



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:00 PM GMT

PDB ID : 4GUA
Title : Alphavirus P23pro-zbd
Authors : Shin, G.; Yost, S.; Miller, M.; Marcotrigiano, J.
Deposited on : 2012-08-29
Resolution : 2.85 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

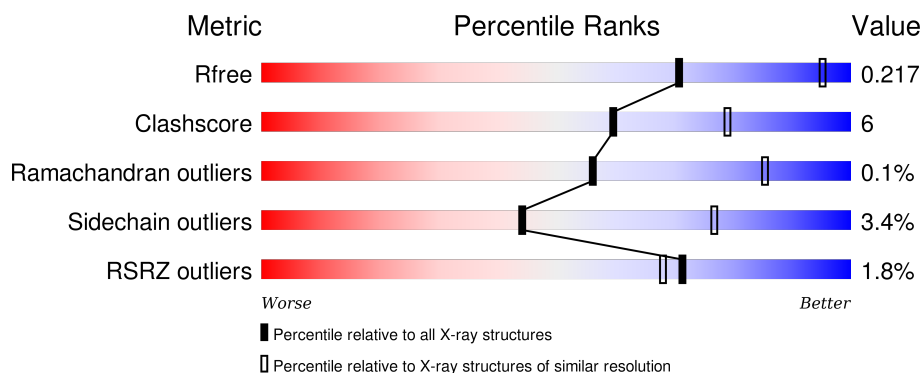
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	670	<div> <div>2%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	B	670	<div> <div>3%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	C	670	<div> <div>%</div> <div>85%</div> <div>13%</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	SO4	A	1703	-	-	-	X
2	SO4	A	1709	-	-	-	X
2	SO4	C	1705	-	-	-	X
2	SO4	C	1706	-	-	-	X
2	SO4	C	1710	-	-	-	X
2	SO4	C	1713	-	-	-	X
3	MES	A	1718	-	-	-	X
3	MES	C	1720	-	-	-	X
3	MES	C	1721	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15707 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 Non-structural polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	662	Total	C	N	O	S	0	0	0
			5118	3238	895	957	28			
1	B	662	Total	C	N	O	S	0	0	0
			5110	3228	895	959	28			
1	C	662	Total	C	N	O	S	0	0	0
			5190	3282	921	959	28			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1006	GLY	-	EXPRESSION TAG	UNP P03317
A	1007	PRO	-	EXPRESSION TAG	UNP P03317
A	1008	LEU	-	EXPRESSION TAG	UNP P03317
A	1009	GLY	-	EXPRESSION TAG	UNP P03317
A	1010	SER	-	EXPRESSION TAG	UNP P03317
B	1006	GLY	-	EXPRESSION TAG	UNP P03317
B	1007	PRO	-	EXPRESSION TAG	UNP P03317
B	1008	LEU	-	EXPRESSION TAG	UNP P03317
B	1009	GLY	-	EXPRESSION TAG	UNP P03317
B	1010	SER	-	EXPRESSION TAG	UNP P03317
C	1006	GLY	-	EXPRESSION TAG	UNP P03317
C	1007	PRO	-	EXPRESSION TAG	UNP P03317
C	1008	LEU	-	EXPRESSION TAG	UNP P03317
C	1009	GLY	-	EXPRESSION TAG	UNP P03317
C	1010	SER	-	EXPRESSION TAG	UNP P03317

- Molecule 2 is SULFATE ION (three-letter code: 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	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
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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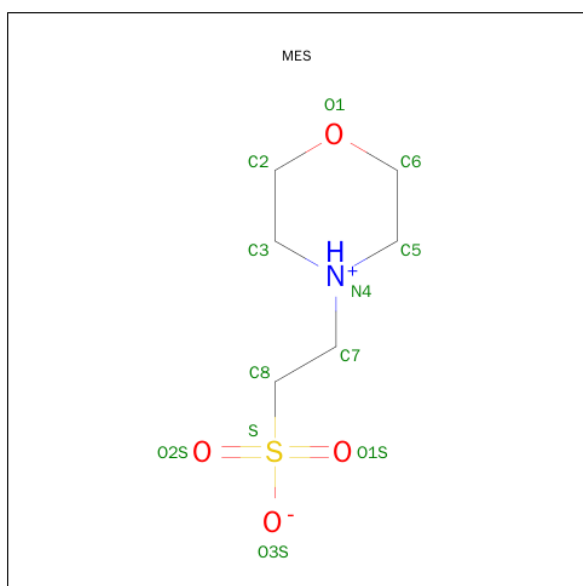
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	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	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).

