



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:20 PM GMT

PDB ID : 3WVQ  
Title : Structure of ATP grasp protein  
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Deposited on : 2014-06-04  
Resolution : 1.96 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

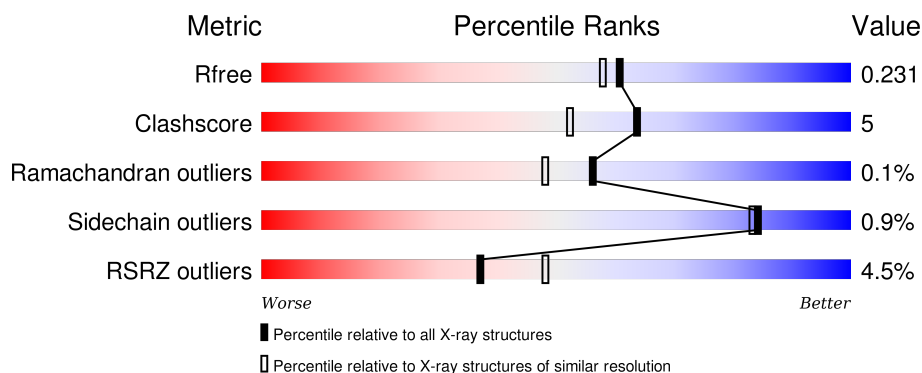
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	447	<div> <div>5%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
1	B	447	<div> <div>2%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
1	C	447	<div> <div>3%</div> <div>87%</div> <div>8%</div> <div>.</div> </div>
1	D	447	<div> <div>7%</div> <div>88%</div> <div>8%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14454 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 PGM1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	Se	0	0	0
			3304	2079	609	608	4	4			
1	B	422	Total	C	N	O	S	Se	0	0	0
			3211	2017	594	592	4	4			
1	C	427	Total	C	N	O	S	Se	0	0	0
			3249	2043	598	600	4	4			
1	D	433	Total	C	N	O	S	Se	0	0	0
			3304	2079	609	608	4	4			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

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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		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

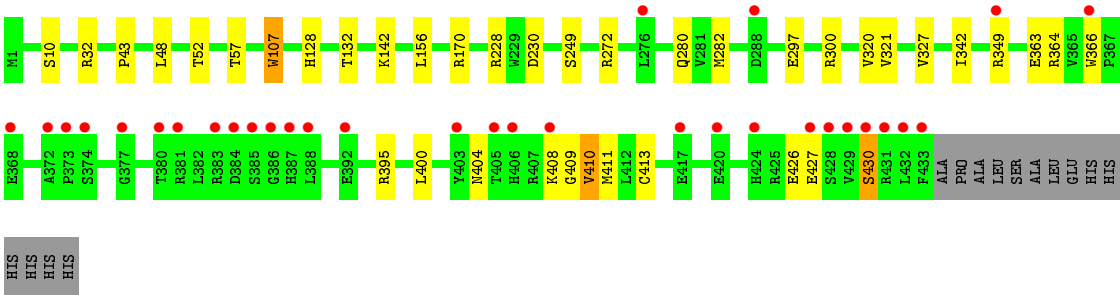
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	308	Total	O	0	0
			308	308		
4	B	329	Total	O	0	0
			329	329		
4	C	346	Total	O	0	0
			346	346		
4	D	316	Total	O	0	0
			316	316		



- Molecule 1: PGM1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.66Å 86.75Å 94.26Å 73.74° 85.93° 68.26°	Depositor
Resolution (Å)	45.18 – 1.96 45.18 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.2 (45.18-1.96) 88.1 (45.18-1.95)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.194 , 0.231 0.194 , 0.231	Depositor DCC
$R_{free}$ test set	7711 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.9	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 154262 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14454	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, 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	0.41	0/3378	0.53	0/4592
1	B	0.43	0/3277	0.55	0/4448
1	C	0.44	0/3318	0.54	0/4505
1	D	0.39	0/3378	0.53	0/4592
All	All	0.42	0/13351	0.54	0/18137

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	3304	0	3251	38	0
1	B	3211	0	3165	34	0
1	C	3249	0	3196	40	0
1	D	3304	0	3251	26	0
2	A	15	0	0	0	0
2	B	20	0	0	1	0
2	C	30	0	0	2	0
2	D	10	0	0	0	0
3	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	6	0	8	0	0
4	A	308	0	0	6	0
4	B	329	0	0	6	0
4	C	346	0	0	5	0
4	D	316	0	0	6	0
All	All	14454	0	12879	136	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 5.

