



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:34 PM GMT

PDB ID : 3ZWB
Title : CRYSTAL STRUCTURE OF RAT PEROXISOMAL MULTIFUNCTIONAL ENZYME TYPE 1 (RPMFE1) COMPLEXED WITH 2TRANS-HEXENOYL-COA
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Deposited on : 2011-07-28
Resolution : 3.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

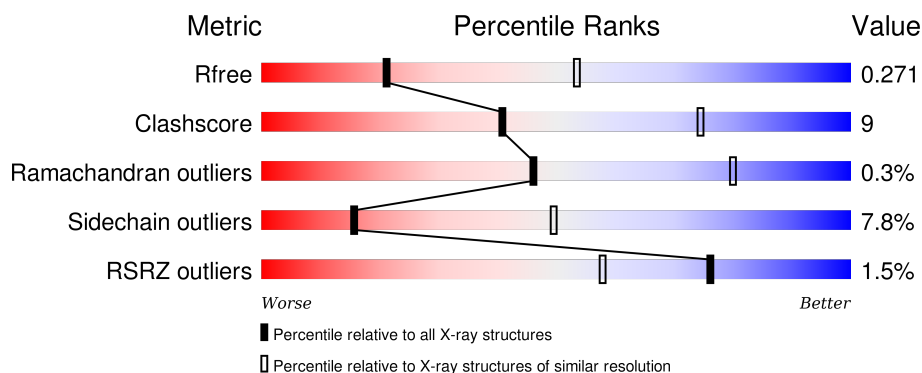
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. 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	742	<div> <div> <div></div> <div>76%</div> <div>20%</div> <div>• •</div> </div> </div>
1	B	742	<div> <div> <div>2%</div> <div>76%</div> <div>20%</div> <div>• •</div> </div> </div>

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	GOL	A	1721	-	-	X	-
4	SO4	B	1720	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11366 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 PEROXISOMAL BIFUNCTIONAL ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	0	0
			5558	3551	976	1008	23			
1	B	721	Total	C	N	O	S	0	0	0
			5530	3535	969	1003	23			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P07896
A	-18	GLY	-	EXPRESSION TAG	UNP P07896
A	-17	SER	-	EXPRESSION TAG	UNP P07896
A	-16	SER	-	EXPRESSION TAG	UNP P07896
A	-15	HIS	-	EXPRESSION TAG	UNP P07896
A	-14	HIS	-	EXPRESSION TAG	UNP P07896
A	-13	HIS	-	EXPRESSION TAG	UNP P07896
A	-12	HIS	-	EXPRESSION TAG	UNP P07896
A	-11	HIS	-	EXPRESSION TAG	UNP P07896
A	-10	HIS	-	EXPRESSION TAG	UNP P07896
A	-9	SER	-	EXPRESSION TAG	UNP P07896
A	-8	SER	-	EXPRESSION TAG	UNP P07896
A	-7	GLY	-	EXPRESSION TAG	UNP P07896
A	-6	LEU	-	EXPRESSION TAG	UNP P07896
A	-5	VAL	-	EXPRESSION TAG	UNP P07896
A	-4	PRO	-	EXPRESSION TAG	UNP P07896
A	-3	ARG	-	EXPRESSION TAG	UNP P07896
A	-2	GLY	-	EXPRESSION TAG	UNP P07896
A	-1	SER	-	EXPRESSION TAG	UNP P07896
A	0	HIS	-	EXPRESSION TAG	UNP P07896
A	123	ALA	GLU	ENGINEERED MUTATION	UNP P07896
B	-19	MET	-	EXPRESSION TAG	UNP P07896
B	-18	GLY	-	EXPRESSION TAG	UNP P07896
B	-17	SER	-	EXPRESSION TAG	UNP P07896
B	-16	SER	-	EXPRESSION TAG	UNP P07896