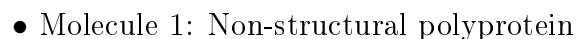
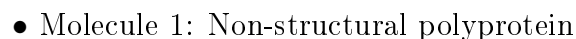


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 1: Non-structural polyprotein





CUU
VAL

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.18Å 147.18Å 360.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.18 – 2.85 73.59 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.18-2.85) 95.9 (73.59-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1066)	Depositor
R, R_{free}	0.186 , 0.217 0.184 , 0.217	Depositor DCC
R_{free} test set	5066 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.5	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 105756 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15707	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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: ZN, SO4, MES

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	0.32	0/5242	0.54	0/7139
1	B	0.32	0/5234	0.53	0/7134
1	C	0.35	0/5314	0.57	0/7218
All	All	0.33	0/15790	0.55	0/21491

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1490	CYS	Peptide
1	B	1343	ASP	Peptide
1	B	1490	CYS	Peptide
1	C	1320	SER	Peptide

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	5118	0	4999	61	0
1	B	5110	0	4959	50	0
1	C	5190	0	5157	68	0
2	A	75	0	0	1	0
2	B	25	0	0	0	0
2	C	90	0	0	4	0
3	A	36	0	37	0	0
3	B	24	0	26	0	0
3	C	36	0	39	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
All	All	15707	0	15217	176	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 6.