All (136) 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:282:MSE:CE	1:A:343:TYR:HB3	1.66	1.25
1:C:282:MSE:CE	1:C:339:SER:HB3	1.73	1.18
1:A:282:MSE:HE1	1:A:343:TYR:CB	1.80	1.11
1:C:282:MSE:HE1	1:C:339:SER:HB3	1.12	1.10
1:C:282:MSE:HE1	1:C:339:SER:CB	1.91	0.98
1:C:253:PHE:HZ	1:C:282:MSE:CE	1.78	0.96
1:A:271:MSE:HE2	1:A:277:PRO:CB	2.00	0.92
1:C:365:VAL:HA	1:C:411:MSE:SE	2.21	0.91
1:A:282:MSE:HE1	1:A:343:TYR:HB3	0.90	0.89
1:C:253:PHE:CZ	1:C:282:MSE:CE	2.57	0.87
1:B:253:PHE:CZ	1:B:282:MSE:HE3	2.10	0.86
1:C:253:PHE:CZ	1:C:282:MSE:HE2	2.11	0.84
1:A:271:MSE:HE2	1:A:277:PRO:CA	2.09	0.82
1:B:253:PHE:HZ	1:B:282:MSE:HE3	1.43	0.81
1:C:253:PHE:HZ	1:C:282:MSE:HE2	1.46	0.80
1:C:253:PHE:HZ	1:C:282:MSE:HE3	1.48	0.78
1:A:22:TRP:HH2	1:A:411:MSE:HE3	1.50	0.77
1:B:383:ARG:NH2	4:B:805:HOH:O	2.22	0.73
1:D:280:GLN:NE2	1:D:363:GLU:OE1	2.20	0.72
1:B:282:MSE:HE1	1:B:339:SER:HB3	1.72	0.71
1:D:170:ARG:NH1	4:D:775:HOH:O	2.23	0.71
1:D:297:GLU:OE1	1:D:300:ARG:NH1	2.24	0.71
1:C:253:PHE:CZ	1:C:282:MSE:HE3	2.22	0.70
1:A:395:ARG:NH2	1:A:417:GLU:OE2	2.22	0.68
1:A:271:MSE:HE2	1:A:277:PRO:HB2	1.75	0.68
1:B:282:MSE:CE	1:B:339:SER:HB3	2.22	0.68
1:D:43:PRO:HB2	1:D:48:LEU:HD21	1.77	0.67
1:A:296:VAL:HG21	1:C:289:GLN:HG2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:ARG:NH2	2:C:504:SO4:O1	2.20	0.66
1:C:366:TRP:O	1:C:407:ARG:NH2	2.28	0.66
1:C:282:MSE:CE	1:C:339:SER:CB	2.59	0.65
1:B:1:MSE:HE2	1:B:95:PHE:CD1	2.31	0.65
1:C:206:LEU:HD21	1:C:212:LEU:HB2	1.78	0.65
1:B:300:ARG:NH2	2:B:505:SO4:O3	2.31	0.64
1:A:22:TRP:CH2	1:A:411:MSE:HE3	2.33	0.64
1:D:427:GLU:O	1:D:430:SER:HB2	1.97	0.63
1:D:32:ARG:NH2	4:D:804:HOH:O	2.26	0.63
1:A:400:LEU:HD11	1:A:413:CYS:HB2	1.79	0.63
1:C:366:TRP:H	1:C:411:MSE:CE	2.13	0.62
1:C:358:ASP:OD1	1:C:359:ARG:NH1	2.33	0.62
1:A:174:ARG:NH2	4:A:884:HOH:O	2.35	0.60
1:D:282:MSE:HE1	1:D:342:ILE:HG21	1.83	0.60
1:B:365:VAL:H	1:B:407:ARG:NH2	1.99	0.60
1:B:32:ARG:NH2	4:B:842:HOH:O	2.27	0.59
1:D:272:ARG:NH1	4:D:811:HOH:O	2.25	0.59
1:A:271:MSE:HE3	1:A:272:ARG:N	2.18	0.59
1:C:365:VAL:HG23	1:C:411:MSE:HE1	1.84	0.58
1:A:271:MSE:HE2	1:A:277:PRO:HA	1.87	0.57
1:A:427:GLU:O	1:A:430:SER:OG	2.20	0.57
1:A:431:ARG:NH2	4:A:851:HOH:O	2.31	0.56
1:C:365:VAL:CG2	1:C:411:MSE:HE1	2.36	0.56