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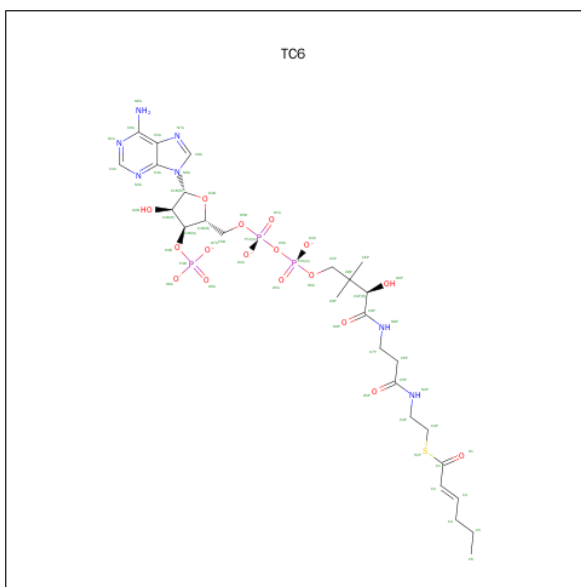
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	EXPRESSION TAG	UNP P07896
B	-14	HIS	-	EXPRESSION TAG	UNP P07896
B	-13	HIS	-	EXPRESSION TAG	UNP P07896
B	-12	HIS	-	EXPRESSION TAG	UNP P07896
B	-11	HIS	-	EXPRESSION TAG	UNP P07896
B	-10	HIS	-	EXPRESSION TAG	UNP P07896
B	-9	SER	-	EXPRESSION TAG	UNP P07896
B	-8	SER	-	EXPRESSION TAG	UNP P07896
B	-7	GLY	-	EXPRESSION TAG	UNP P07896
B	-6	LEU	-	EXPRESSION TAG	UNP P07896
B	-5	VAL	-	EXPRESSION TAG	UNP P07896
B	-4	PRO	-	EXPRESSION TAG	UNP P07896
B	-3	ARG	-	EXPRESSION TAG	UNP P07896
B	-2	GLY	-	EXPRESSION TAG	UNP P07896
B	-1	SER	-	EXPRESSION TAG	UNP P07896
B	0	HIS	-	EXPRESSION TAG	UNP P07896
B	123	ALA	GLU	ENGINEERED MUTATION	UNP P07896

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is (2E)-HEXENOYL-COA (three-letter code: TC6) (formula: C₂₇H₄₀N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

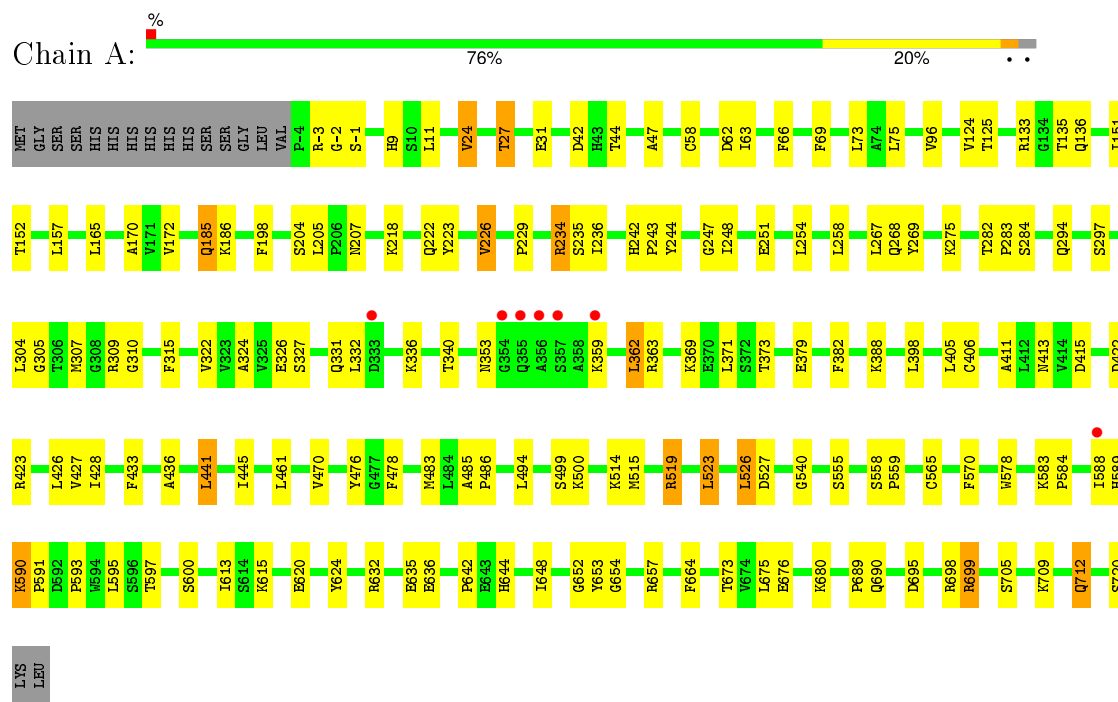
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	64	Total	O	0	0
			64	64		
5	B	72	Total	O	0	0
			72	72		