All (176) 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:C:1280:ARG:NH2	1:C:1550:GLU:OE2	2.06	0.87
1:A:1343:ASP:HB2	1:A:1344:GLY:HA2	1.61	0.82
1:A:1342:ARG:NH2	1:A:1444:ASN:O	2.14	0.80
1:B:1492:ASP:OD1	1:B:1493:LYS:N	2.18	0.76
1:A:1321:ARG:HD3	1:A:1321:ARG:H	1.52	0.75
1:C:1343:ASP:HB2	1:C:1344:GLY:HA2	1.71	0.73
1:A:1596:VAL:HG23	1:A:1597:ASP:N	2.05	0.71
1:A:1343:ASP:HB2	1:A:1344:GLY:CA	2.21	0.70
1:C:1336:SER:HB2	1:C:1342:ARG:HD3	1.72	0.70
1:A:1080:LYS:HD3	1:A:1082:SER:OG	1.92	0.70
1:A:1121:ARG:HG3	1:A:1121:ARG:O	1.94	0.67
1:A:1343:ASP:CB	1:A:1344:GLY:HA2	2.25	0.67
1:A:1071:MET:HE1	1:A:1118:LEU:HD13	1.77	0.66
1:A:1555:HIS:NE2	1:A:1559:LYS:HD2	2.09	0.66
1:C:1620:ARG:NH2	1:C:1633:THR:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1012:ASN:N	1:B:1013:PRO:CD	2.59	0.66
1:A:1596:VAL:CG2	1:A:1597:ASP:N	2.58	0.65
1:B:1522:GLU:OE1	1:B:1522:GLU:N	2.26	0.64
1:C:1343:ASP:HB3	1:C:1345:VAL:HG23	1.80	0.63
1:A:1388:TRP:CZ2	1:A:1410:LYS:HD2	2.33	0.63
1:C:1012:ASN:N	1:C:1013:PRO:HD3	2.15	0.62
1:A:1584:GLY:O	1:A:1585:GLU:HB3	1.99	0.62
1:C:1343:ASP:HB2	1:C:1344:GLY:CA	2.29	0.61
1:A:1142:ARG:HB3	1:A:1142:ARG:CZ	2.31	0.60
1:A:1321:ARG:HD3	1:A:1321:ARG:N	2.17	0.60
1:C:1123:PRO:O	1:C:1126:GLN:HB2	2.01	0.60
1:C:1137:GLN:NE2	1:C:1673:ILE:HG21	2.16	0.60
1:C:1596:VAL:HG12	1:C:1597:ASP:N	2.17	0.60
1:A:1344:GLY:O	1:A:1345:VAL:HG22	2.02	0.60
1:B:1084:PRO:HG2	1:B:1101:ASN:O	2.02	0.59
1:C:1645:ILE:HD12	1:C:1645:ILE:N	2.17	0.59
1:C:1181:LYS:N	2:C:1714:SO4:O4	2.36	0.58
1:A:1596:VAL:HG23	1:A:1597:ASP:H	1.68	0.58
1:A:1469:GLU:OE1	1:A:1469:GLU:N	2.36	0.58
1:B:1521:ASP:N	1:B:1522:GLU:OE1	2.36	0.58
1:C:1596:VAL:CG1	1:C:1597:ASP:N	2.67	0.58
1:B:1232:ILE:N	1:B:1232:ILE:HD12	2.19	0.58
1:B:1387:ARG:HG2	1:B:1388:TRP:CE2	2.39	0.57
1:C:1120:ARG:HG3	1:C:1121:ARG:N	2.18	0.56
1:C:1341:THR:HG22	1:C:1342:ARG:H	1.70	0.56
1:A:1329:HIS:HB2	1:A:1481:ARG:O	2.06	0.55
1:C:1261:LEU:HB3	1:C:1517:MET:CG	2.36	0.55
1:A:1280:ARG:NH2	1:A:1550:GLU:OE2	2.40	0.54
1:B:1520:ASP:OD1	1:B:1522:GLU:OE1	2.25	0.54
1:C:1620:ARG:NH1	2:C:1717:SO4:O2	2.40	0.54
1:C:1261:LEU:HB3	1:C:1517:MET:HG3	1.89	0.54
1:A:1084:PRO:HG2	1:A:1101:ASN:O	2.08	0.54
1:C:1347:ALA:O	1:C:1349:PRO:HD3	2.07	0.54
1:C:1341:THR:HG22	1:C:1342:ARG:N	2.23	0.53
1:B:1321:ARG:NH1	1:B:1322:THR:OG1	2.42	0.53
1:B:1343:ASP:OD2	1:B:1449:LYS:NZ	2.42	0.52
1:C:1620:ARG:HB2	3:C:1721:MES:H21	1.92	0.52
1:B:1300:ARG:HG3	1:B:1300:ARG:O	2.09	0.52
1:A:1468:LEU:C	1:A:1468:LEU:HD23	2.30	0.52
1:C:1570:ASN:OD1	1:C:1573:GLU:HG3	2.09	0.52
1:B:1127:LEU:N	1:B:1127:LEU:HD13	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1012:ASN:N	1:B:1013:PRO:HD3	2.25	0.51
1:B:1202:TRP:CE3	1:B:1211:ALA:HA	2.45	0.51
1:B:1468:LEU:HD23	1:B:1468:LEU:C	2.30	0.51
1:C:1355:ARG:HD2	1:C:1493:LYS:NZ	2.26	0.51