1:B:165:ARG:NH1	1:B:226:ASP:OD1	2.39	0.55
1:B:349:ARG:NH1	4:B:719:HOH:O	2.39	0.55
1:B:395:ARG:NH2	1:B:417:GLU:OE2	2.38	0.54
1:B:196:GLU:OE2	1:B:228:ARG:NH2	2.22	0.53
1:B:322:THR:HB	1:B:323:PRO:HD2	1.90	0.53
1:D:400:LEU:HD11	1:D:413:CYS:HB2	1.90	0.53
1:D:395:ARG:NH2	4:D:899:HOH:O	2.40	0.53
1:D:364:ARG:NH1	1:D:426:GLU:OE1	2.41	0.51
1:A:294:ASP:OD2	4:A:878:HOH:O	2.20	0.51
1:C:300:ARG:NH2	2:C:506:SO4:O2	2.43	0.50
1:C:174:ARG:HD3	4:C:743:HOH:O	2.11	0.50
1:A:10:SER:HB2	1:A:107:TRP:CZ3	2.47	0.49
1:C:2:ARG:NH2	4:C:879:HOH:O	2.44	0.49
1:D:43:PRO:HB2	1:D:48:LEU:CD2	2.40	0.49
1:C:364:ARG:HD2	1:C:426:GLU:OE2	2.12	0.49
1:B:225:LEU:O	1:B:229:TRP:HB2	2.13	0.49
1:B:377:GLY:O	1:B:381:ARG:HG2	2.13	0.49
1:A:22:TRP:HH2	1:A:411:MSE:CE	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:GLU:O	1:B:301:ARG:HG3	2.12	0.48
1:D:427:GLU:O	1:D:430:SER:CB	2.61	0.48
1:C:170:ARG:NH1	4:C:802:HOH:O	2.46	0.48
1:A:282:MSE:HE2	1:A:343:TYR:HB3	1.83	0.48
1:B:170:ARG:NH1	4:B:807:HOH:O	2.46	0.48
1:A:268:HIS:CE1	1:A:283:PRO:HB2	2.48	0.48
1:D:128:HIS:O	1:D:132:THR:HG23	2.13	0.48
1:B:282:MSE:CE	1:B:343:TYR:HD2	2.27	0.47
1:A:282:MSE:HE1	1:A:343:TYR:CD2	2.49	0.47
1:B:196:GLU:HG2	1:B:210:ARG:HG2	1.96	0.47
1:C:210:ARG:HG3	1:C:211:ALA:N	2.28	0.47
1:C:145:PHE:CE2	1:C:156:LEU:HD11	2.49	0.47
1:A:170:ARG:NH2	4:A:651:HOH:O	2.47	0.47
1:A:282:MSE:HE1	1:A:343:TYR:CG	2.45	0.47
1:A:184:LEU:HD22	1:A:242:VAL:HG22	1.96	0.47
1:B:179:GLY:O	4:B:791:HOH:O	2.21	0.47
1:D:10:SER:HB2	1:D:107:TRP:CZ3	2.50	0.47
1:B:282:MSE:HE3	1:B:339:SER:HB3	1.97	0.46
1:B:1:MSE:CE	1:B:95:PHE:CD1	2.99	0.46
1:A:271:MSE:CE	1:A:277:PRO:CA	2.89	0.46
1:B:364:ARG:HD2	1:B:426:GLU:OE2	2.16	0.46
1:A:296:VAL:HG21	1:C:289:GLN:CG	2.43	0.46
1:B:28:VAL:HG12	1:B:51:VAL:HG11	1.97	0.46
1:B:128:HIS:O	1:B:132:THR:HG23	2.16	0.45
1:C:253:PHE:CE2	1:C:282:MSE:HE2	2.48	0.45
1:A:92:ARG:NH1	4:A:671:HOH:O	2.47	0.45
1:D:52:THR:HB	1:D:57:THR:O	2.17	0.45
1:D:364:ARG:HD2	1:D:426:GLU:OE2	2.17	0.45
1:B:408:LYS:HA	1:B:408:LYS:HD3	1.73	0.45
1:B:156:LEU:HD12	1:B:156:LEU:HA	1.77	0.45
1:A:364:ARG:HG3	1:A:365:VAL:O	2.17	0.45
1:C:1:MSE:HE2	1:C:95:PHE:CD1	2.52	0.45
1:A:225:LEU:O	1:A:229:TRP:HB2	2.16	0.44
1:C:170:ARG:NH2	4:C:689:HOH:O	2.51	0.44