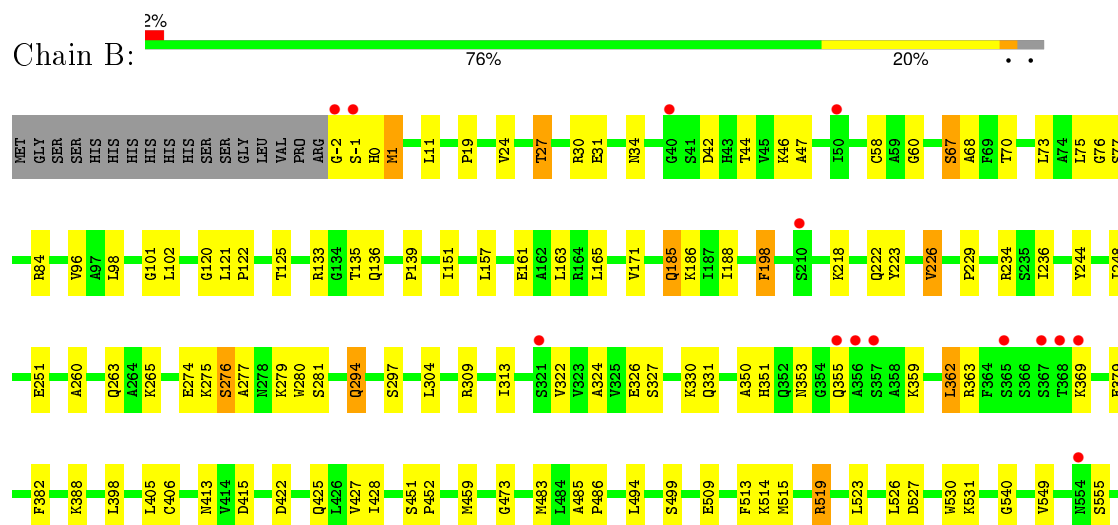
3 Residue-property plots

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: PEROXISOMAL BIFUNCTIONAL ENZYME



• Molecule 1: PEROXISOMAL BIFUNCTIONAL ENZYME



S558	P559	C565	F570	R587	I588	H589	K590	L595	S596	T597	F598	L599	S600	Q601	E609	I613	S614	K615	E620	Y624	E629	I630	F631	R632	I633	M638	D646	R657	M663	F664	T673	K674	L675	E676	P689	Q690	D695	R699	S705	K709	
Q712	P717	H718	GLY	SER	LYS	LEU																																			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.38Å 125.49Å 224.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.11 – 3.10 57.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (112.11-3.10) 97.5 (57.98-3.10)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.221 , 0.276 0.217 , 0.271	Depositor DCC
R_{free} test set	1698 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 33528 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11366	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: TC6, 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	0.58	0/5687	0.68	3/7704 (0.0%)
1	B	0.59	0/5658	0.68	2/7666 (0.0%)
All	All	0.58	0/11345	0.68	5/15370 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	B	234	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	B	234	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	A	234	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	675	LEU	CA-CB-CG	5.92	128.91	115.30

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	5558	0	5666	101	0
1	B	5530	0	5638	96	0
2	A	12	0	16	5	0
3	A	55	0	40	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	55	0	40	4	0
4	A	5	0	0	0	0
4	B	15	0	0	2	0
5	A	64	0	0	10	0
5	B	72	0	0	16	0
All	All	11366	0	11400	195	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 9.