1:A:1096:VAL:CG1	1:A:1097:ALA:N	2.73	0.51
1:B:1088:HIS:HB2	1:B:1098:HIS:CD2	2.47	0.50
1:C:1343:ASP:CB	1:C:1345:VAL:HG23	2.41	0.50
1:B:1052:ASP:O	1:B:1053:LYS:HD3	2.11	0.50
1:B:1565:LYS:HD3	1:B:1663:THR:OG1	2.11	0.50
1:B:1116:ALA:O	1:B:1119:SER:OG	2.21	0.49
1:A:1318:ASP:OD1	1:A:1323:ARG:NH2	2.45	0.49
1:C:1318:ASP:OD1	1:C:1323:ARG:NH2	2.45	0.49
1:A:1585:GLU:O	1:A:1586:THR:HG22	2.12	0.49
1:A:1120:ARG:HG3	1:A:1121:ARG:N	2.27	0.49
1:B:1515:GLU:OE2	1:C:1226:ARG:CD	2.60	0.49
1:C:1596:VAL:HG12	1:C:1597:ASP:O	2.13	0.48
1:C:1255:THR:OG1	3:C:1720:MES:H31	2.14	0.48
1:B:1361:CYS:HB2	1:B:1363:GLU:OE1	2.14	0.48
1:C:1277:TYR:CD1	1:C:1277:TYR:N	2.82	0.48
1:A:1293:PHE:CE2	1:A:1317:LEU:HB2	2.48	0.48
1:A:1199:ARG:HH11	1:A:1199:ARG:HG3	1.78	0.48
1:B:1329:HIS:HB2	1:B:1481:ARG:O	2.13	0.48
1:A:1491:LEU:HD13	1:A:1495:TRP:CE3	2.50	0.47
1:B:1261:LEU:HB3	1:B:1517:MET:HG3	1.95	0.47
1:C:1540:THR:HG22	2:C:1701:SO4:O2	2.15	0.47
1:A:1137:GLN:NE2	1:A:1673:ILE:HG21	2.29	0.47
1:B:1628:ASN:HD22	1:B:1628:ASN:N	2.13	0.47
1:B:1183:HIS:NE2	1:B:1199:ARG:HG2	2.29	0.47
1:A:1261:LEU:HB3	1:A:1517:MET:HG3	1.96	0.47
1:C:1493:LYS:N	1:C:1493:LYS:HD3	2.30	0.46
1:A:1584:GLY:O	1:A:1585:GLU:CB	2.64	0.46
1:B:1277:TYR:CD1	1:B:1277:TYR:N	2.83	0.46
1:B:1596:VAL:HG22	1:B:1597:ASP:H	1.80	0.46
1:A:1581:TYR:O	1:A:1625:ARG:NH1	2.47	0.46
1:B:1022:TRP:CE2	1:B:1055:HIS:HB3	2.51	0.46
1:A:1080:LYS:HD2	1:A:1110:TYR:O	2.16	0.46
1:C:1586:THR:HG23	1:C:1589:ALA:H	1.80	0.46
1:A:1080:LYS:HB3	1:A:1109:GLY:O	2.16	0.45
1:A:1080:LYS:HD3	1:A:1082:SER:HG	1.82	0.45
1:C:1012:ASN:N	1:C:1013:PRO:CD	2.79	0.45
1:A:1181:LYS:N	1:A:1181:LYS:HD3	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1166:LYS:HG2	1:B:1307:ASN:ND2	2.30	0.45
1:C:1316:GLN:HB3	1:C:1509:VAL:HG21	1.97	0.45
1:C:1355:ARG:HD2	1:C:1493:LYS:HZ3	1.81	0.45
1:A:1042:TRP:HB3	1:A:1049:PHE:CD2	2.52	0.45
1:A:1344:GLY:O	1:A:1345:VAL:CG2	2.64	0.45
1:C:1373:LEU:HD13	1:C:1375:ARG:NH2	2.32	0.45
1:C:1321:ARG:HE	1:C:1513:LYS:HB3	1.82	0.45
1:B:1387:ARG:O	1:B:1387:ARG:HG3	2.17	0.44
1:C:1121:ARG:HG3	1:C:1121:ARG:O	2.16	0.44
1:C:1565:LYS:NZ	1:C:1569:PRO:O	2.50	0.44
1:B:1222:PRO:CB	1:C:1508:SER:HB3	2.47	0.44
1:B:1203:ILE:HD11	1:B:1224:GLN:HG3	2.00	0.44
1:B:1222:PRO:HB3	1:C:1508:SER:HB3	1.99	0.44
1:C:1084:PRO:HG2	1:C:1101:ASN:O	2.17	0.44
1:A:1594:CYS:HA	1:A:1595:PRO:HD3	1.87	0.44
1:C:1468:LEU:HD23	1:C:1468:LEU:C	2.38	0.44
1:A:1388:TRP:CE2	1:A:1410:LYS:HD2	2.52	0.44
1:B:1468:LEU:HD12	1:B:1495:TRP:CD2	2.53	0.44
1:A:1343:ASP:OD1	1:A:1343:ASP:N	2.50	0.43
1:A:1493:LYS:O	1:A:1497:GLU:HG3	2.18	0.43
1:A:1088:HIS:O	1:A:1097:ALA:HA	2.19	0.43
1:C:1346:GLY:HA3	1:C:1347:ALA:HA	1.80	0.43
1:C:1022:TRP:CE2	1:C:1055:HIS:HB3	2.53	0.43
1:A:1202:TRP:CE3	1:A:1211:ALA:HA	2.53	0.43
