN:HB2	2.01	0.43
1:B:546:LEU:O	1:B:550:ILE:HG13	2.19	0.43
1:B:5:ILE:N	1:B:189:GLU:O	2.50	0.43
1:A:49:THR:HG23	1:A:156:GLN:HB2	1.99	0.43
1:B:328:SER:O	1:B:332:ILE:HG13	2.19	0.43
1:B:239:HIS:N	1:B:263:ASN:HB3	2.34	0.43
1:B:375:TRP:NE1	1:B:392:GLU:OE1	2.52	0.42
1:B:276:ASP:HB3	1:B:281:TYR:CD2	2.54	0.42
1:A:5:ILE:HA	1:A:6:PRO:HD3	1.84	0.42
1:B:129:PRO:HG3	1:B:274:HIS:HA	2.01	0.42
1:B:221:LEU:HG	1:B:419:ALA:HB1	2.01	0.42
1:B:510:SER:O	1:B:511:ARG:HG3	2.19	0.42
1:A:184:GLY:N	1:A:202:VAL:HG13	2.34	0.42
1:B:100:THR:N	1:B:101:PRO:CD	2.83	0.42
1:A:406:ASP:HB3	1:A:409:TRP:HB3	2.02	0.42
1:A:351:MET:O	1:A:511:ARG:NH2	2.46	0.42
1:A:422:ASN:ND2	1:A:428:PHE:HA	2.35	0.42
1:B:39:LEU:HD21	1:B:74:ALA:CA	2.47	0.42
1:A:344:LEU:HD23	1:A:366:ILE:HG21	2.02	0.42
1:B:344:LEU:HB2	4:B:738:HOH:O	2.19	0.42
1:B:295:LYS:NZ	1:B:295:LYS:HB3	2.35	0.42
1:B:147:ALA:HB2	1:B:403:ARG:CB	2.50	0.42
1:B:493:ASP:O	1:B:495:SER:N	2.53	0.42
1:A:468:LYS:C	1:A:470:LYS:H	2.23	0.42
1:A:351:MET:HE2	1:A:511:ARG:HH21	1.85	0.42
1:B:163:LYS:HG2	1:B:163:LYS:O	2.19	0.42
1:A:33:ALA:HA	1:A:38:TYR:CD2	2.55	0.42
1:A:59:ASN:ND2	1:A:59:ASN:N	2.60	0.42
1:A:124:THR:CG2	1:A:310:ASP:HB3	2.48	0.41
1:B:512:ILE:C	1:B:513:ILE:HD12	2.41	0.41
1:A:29:LYS:HZ3	1:A:134:HIS:HA	1.82	0.41
1:A:147:ALA:HB2	1:A:403:ARG:HB3	2.02	0.41
1:B:61:LEU:HD22	1:B:87:ILE:HD13	2.02	0.41
1:A:29:LYS:HZ1	1:A:134:HIS:HA	1.82	0.41
1:A:367:LYS:HD2	1:A:367:LYS:HA	1.87	0.41
1:B:211:GLN:HA	1:B:214:GLN:NE2	2.35	0.41
1:B:63:VAL:HA	1:B:121:ILE:O	2.20	0.41
1:B:133:GLU:HB2	1:B:134:HIS:CE1	2.55	0.41
1:B:30:VAL:O	1:B:33:ALA:N	2.54	0.41
1:A:207:GLN:HE21	1:A:207:GLN:CA	2.33	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:508:ASP:C	1:B:508:ASP:OD1	2.58	0.41
1:A:175:GLU:H	1:A:175:GLU:HG2	1.45	0.41
1:B:536:GLN:O	1:B:538:ILE:N	2.53	0.41
1:A:401:HIS:HE1	1:A:406:ASP:OD2	2.04	0.41
1:A:511:ARG:NH1	1:A:531:GLU:OE2	2.50	0.41
1:B:26:LEU:HD11	1:B:28:LYS:CE	2.50	0.41
1:A:53:ASP:O	1:A:57:PRO:HD3	2.20	0.41
1:B:364:ASN:N	1:B:364:ASN:HD22	2.18	0.41
1:B:375:TRP:HZ2	4:B:702:HOH:O	2.03	0.41
1:B:167:TYR:CE1	1:B:169:THR:OG1	2.73	0.41
1:B:277:PRO:CD	1:B:308:ASP:HB3	2.50	0.41
1:B:516:LEU:HD12	1:B:516:LEU:HA	1.85	0.41
1:A:226:PHE:HE2	1:A:256:CYS:HB3	1.86	0.41
1:A:475:GLU:HA	1:A:481:ASN:HB2	2.02	0.41