All (195) 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:161:GLU:HB2	5:B:2018:HOH:O	1.48	1.14
1:B:30:ARG:HD2	5:B:2003:HOH:O	1.60	1.01
1:B:717:PRO:HA	5:B:2070:HOH:O	1.66	0.95
1:A:307:MET:HG3	2:A:1721:GOL:H31	1.50	0.91
1:A:555:SER:HB2	1:A:689:PRO:HD2	1.58	0.84
1:B:615:LYS:HB3	5:B:2056:HOH:O	1.77	0.84
1:A:307:MET:HB2	2:A:1721:GOL:H32	1.60	0.84
1:A:24:VAL:HG12	1:A:58:CYS:SG	2.17	0.84
1:B:135:THR:HG22	1:B:251:GLU:OE2	1.80	0.82
1:A:519:ARG:HD3	1:A:589:HIS:CE1	2.17	0.80
1:B:304:LEU:HD11	1:B:324:ALA:HB1	1.63	0.79
1:A:304:LEU:HD11	1:A:324:ALA:HB1	1.70	0.73
1:A:244:TYR:CZ	1:A:248:ILE:HD11	2.27	0.69
1:A:9:HIS:HB3	1:A:185:GLN:HE22	1.56	0.69
1:A:635:GLU:HG2	5:A:2062:HOH:O	1.93	0.69
1:A:135:THR:HG21	1:A:235:SER:OG	1.93	0.69
1:B:587:ARG:HB3	5:B:2050:HOH:O	1.92	0.68
1:A:405:LEU:HB2	1:A:427:VAL:HG22	1.74	0.67
1:B:405:LEU:HB2	1:B:427:VAL:HG22	1.77	0.66
1:A:515:MET:HG2	1:A:519:ARG:HB2	1.78	0.65
1:A:307:MET:HB2	2:A:1721:GOL:C3	2.26	0.65
1:B:322:VAL:HB	1:B:362:LEU:HB3	1.79	0.64
1:B:218:LYS:HE3	1:B:222:GLN:OE1	1.98	0.64
1:A:135:THR:HG22	1:A:251:GLU:OE2	1.98	0.64
1:B:695:ASP:HA	5:B:2063:HOH:O	1.97	0.63
1:B:406:CYS:HA	1:B:428:ILE:O	1.99	0.63
1:B:555:SER:HB2	1:B:689:PRO:HD2	1.79	0.63
1:B:515:MET:HG2	1:B:519:ARG:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:VAL:HA	1:B:263:GLN:HE22	1.62	0.63
3:B:1721:TC6:H3PA	5:B:2013:HOH:O	1.99	0.62
1:A:27:THR:O	1:A:31:GLU:HG3	1.99	0.62
1:A:-2:GLY:HA2	1:A:31:GLU:OE2	2.00	0.62
1:B:630:ALA:HA	1:B:633:ILE:HD12	1.82	0.62
1:B:67:SER:HA	5:B:2006:HOH:O	2.00	0.61
1:A:654:GLY:N	5:A:2055:HOH:O	2.30	0.61
1:B:632:ARG:HH12	1:B:690:GLN:HG2	1.64	0.61
1:B:24:VAL:HG11	1:B:75:LEU:HD13	1.81	0.61
1:B:-2:GLY:HA3	1:B:1:MET:SD	2.41	0.60
1:A:433:PHE:HE2	1:A:653:TYR:CZ	2.19	0.60
1:B:632:ARG:NH1	1:B:690:GLN:HG2	2.17	0.60
1:B:226:VAL:HG22	1:B:229:PRO:CD	2.32	0.59
1:B:519:ARG:HD3	1:B:589:HIS:CE1	2.38	0.59
1:A:269:TYR:CE2	1:A:664:PHE:HB2	2.38	0.59
1:A:441:LEU:HD12	1:A:652:GLY:HA3	1.83	0.59
1:A:527:ASP:HB3	1:A:570:PHE:CD1	2.38	0.59
1:A:406:CYS:HA	1:A:428:ILE:O	2.03	0.58
1:A:151:ILE:HD12	1:A:236:ILE:HD11	1.84	0.58
1:B:425:GLN:HB2	5:B:2033:HOH:O	2.02	0.58
1:B:350:ALA:HA	1:B:353:ASN:HB2	1.86	0.57
1:B:589:HIS:HE1	5:B:2042:HOH:O	1.87	0.56
1:A:499:SER:HB2	1:A:613:ILE:HD12	1.87	0.56
1:B:84:ARG:NE	5:B:2010:HOH:O	2.38	0.56
1:A:307:MET:CG	2:A:1721:GOL:H31	2.28	0.55
1:A:555:SER:CB	1:A:689:PRO:HD2	2.34	0.55
1:B:485:ALA:HB3	1:B:486:PRO:HD3	1.89	0.55
1:A:223:TYR:O	1:A:226:VAL:HG13	2.07	0.55
1:A:500:LYS:HD3	1:B:330:LYS:NZ	2.22	0.55
1:A:712:GLN:OE1	1:A:712:GLN:HA	2.07	0.54
1:A:433:PHE:CE1	1:A:441:LEU:HD13	2.43	0.53
1:A:485:ALA:HB3	1:A:486:PRO:HD3	1.90	0.53
1:A:565:CYS:O	1:B:570:PHE:CE2	2.61	0.53
1:A:441:LEU:HD11	1:A:648:ILE:HG23	1.90	0.53
1:B:42:ASP:OD1	1:B:44:THR:OG1	2.16	0.53
1:A:124:VAL:HG11	1:A:152:THR:O	2.08	0.53
1:A:322:VAL:HB	1:A:362:LEU:HB3	1.91	0.53
1:A:483:MET:O	1:A:486:PRO:HD2	2.09	0.53
1:B:527:ASP:HB3	1:B:570:PHE:CD1	2.44	0.52
1:B:275:LYS:NZ	3:B:1721:TC6:O1A	2.34	0.52