1:B:142:LYS:NZ	4:B:634:HOH:O	2.33	0.44
1:A:196:GLU:OE2	1:A:228:ARG:NH2	2.44	0.44
1:C:278:ASP:HB2	1:C:365:VAL:HG12	1.99	0.44
1:C:128:HIS:O	1:C:132:THR:HG23	2.18	0.44
1:C:278:ASP:OD1	4:C:655:HOH:O	2.21	0.43
1:D:230:ASP:OD1	4:D:913:HOH:O	2.21	0.43
1:D:321:VAL:HG22	1:D:327:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:PHE:CE2	1:B:282:MSE:HE3	2.53	0.43
1:B:400:LEU:HD11	1:B:413:CYS:HB2	2.00	0.43
1:C:178:GLU:OE1	1:C:244:ARG:NH2	2.51	0.43
1:A:145:PHE:CE2	1:A:156:LEU:HD11	2.54	0.42
1:C:373:PRO:HG2	1:C:377:GLY:HA3	2.01	0.42
1:D:366:TRP:HB2	1:D:410:VAL:O	2.19	0.42
1:B:366:TRP:HA	1:B:367:PRO:HD3	1.88	0.42
1:C:282:MSE:HE1	1:C:339:SER:CA	2.48	0.42
1:D:142:LYS:NZ	4:D:749:HOH:O	2.35	0.42
1:C:52:THR:HB	1:C:57:THR:O	2.20	0.42
1:C:400:LEU:HD11	1:C:413:CYS:HB2	2.02	0.42
1:B:403:TYR:OH	1:B:408:LYS:HD2	2.20	0.42
1:A:178:GLU:OE1	1:A:244:ARG:NH2	2.50	0.42
1:C:282:MSE:HE2	1:C:339:SER:HB3	1.87	0.41
1:B:2:ARG:CZ	1:B:32:ARG:HH21	2.33	0.41
1:A:271:MSE:HE3	1:A:272:ARG:H	1.85	0.41
1:D:349:ARG:HB3	1:D:349:ARG:HE	1.67	0.41
1:D:404:ASN:O	1:D:408:LYS:N	2.54	0.41
1:A:390:ASP:HA	1:A:391:PRO:HD3	1.93	0.41
1:D:249:SER:HB3	1:D:320:VAL:HB	2.02	0.41
1:A:271:MSE:CE	1:A:277:PRO:HB2	2.47	0.40
1:D:366:TRP:CE2	1:D:409:GLY:HA3	2.57	0.40
1:A:367:PRO:HB2	1:A:370:TRP:CD1	2.56	0.40
1:D:228:ARG:HD2	1:D:228:ARG:HA	1.91	0.40
1:A:234:GLU:HA	4:A:809:HOH:O	2.21	0.40
1:C:1:MSE:CE	1:C:95:PHE:CD1	3.05	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	431/447 (96%)	423 (98%)	7 (2%)	1 (0%)	52	43
1	B	416/447 (93%)	410 (99%)	6 (1%)	0	100	100
1	C	421/447 (94%)	413 (98%)	8 (2%)	0	100	100
1	D	431/447 (96%)	423 (98%)	7 (2%)	1 (0%)	52	43
All	All	1699/1788 (95%)	1669 (98%)	28 (2%)	2 (0%)	56	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	410	VAL
1	A	410	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	330/337 (98%)	327 (99%)	3 (1%)	84	83
1	B	321/337 (95%)	317 (99%)	4 (1%)	78	75
1	C	324/337 (96%)	323 (100%)	1 (0%)	94	94
1	D	330/337 (98%)	326 (99%)	4 (1%)	78	75
All	All	1305/1348 (97%)	1293 (99%)	12 (1%)	84	83

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	TRP
1	A	358	ASP
1	A	392	GLU
1	B	107	TRP
1	B	228	ARG
1	B	271	MSE
1	B	410	VAL
1	C	107	TRP
1	D	107	TRP