1:B:435:VAL:O	1:B:438:TYR:HB3	2.20	0.41
1:B:231:PHE:HD1	1:B:428:PHE:HZ	1.69	0.41
1:B:49:THR:HG23	1:B:156:GLN:CB	2.50	0.41
1:A:473:TYR:CE1	1:A:477:LEU:HD21	2.56	0.41
1:B:277:PRO:HD3	1:B:308:ASP:CA	2.51	0.41
1:B:329:LEU:HG	1:B:391:GLY:HA3	2.03	0.41
1:A:66:ASP:O	1:A:68:ARG:N	2.48	0.40
1:B:490:ASP:HA	1:B:491:PRO:HD3	1.90	0.40
1:B:44:GLN:HG2	1:B:167:TYR:CB	2.51	0.40
1:B:203:VAL:CG2	1:B:204:ASP:N	2.84	0.40
1:B:72:ARG:O	1:B:75:ILE:HB	2.22	0.40
1:B:331:VAL:HG11	1:B:414:TRP:CH2	2.57	0.40
1:A:241:VAL:O	1:A:244:PRO:HD2	2.22	0.40
1:B:211:GLN:HA	1:B:214:GLN:HE21	1.86	0.40
1:A:380:ASN:HA	1:A:380:ASN:HD22	1.69	0.40
1:A:550:ILE:O	1:A:554:LEU:HG	2.22	0.40
1:B:483:ALA:HA	1:B:503:ARG:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	568/572 (99%)	531 (94%)	28 (5%)	9 (2%)	14	18
1	B	568/572 (99%)	515 (91%)	44 (8%)	9 (2%)	14	18
All	All	1136/1144 (99%)	1046 (92%)	72 (6%)	18 (2%)	14	18

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	SER
1	A	127	HIS
1	B	494	GLN
1	A	115	GLY
1	A	133	GLU
1	B	115	GLY
1	B	424	ASN
1	A	479	GLN
1	B	166	GLU
1	A	4	VAL
1	A	67	GLY
1	B	4	VAL
1	B	133	GLU
1	B	537	GLN
1	A	402	ILE
1	A	494	GLN
1	B	402	ILE
1	B	298	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	479/481 (100%)	463 (97%)	16 (3%)	50	71
1	B	479/481 (100%)	456 (95%)	23 (5%)	35	53
All	All	958/962 (100%)	919 (96%)	39 (4%)	41	61

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	59	ASN
1	A	97	LEU
1	A	116	ASN
1	A	175	GLU
1	A	182	GLN
1	A	205	THR
1	A	207	GLN
1	A	225	LEU
1	A	234	ARG
1	A	329	LEU
1	A	351	MET
1	A	367	LYS
1	A	393	GLU
1	A	505	VAL
1	A	516	LEU
1	B	51	ARG
1	B	91	HIS
1	B	134	HIS
1	B	139	ILE
1	B	142	ASN
1	B	187	LYS
1	B	205	THR
1	B	230	ASP
1	B	234	ARG
1	B	258	LYS
1	B	262	LEU
1	B	296	ASP
1	B	325	PRO
1	B	329	LEU
1	B	344	LEU
1	B	351	MET
1	B	389	LEU
1	B	393	GLU
1	B	405	LYS
1	B	441	GLN
1	B	454	GLN
1	B	516	LEU
1	B	542	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	19	GLN
1	A	37	ASN
1	A	41	ASN
1	A	59	ASN
1	A	73	GLN
1	A	85	ASN
1	A	105	HIS
1	A	116	ASN
1	A	128	ASN
1	A	142	ASN
1	A	207	GLN
1	A	214	GLN
1	A	239	HIS
1	A	263	ASN
1	A	320	GLN
1	A	335	ASN
1	A	337	ASN
1	A	364	ASN
1	A	380	ASN
1	A	401	HIS
1	A	422	ASN
1	A	441	GLN
1	A	461	ASN
1	A	472	GLN
1	A	476	GLN
1	A	479	GLN
1	A	500	GLN
1	A	561	GLN
1	A	566	ASN
1	B	14	GLN
1	B	19	GLN
1	B	37	ASN