1:A:226:VAL:HG22	1:A:229:PRO:CD	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:SER:HB2	4:B:1720:SO4:O4	2.09	0.52
1:B:244:TYR:CZ	1:B:248:ILE:HD11	2.45	0.51
1:B:615:LYS:HD2	5:B:2055:HOH:O	2.09	0.51
1:A:340:THR:HB	5:A:2022:HOH:O	2.09	0.51
1:B:133:ARG:HD3	1:B:248:ILE:HD12	1.93	0.51
1:A:62:ASP:OD1	3:A:1723:TC6:H2A	2.11	0.51
1:A:42:ASP:OD1	1:A:44:THR:OG1	2.19	0.51
1:B:379:GLU:OE2	1:B:388:LYS:HE2	2.11	0.50
1:B:76:GLY:N	4:B:1720:SO4:O2	2.44	0.50
1:A:590:LYS:HD3	1:A:591:PRO:HD2	1.93	0.50
1:B:483:MET:O	1:B:486:PRO:HD2	2.11	0.50
3:A:1723:TC6:H8A	3:A:1723:TC6:OAP	2.11	0.50
1:B:24:VAL:HG23	1:B:58:CYS:SG	2.51	0.50
1:A:170:ALA:HA	5:A:2013:HOH:O	2.11	0.50
1:A:635:GLU:CG	5:A:2062:HOH:O	2.54	0.49
1:A:135:THR:CG2	1:A:251:GLU:HG3	2.42	0.49
1:B:499:SER:HB2	1:B:613:ILE:HD12	1.93	0.49
1:B:405:LEU:O	1:B:427:VAL:HA	2.12	0.49
1:B:151:ILE:HD12	1:B:236:ILE:HD11	1.94	0.49
1:A:593:PRO:HA	1:B:330:LYS:HG3	1.93	0.49
1:A:413:ASN:OD1	1:A:415:ASP:HB2	2.13	0.49
1:A:282:THR:C	1:A:284:SER:H	2.15	0.49
1:A:494:LEU:HD22	1:A:613:ILE:HG21	1.95	0.48
1:B:712:GLN:HA	1:B:712:GLN:OE1	2.12	0.48
1:A:423:ARG:HD3	1:A:426:LEU:HD12	1.95	0.48
1:A:699:ARG:HG3	5:A:2063:HOH:O	2.13	0.48
1:B:198:PHE:HE2	5:B:2010:HOH:O	1.96	0.48
1:A:226:VAL:HG22	1:A:229:PRO:HD2	1.94	0.48
1:B:494:LEU:HD22	1:B:613:ILE:HG21	1.95	0.48
1:A:632:ARG:NH1	1:A:690:GLN:HG2	2.29	0.48
1:A:223:TYR:HB3	1:A:226:VAL:HG13	1.96	0.48
1:A:11:LEU:HD23	1:A:47:ALA:HB3	1.96	0.48
1:B:31:GLU:HA	1:B:34:ASN:HB2	1.95	0.48
1:A:315:PHE:CE1	1:A:461:LEU:HD21	2.49	0.47
1:A:135:THR:HG21	1:A:251:GLU:HG3	1.95	0.47
1:A:24:VAL:HG21	1:A:75:LEU:HD13	1.97	0.47
1:B:326:GLU:HG2	1:B:331:GLN:HB3	1.97	0.47
1:A:136:GLN:HG3	1:A:248:ILE:HD13	1.95	0.47
1:A:405:LEU:O	1:A:427:VAL:HA	2.14	0.47
1:A:242:HIS:HB3	1:A:243:PRO:HD2	1.96	0.47
1:A:632:ARG:HH12	1:A:690:GLN:HG2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:THR:O	1:B:31:GLU:HG3	2.14	0.47
1:A:133:ARG:HD3	1:A:248:ILE:HD12	1.97	0.47
1:B:19:PRO:HA	5:B:2002:HOH:O	2.15	0.46
1:B:473:GLY:HA3	1:B:638:MET:SD	2.55	0.46
1:A:519:ARG:CD	1:A:589:HIS:CE1	2.92	0.46
1:B:98:LEU:O	1:B:101:GLY:N	2.41	0.46
1:A:583:LYS:HG3	1:A:584:PRO:O	2.15	0.46
1:A:680:LYS:HD2	2:A:1722:GOL:H2	1.97	0.46
1:A:310:GLY:HA3	1:A:436:ALA:HB3	1.98	0.45
1:B:309:ARG:O	1:B:313:ILE:HG13	2.16	0.45
1:B:620:GLU:O	1:B:624:TYR:HB2	2.16	0.45
1:A:305:GLY:O	1:A:309:ARG:HG3	2.17	0.45
1:A:136:GLN:NE2	1:A:247:GLY:HA3	2.32	0.45
1:A:244:TYR:CE1	1:A:248:ILE:HD11	2.50	0.45
1:A:326:GLU:HG2	1:A:331:GLN:HB3	1.99	0.45
1:B:226:VAL:HG22	1:B:229:PRO:HD2	1.98	0.45
1:B:11:LEU:HD23	1:B:47:ALA:HB3	1.99	0.45
1:A:63:ILE:HA	1:A:66:PHE:CE1	2.52	0.45
1:B:276:SER:O	1:B:277:ALA:C	2.54	0.44
1:B:136:GLN:O	1:B:139:PRO:HD2	2.18	0.44
1:B:46:LYS:HB3	1:B:188:ILE:HD11	1.99	0.44
1:A:642:PRO:HD3	1:A:712:GLN:HG2	1.98	0.44
1:A:282:THR:C	1:A:284:SER:N	2.71	0.44
1:B:274:GLU:O	1:B:277:ALA:HB3	2.18	0.44
1:A:267:LEU:HA	1:A:267:LEU:HD23	1.57	0.44
3:B:1721:TC6:H2B	3:B:1721:TC6:O1A	2.18	0.44
1:A:411:ALA:HB1	1:A:476:TYR:HE1	1.83	0.44