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Mol	Chain	Res	Type
1	D	156	LEU
1	D	411	MSE
1	D	430	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	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 carbohydrates 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	A	501	-	4,4,4	0.25	0	6,6,6	0.21	0
2	SO4	A	502	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	A	503	-	4,4,4	0.16	0	6,6,6	0.23	0
2	SO4	B	501	-	4,4,4	0.18	0	6,6,6	0.36	0
2	SO4	B	502	-	4,4,4	0.25	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	B	503	-	5,5,5	0.30	0	5,5,5	0.87	0
2	SO4	B	504	-	4,4,4	0.29	0	6,6,6	0.15	0
2	SO4	B	505	-	4,4,4	0.19	0	6,6,6	0.14	0
2	SO4	C	501	-	4,4,4	0.29	0	6,6,6	0.16	0
2	SO4	C	502	-	4,4,4	0.20	0	6,6,6	0.27	0
2	SO4	C	503	-	4,4,4	0.24	0	6,6,6	0.19	0
2	SO4	C	504	-	4,4,4	0.15	0	6,6,6	0.20	0
3	GOL	C	505	-	5,5,5	0.32	0	5,5,5	0.72	0
2	SO4	C	506	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	C	507	-	4,4,4	0.22	0	6,6,6	0.21	0
2	SO4	D	501	-	4,4,4	0.12	0	6,6,6	0.16	0
2	SO4	D	502	-	4,4,4	0.23	0	6,6,6	0.14	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
2	SO4	A	501	-	-	0/0/0/0	0/0/0/0
2	SO4	A	502	-	-	0/0/0/0	0/0/0/0
2	SO4	A	503	-	-	0/0/0/0	0/0/0/0
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	502	-	-	0/0/0/0	0/0/0/0
3	GOL	B	503	-	-	0/4/4/4	0/0/0/0
2	SO4	B	504	-	-	0/0/0/0	0/0/0/0
2	SO4	B	505	-	-	0/0/0/0	0/0/0/0
2	SO4	C	501	-	-	0/0/0/0	0/0/0/0
2	SO4	C	502	-	-	0/0/0/0	0/0/0/0
2	SO4	C	503	-	-	0/0/0/0	0/0/0/0
2	SO4	C	504	-	-	0/0/0/0	0/0/0/0
3	GOL	C	505	-	-	0/4/4/4	0/0/0/0
2	SO4	C	506	-	-	0/0/0/0	0/0/0/0
2	SO4	C	507	-	-	0/0/0/0	0/0/0/0
2	SO4	D	501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	502	-	-	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	505	SO4	1	0
2	C	504	SO4	1	0
2	C	506	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	429/447 (95%)	0.34	24 (5%)	28 39	11, 20, 35, 43	0
1	B	418/447 (93%)	0.12	7 (1%)	73 81	11, 19, 31, 45	0
1	C	423/447 (94%)	0.15	13 (3%)	52 62	10, 19, 34, 47	0
1	D	429/447 (95%)	0.30	32 (7%)	17 26	11, 21, 37, 46	0
All	All	1699/1788 (95%)	0.23	76 (4%)	37 48	10, 20, 35, 47	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	380	THR	4.8
1	D	429	VAL	4.8
1	C	409	GLY	4.7
1	A	431	ARG	4.3