1:B:1328:HIS:CE1	1:B:1660:ASN:HB3	2.53	0.43
1:C:1166:LYS:HG2	1:C:1307:ASN:ND2	2.34	0.43
1:C:1321:ARG:HE	1:C:1513:LYS:CB	2.32	0.43
1:C:1138:THR:OG1	1:C:1140:ARG:HG2	2.19	0.43
1:B:1348:ALA:HA	1:B:1349:PRO:HD3	1.87	0.43
1:A:1420:PHE:CG	1:A:1467:ARG:NH1	2.87	0.43
1:A:1121:ARG:CG	1:A:1121:ARG:O	2.63	0.43
1:B:1638:THR:HG22	1:B:1638:THR:O	2.19	0.43
1:C:1402:ALA:HA	1:C:1414:HIS:O	2.18	0.43
1:C:1150:LEU:HD13	1:C:1241:HIS:HB2	2.00	0.43
1:C:1174:LYS:HB3	1:C:1194:GLU:O	2.19	0.43
1:A:1570:ASN:OD1	1:A:1573:GLU:HG3	2.19	0.43
1:B:1261:LEU:HB3	1:B:1517:MET:CG	2.48	0.43
1:A:1420:PHE:CD2	1:A:1467:ARG:NH1	2.87	0.42
1:C:1358:ILE:HG21	1:C:1380:VAL:HG13	2.01	0.42
1:C:1237:LYS:HD2	1:C:1237:LYS:HA	1.77	0.42
1:A:1363:GLU:O	1:A:1410:LYS:NZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1202:TRP:CE3	1:C:1211:ALA:HA	2.54	0.42
1:C:1343:ASP:CB	1:C:1344:GLY:HA2	2.43	0.42
1:A:1277:TYR:N	1:A:1277:TYR:CD1	2.86	0.42
1:B:1014:PHE:CZ	1:B:1024:LYS:HA	2.55	0.42
1:B:1673:ILE:O	1:B:1673:ILE:HD12	2.20	0.42
1:C:1577:GLN:OE1	1:C:1593:LYS:HE2	2.19	0.42
1:B:1293:PHE:CE2	1:B:1317:LEU:HB2	2.55	0.42
1:C:1453:ILE:O	1:C:1488:ILE:HA	2.20	0.42
1:A:1022:TRP:CE2	1:A:1055:HIS:HB3	2.55	0.42
1:A:1522:GLU:HG3	1:A:1523:LEU:N	2.34	0.42
1:C:1583:LEU:HD21	1:C:1632:VAL:HG23	2.02	0.42
1:B:1387:ARG:HB2	1:B:1387:ARG:HE	1.75	0.42
1:A:1162:VAL:O	1:A:1162:VAL:HG23	2.20	0.41
1:C:1336:SER:HB2	1:C:1342:ARG:CD	2.48	0.41
1:A:1293:PHE:CG	1:A:1314:PHE:HB3	2.55	0.41
1:A:1195:ALA:HB3	1:A:1200:ILE:HD11	2.01	0.41
1:B:1342:ARG:HG2	1:B:1343:ASP:N	2.35	0.41
1:C:1599:ASN:HA	1:C:1600:PRO:HD3	1.79	0.41
1:A:1336:SER:HB2	1:A:1342:ARG:HD2	2.03	0.41
1:B:1387:ARG:HG2	1:B:1388:TRP:CD2	2.56	0.41
1:C:1475:LEU:HD23	1:C:1475:LEU:C	2.41	0.41
1:A:1344:GLY:C	1:A:1345:VAL:CG2	2.90	0.41
1:B:1052:ASP:C	1:B:1053:LYS:HD3	2.40	0.41
1:B:1512:LEU:HD12	1:B:1512:LEU:N	2.35	0.41
1:A:1540:THR:HB	2:A:1707:SO4:O3	2.21	0.41
1:B:1299:ALA:HA	1:B:1344:GLY:HA2	2.02	0.41
1:C:1262:ASN:ND2	2:C:1706:SO4:O2	2.53	0.41
1:C:1336:SER:CB	1:C:1342:ARG:HD3	2.46	0.40
1:A:1096:VAL:HG12	1:A:1097:ALA:N	2.35	0.40
1:C:1345:VAL:O	1:C:1346:GLY:C	2.59	0.40
1:B:1232:ILE:N	1:B:1232:ILE:CD1	2.84	0.40
1:B:1670:ARG:HG3	1:B:1671:LYS:N	2.36	0.40
1:C:1326:THR:HB	1:C:1327:PRO:HD2	2.03	0.40
1:B:1293:PHE:CG	1:B:1314:PHE:HB3	2.55	0.40
1:C:1067:LYS:HA	1:C:1067:LYS:HD3	1.91	0.40
1:A:1067:LYS:O	1:A:1133:GLN:HG3	2.21	0.40
1:C:1478:ALA:O	1:C:1481:ARG:HB2	2.22	0.40
1:C:1355:ARG:HA	1:C:1490:CYS:O	2.22	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	660/670 (98%)	641 (97%)	18 (3%)	1 (0%)	52	82
1	B	660/670 (98%)	643 (97%)	17 (3%)	0	100	100
1	C	660/670 (98%)	645 (98%)	15 (2%)	0	100	100
All	All	1980/2010 (98%)	1929 (97%)	50 (2%)	1 (0%)	56	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1586	THR