1:B:294:GLN:HE21	1:B:294:GLN:HB3	1.58	0.44
1:A:523:LEU:HD23	5:A:2041:HOH:O	2.17	0.44
1:A:-1:SER:CA	1:A:31:GLU:OE1	2.66	0.44
1:A:635:GLU:CB	5:A:2062:HOH:O	2.66	0.44
1:A:470:VAL:CG1	1:A:644:HIS:HB3	2.48	0.43
1:A:332:LEU:O	1:A:336:LYS:HG3	2.17	0.43
1:B:136:GLN:HG3	1:B:248:ILE:HD13	2.00	0.43
1:B:223:TYR:O	1:B:226:VAL:HG13	2.18	0.43
1:A:578:TRP:O	1:A:595:LEU:HD22	2.18	0.43
1:B:102:LEU:HD23	1:B:121:LEU:HG	2.01	0.43
1:B:369:LYS:HG3	1:B:398:LEU:HD22	2.01	0.42
1:B:595:LEU:HG	1:B:599:LEU:CD2	2.49	0.42
1:B:185:GLN:H	1:B:185:GLN:HG2	1.69	0.42
1:B:646:ASP:OD2	1:B:663:MET:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LYS:HG3	1:A:398:LEU:HD22	2.01	0.42
1:B:615:LYS:HD3	5:B:2054:HOH:O	2.19	0.42
1:B:530:TRP:CE3	1:B:565:CYS:HB3	2.54	0.42
1:A:379:GLU:OE2	1:A:388:LYS:HE2	2.20	0.42
1:A:565:CYS:O	1:B:570:PHE:HE2	2.03	0.42
1:B:595:LEU:HD12	1:B:598:PHE:HD2	1.85	0.42
1:A:24:VAL:CG1	1:A:58:CYS:SG	3.00	0.42
1:B:609:GLU:O	1:B:609:GLU:HG2	2.20	0.42
1:A:698:ARG:NH2	5:A:2060:HOH:O	2.53	0.42
1:A:620:GLU:O	1:A:624:TYR:HB2	2.19	0.42
1:B:133:ARG:HD2	1:B:244:TYR:OH	2.20	0.42
1:A:254:LEU:O	1:A:258:LEU:HB2	2.20	0.42
1:B:120:GLY:O	1:B:122:PRO:HD3	2.20	0.42
1:B:276:SER:O	1:B:279:LYS:N	2.52	0.41
1:A:411:ALA:HB1	1:A:476:TYR:CE1	2.55	0.41
1:B:558:SER:HA	1:B:559:PRO:HD3	1.77	0.41
1:A:133:ARG:CD	1:A:248:ILE:HD12	2.50	0.41
1:A:526:LEU:HD23	1:A:526:LEU:N	2.35	0.41
1:B:531:LYS:HG2	5:B:2044:HOH:O	2.20	0.41
1:A:558:SER:HA	1:A:559:PRO:HD3	1.70	0.41
1:B:163:LEU:HD22	1:B:171:VAL:HG23	2.01	0.41
1:B:483:MET:CE	1:B:630:ALA:HB2	2.50	0.41
1:A:282:THR:O	1:A:284:SER:N	2.53	0.41
1:B:509:GLU:HA	1:B:513:PHE:O	2.20	0.41
1:A:218:LYS:HE3	1:A:222:GLN:OE1	2.20	0.41
1:B:555:SER:CB	1:B:689:PRO:HD2	2.48	0.41
1:B:353:ASN:HB3	1:B:355:GLN:H	1.85	0.41
1:A:411:ALA:HA	5:A:2031:HOH:O	2.21	0.41
1:B:413:ASN:OD1	1:B:415:ASP:HB2	2.20	0.41
1:B:322:VAL:O	1:B:362:LEU:HA	2.21	0.41
1:A:207:ASN:N	1:A:207:ASN:OD1	2.51	0.41
1:A:445:ILE:HG21	1:A:478:PHE:CE1	2.56	0.41
1:B:68:ALA:HB2	1:B:260:ALA:HA	2.02	0.41
1:B:265:LYS:HD3	1:B:664:PHE:HZ	1.86	0.41
1:A:500:LYS:HD3	1:B:330:LYS:HZ3	1.85	0.41
1:B:275:LYS:HA	1:B:275:LYS:HD3	1.88	0.40
1:A:268:GLN:O	1:A:269:TYR:C	2.60	0.40
1:A:632:ARG:O	1:A:636:GLU:HG3	2.21	0.40
1:B:280:TRP:CD1	1:B:459:MET:HG3	2.57	0.40
1:B:135:THR:HG21	1:B:251:GLU:HG3	2.03	0.40
1:B:629:GLU:O	1:B:632:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:SER:HA	1:B:452:PRO:HD2	1.91	0.40
1:B:60:GLY:HA3	3:B:1721:TC6:H3P	2.03	0.40
1:A:204:SER:O	1:A:205:LEU:HD12	2.22	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	723/742 (97%)	668 (92%)	53 (7%)	2 (0%)	46	80
1	B	719/742 (97%)	669 (93%)	48 (7%)	2 (0%)	46	80
All	All	1442/1484 (97%)	1337 (93%)	101 (7%)	4 (0%)	46	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	-1	SER
1	A	283	PRO
1	A	540	GLY
1	B	540	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	593/608 (98%)	547 (92%)	46 (8%)	16	49
1	B	590/608 (97%)	544 (92%)	46 (8%)	16	49
All	All	1183/1216 (97%)	1091 (92%)	92 (8%)	16	49