1	B	406	HIS	4.3
1	D	432	LEU	4.3
1	D	406	HIS	4.2
1	D	424	HIS	4.1
1	D	384	ASP	3.7
1	A	380	THR	3.6
1	C	408	LYS	3.6
1	C	368	GLU	3.5
1	D	431	ARG	3.5
1	D	385	SER	3.4
1	A	408	LYS	3.3
1	A	427	GLU	3.2
1	D	403	TYR	3.2
1	D	427	GLU	3.2
1	A	384	ASP	3.2
1	D	392	GLU	3.2
1	C	365	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	430	SER	3.1
1	D	373	PRO	3.1
1	B	323	PRO	3.0
1	D	408	LYS	3.0
1	A	392	GLU	3.0
1	A	432	LEU	2.9
1	D	276	LEU	2.9
1	D	428	SER	2.8
1	C	366	TRP	2.8
1	A	387	HIS	2.8
1	A	373	PRO	2.8
1	D	386	GLY	2.7
1	C	403	TYR	2.7
1	C	373	PRO	2.6
1	D	368	GLU	2.6
1	D	377	GLY	2.6
1	D	349	ARG	2.6
1	D	420	GLU	2.5
1	A	386	GLY	2.5
1	A	144	ALA	2.5
1	D	405	THR	2.5
1	D	381	ARG	2.5
1	A	424	HIS	2.5
1	D	374	SER	2.5
1	B	433	PHE	2.5
1	A	381	ARG	2.5
1	A	349	ARG	2.4
1	B	405	THR	2.4
1	A	406	HIS	2.4
1	A	369	GLY	2.3
1	D	383	ARG	2.3
1	D	417	GLU	2.3
1	C	371	GLU	2.3
1	C	369	GLY	2.3
1	A	371	GLU	2.2
1	A	141	SER	2.2
1	C	433	PHE	2.2
1	D	372	ALA	2.2
1	B	227	GLU	2.2
1	A	147	ALA	2.1
1	D	433	PHE	2.1
1	C	349	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	428	SER	2.1
1	C	432	LEU	2.1
1	A	139	GLY	2.1
1	A	377	GLY	2.1
1	B	409	GLY	2.1
1	D	366	TRP	2.1
1	D	288	ASP	2.1
1	D	388	LEU	2.1
1	B	408	LYS	2.1
1	A	161	VAL	2.1
1	A	145	PHE	2.0
1	C	376	ALA	2.0
1	D	387	HIS	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 carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	503	6/6	0.91	0.16	1.97	17,24,30,31	0
2	SO4	A	501	5/5	0.98	0.12	1.02	29,34,36,37	0
2	SO4	D	502	5/5	0.96	0.10	0.40	33,35,37,42	0
2	SO4	B	504	5/5	0.99	0.10	-0.39	26,27,33,33	0
3	GOL	C	505	6/6	0.93	0.12	-0.40	16,23,27,28	0
2	SO4	B	502	5/5	0.98	0.09	-1.06	33,38,43,44	0
2	SO4	C	501	5/5	0.99	0.09	-1.20	26,26,35,38	0
2	SO4	A	503	5/5	0.93	0.12	-	33,44,45,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	D	501	5/5	0.97	0.15	-	34,34,44,45	0
2	SO4	B	501	5/5	0.99	0.07	-	20,23,30,33	0
2	SO4	C	504	5/5	0.94	0.15	-	35,37,43,51	0
2	SO4	C	506	5/5	0.97	0.14	-	30,42,46,49	0
2	SO4	C	507	5/5	0.97	0.09	-	34,37,44,44	0
2	SO4	A	502	5/5	0.98	0.11	-	33,37,41,44	0
2	SO4	C	502	5/5	0.99	0.08	-	22,23,27,30	0
2	SO4	B	505	5/5	0.97	0.11	-	30,40,47,48	0
2	SO4	C	503	5/5	0.97	0.12	-	39,40,43,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.