1	B	44	GLN
1	B	48	ASN
1	B	85	ASN
1	B	91	HIS
1	B	142	ASN
1	B	179	ASN
1	B	207	GLN
1	B	214	GLN
1	B	263	ASN
1	B	314	ASN

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Mol	Chain	Res	Type
1	B	320	GLN
1	B	335	ASN
1	B	337	ASN
1	B	364	ASN
1	B	380	ASN
1	B	422	ASN
1	B	461	ASN
1	B	472	GLN
1	B	479	GLN
1	B	481	ASN
1	B	561	GLN
1	B	566	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	SO4	A	601	2	4,4,4	0.29	0	6,6,6	0.14	0
3	SO4	A	603	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	B	602	2	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	B	604	-	4,4,4	0.28	0	6,6,6	0.10	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	SO4	A	601	2	-	0/0/0/0	0/0/0/0
3	SO4	A	603	-	-	0/0/0/0	0/0/0/0
3	SO4	B	602	2	-	0/0/0/0	0/0/0/0
3	SO4	B	604	-	-	0/0/0/0	0/0/0/0

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	570/572 (99%)	0.02	11 (1%) 64 61	11, 29, 52, 85	0
1	B	570/572 (99%)	0.32	41 (7%) 15 13	10, 31, 54, 86	0
All	All	1140/1144 (99%)	0.17	52 (4%) 32 29	10, 30, 53, 86	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	522	VAL	7.2
1	A	522	VAL	6.8
1	B	521	SER	6.1
1	B	520	GLY	5.4
1	B	134	HIS	4.2
1	B	23	THR	3.8
1	B	375	TRP	3.8
1	B	296	ASP	3.8
1	B	22	GLY	3.7
1	B	295	LYS	3.6
1	B	12	VAL	3.5
1	A	521	SER	3.5
1	B	13	THR	3.4
1	B	519	THR	3.2
1	B	426	ASP	3.2
1	B	518	GLY	3.1
1	B	3	GLN	3.1
1	B	227	SER	3.1
1	B	114	VAL	2.9
1	B	424	ASN	2.9
1	B	425	THR	2.9
1	B	229	LYS	2.8
1	B	14	GLN	2.7
1	B	294	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	133	GLU	2.6
1	A	121	ILE	2.6
1	A	375	TRP	2.6
1	B	427	HIS	2.6
1	B	132	LYS	2.5
1	B	297	VAL	2.5
1	B	164	ILE	2.5
1	A	14	GLN	2.5
1	B	161	THR	2.5
1	B	165	LYS	2.4
1	B	183	ILE	2.4
1	B	11	GLN	2.4
1	A	544	THR	2.4
1	B	16	TYR	2.3
1	B	495	SER	2.3
1	A	134	HIS	2.3
1	B	489	VAL	2.2
1	B	35	GLN	2.2
1	A	63	VAL	2.2
1	B	36	PRO	2.2
1	A	126	SER	2.1
1	B	135	GLY	2.1
1	B	541	GLU	2.1
1	B	496	VAL	2.1
1	A	29	LYS	2.1
1	B	272	GLY	2.1
1	B	163	LYS	2.0
1	A	193	LEU	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	B	602	5/5	0.21	0.15	71,73,77,80	0
3	SO4	A	603	5/5	0.11	-0.94	38,39,41,42	0
3	SO4	B	604	5/5	0.07	-1.23	47,47,52,54	0
3	SO4	A	601	5/5	0.12	-1.62	38,41,50,52	0
2	ZN	A	700	1/1	0.10	-1.98	21,21,21,21	0
2	ZN	B	700	1/1	0.09	-1.98	33,33,33,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.