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	ARG
1	A	24	VAL
1	A	27	THR
1	A	69	PHE
1	A	73	LEU
1	A	96	VAL
1	A	125	THR
1	A	157	LEU
1	A	165	LEU
1	A	172	VAL
1	A	185	GLN
1	A	186	LYS
1	A	198	PHE
1	A	226	VAL
1	A	234	ARG
1	A	275	LYS
1	A	294	GLN
1	A	297	SER
1	A	327	SER
1	A	353	ASN
1	A	359	LYS
1	A	362	LEU
1	A	363	ARG
1	A	371	LEU
1	A	373	THR
1	A	382	PHE
1	A	422	ASP
1	A	441	LEU
1	A	514	LYS
1	A	519	ARG
1	A	523	LEU
1	A	526	LEU
1	A	588	ILE
1	A	590	LYS
1	A	597	THR

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Mol	Chain	Res	Type
1	A	600	SER
1	A	615	LYS
1	A	657	ARG
1	A	673	THR
1	A	676	GLU
1	A	695	ASP
1	A	699	ARG
1	A	705	SER
1	A	709	LYS
1	A	712	GLN
1	A	720	SER
1	B	0	HIS
1	B	1	MET
1	B	27	THR
1	B	67	SER
1	B	70	THR
1	B	73	LEU
1	B	96	VAL
1	B	125	THR
1	B	157	LEU
1	B	165	LEU
1	B	185	GLN
1	B	186	LYS
1	B	198	PHE
1	B	226	VAL
1	B	276	SER
1	B	281	SER
1	B	294	GLN
1	B	297	SER
1	B	327	SER
1	B	351	HIS
1	B	359	LYS
1	B	362	LEU
1	B	363	ARG
1	B	382	PHE
1	B	422	ASP
1	B	514	LYS
1	B	519	ARG
1	B	523	LEU
1	B	526	LEU
1	B	549	VAL
1	B	588	ILE

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Mol	Chain	Res	Type
1	B	590	LYS
1	B	597	THR
1	B	599	LEU
1	B	600	SER
1	B	601	GLN
1	B	615	LYS
1	B	657	ARG
1	B	673	THR
1	B	675	LEU
1	B	676	GLU
1	B	695	ASP
1	B	699	ARG
1	B	705	SER
1	B	709	LYS
1	B	712	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	A	589	HIS
1	A	679	GLN
1	B	294	GLN
1	B	353	ASN
1	B	489	ASN
1	B	589	HIS
1	B	658	HIS
1	B	679	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 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	GOL	A	1721	-	5,5,5	0.39	0	5,5,5	0.49	0
2	GOL	A	1722	-	5,5,5	0.41	0	5,5,5	0.75	0
3	TC6	A	1723	-	45,57,57	1.85	5 (11%)	58,83,83	2.05	11 (18%)
4	SO4	A	1724	-	4,4,4	0.29	0	6,6,6	0.28	0
4	SO4	B	1719	-	4,4,4	0.16	0	6,6,6	0.27	0
4	SO4	B	1720	-	4,4,4	0.26	0	6,6,6	0.33	0
3	TC6	B	1721	-	45,57,57	1.76	5 (11%)	58,83,83	2.04	10 (17%)
4	SO4	B	1722	-	4,4,4	0.17	0	6,6,6	0.49	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	GOL	A	1721	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1722	-	-	0/4/4/4	0/0/0/0
3	TC6	A	1723	-	-	0/51/72/72	0/3/3/3
4	SO4	A	1724	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1719	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1720	-	-	0/0/0/0	0/0/0/0
3	TC6	B	1721	-	-	0/51/72/72	0/3/3/3
4	SO4	B	1722	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1721	TC6	C4-C3	-2.92	1.37	1.50
3	A	1723	TC6	C4-C3	-2.19	1.40	1.50
3	B	1721	TC6	C2-C3	2.07	1.37	1.31
3	B	1721	TC6	O4B-C1B	2.90	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1723	TC6	C2-C3	3.10	1.40	1.31
3	A	1723	TC6	O4B-C1B	3.65	1.45	1.41
3	B	1721	TC6	P3B-O7A	6.40	1.63	1.51
3	A	1723	TC6	P3B-O7A	6.46	1.63	1.51
3	B	1721	TC6	P3B-O8A	6.55	1.63	1.51
3	A	1723	TC6	P3B-O8A	7.58	1.65	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1723	TC6	N3A-C2A-N1A	-10.18	121.10	128.89
3	B	1721	TC6	N3A-C2A-N1A	-10.03	121.22	128.89
3	B	1721	TC6	O8A-P3B-O7A	-4.67	102.49	112.85
3	A	1723	TC6	C4-C3-C2	-4.49	117.26	126.16
3	B	1721	TC6	P2A-O3A-P1A	-4.03	121.41	132.73
3	A	1723	TC6	C4B-O4B-C1B	-3.23	106.17	109.72
3	B	1721	TC6	C4B-O4B-C1B	-3.14	106.27	109.72
3	A	1723	TC6	O8A-P3B-O7A	-3.00	106.20	112.85
3	B	1721	TC6	C4-C3-C2	-2.90	120.40	126.16
3	A	1723	TC6	C5B-C4B-C3B	-2.82	104.16	114.31
3	B	1721	TC6	C4A-C5A-N7A	-2.28	107.38	109.48
3	A	1723	TC6	P2A-O3A-P1A	-2.20	126.55	132.73
3	B	1721	TC6	C6P-C5P-N4P	-2.16	112.71	116.46
3	A	1723	TC6	C2B-C1B-N9A	-2.04	111.18	114.29
3	A	1723	TC6	CDP-CBP-CAP	2.02	113.03	109.34
3	A	1723	TC6	CEP-CBP-CCP	3.10	112.53	108.50
3	B	1721	TC6	CEP-CBP-CCP	3.16	112.60	108.50
3	B	1721	TC6	O6A-CCP-CBP	3.21	115.70	110.55
3	B	1721	TC6	CDP-CBP-CAP	3.29	115.36	109.34
3	A	1723	TC6	O4B-C1B-N9A	3.39	115.20	108.10
3	A	1723	TC6	O6A-CCP-CBP	3.54	116.24	110.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1721	GOL	4	0
2	A	1722	GOL	1	0
3	A	1723	TC6	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1720	SO4	2	0
3	B	1721	TC6	4	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	725/742 (97%)	-0.21	7 (0%) 84 69	9, 38, 68, 114	0
1	B	721/742 (97%)	-0.07	14 (1%) 70 48	16, 37, 69, 114	0
All	All	1446/1484 (97%)	-0.14	21 (1%) 76 58	9, 37, 69, 114	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	356	ALA	4.5
1	B	368	THR	3.9
1	A	357	SER	3.7
1	B	357	SER	3.6
1	B	-2	GLY	3.5
1	A	356	ALA	3.3
1	B	-1	SER	3.1
1	B	554	ASN	2.9
1	B	355	GLN	2.9
1	B	367	SER	2.7
1	A	354	GLY	2.6
1	B	369	LYS	2.3
1	A	355	GLN	2.3
1	B	50	ILE	2.3
1	A	359	LYS	2.3
1	B	40	GLY	2.2
1	B	365	SER	2.2
1	B	321	SER	2.1
1	A	333	ASP	2.1
1	A	588	ILE	2.1
1	B	210	SER	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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	B	1720	5/5	0.86	0.25	2.72	88,88,89,89	0
2	GOL	A	1721	6/6	0.75	0.24	1.79	43,45,46,47	0
4	SO4	B	1719	5/5	0.93	0.20	0.18	88,88,88,89	0
3	TC6	A	1723	55/55	0.92	0.19	0.07	39,57,63,64	0
3	TC6	B	1721	55/55	0.95	0.14	-1.04	23,36,40,41	0
2	GOL	A	1722	6/6	0.90	0.19	-1.21	51,52,53,53	0
4	SO4	B	1722	5/5	0.93	0.12	-2.76	76,76,77,77	0
4	SO4	A	1724	5/5	0.97	0.12	-	33,34,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.