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	551/574 (96%)	533 (97%)	18 (3%)	45	78
1	B	548/574 (96%)	526 (96%)	22 (4%)	38	72
1	C	566/574 (99%)	549 (97%)	17 (3%)	48	80
All	All	1665/1722 (97%)	1608 (97%)	57 (3%)	44	77

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1079	SER
1	A	1117	GLU

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Mol	Chain	Res	Type
1	A	1120	ARG
1	A	1134	LEU
1	A	1142	ARG
1	A	1181	LYS
1	A	1191	GLU
1	A	1280	ARG
1	A	1291	ARG
1	A	1321	ARG
1	A	1343	ASP
1	A	1481	ARG
1	A	1517	MET
1	A	1565	LYS
1	A	1592	GLU
1	A	1596	VAL
1	A	1612	CYS
1	A	1642	LYS
1	B	1096	VAL
1	B	1127	LEU
1	B	1134	LEU
1	B	1140	ARG
1	B	1169	GLN
1	B	1181	LYS
1	B	1280	ARG
1	B	1321	ARG
1	B	1343	ASP
1	B	1387	ARG
1	B	1469	GLU
1	B	1481	ARG
1	B	1491	LEU
1	B	1503	LEU
1	B	1505	LEU
1	B	1508	SER
1	B	1536	LYS
1	B	1598	HIS
1	B	1612	CYS
1	B	1616	MET
1	B	1626	SER
1	B	1628	ASN
1	C	1134	LEU
1	C	1140	ARG
1	C	1237	LYS
1	C	1280	ARG

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Mol	Chain	Res	Type
1	C	1343	ASP
1	C	1355	ARG
1	C	1384	ILE
1	C	1395	SER
1	C	1473	ASN
1	C	1481	ARG
1	C	1493	LYS
1	C	1503	LEU
1	C	1505	LEU
1	C	1507	GLU
1	C	1522	GLU
1	C	1612	CYS
1	C	1642	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1628	ASN
1	C	1414	HIS

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](#)

Of 49 ligands modelled in this entry, 3 are monoatomic - leaving 46 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	$\# Z > 2$
2	SO4	A	1701	-	4,4,4	0.18	0	6,6,6	0.26	0
2	SO4	A	1702	-	4,4,4	0.16	0	6,6,6	0.08	0
2	SO4	A	1703	-	4,4,4	0.16	0	6,6,6	0.17	0
2	SO4	A	1704	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	1705	-	4,4,4	0.14	0	6,6,6	0.13	0
2	SO4	A	1706	-	4,4,4	0.18	0	6,6,6	0.12	0
2	SO4	A	1707	-	4,4,4	0.20	0	6,6,6	0.11	0
2	SO4	A	1708	-	4,4,4	0.15	0	6,6,6	0.20	0
2	SO4	A	1709	-	4,4,4	0.16	0	6,6,6	0.19	0
2	SO4	A	1710	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	1711	-	4,4,4	0.18	0	6,6,6	0.17	0
2	SO4	A	1712	-	4,4,4	0.21	0	6,6,6	0.09	0
2	SO4	A	1713	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	A	1714	-	4,4,4	0.16	0	6,6,6	0.17	0
2	SO4	A	1715	-	4,4,4	0.18	0	6,6,6	0.17	0
3	MES	A	1716	-	11,12,12	0.64	0	14,16,16	2.72	6 (42%)
3	MES	A	1717	-	11,12,12	0.65	0	14,16,16	2.34	5 (35%)
3	MES	A	1718	-	11,12,12	0.63	0	14,16,16	1.62	3 (21%)
2	SO4	B	1701	-	4,4,4	0.18	0	6,6,6	0.08	0
2	SO4	B	1702	-	4,4,4	0.14	0	6,6,6	0.22	0
2	SO4	B	1703	-	4,4,4	0.22	0	6,6,6	0.10	0
2	SO4	B	1704	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	B	1705	-	4,4,4	0.16	0	6,6,6	0.26	0
3	MES	B	1706	-	11,12,12	0.62	0	14,16,16	1.86	4 (28%)
3	MES	B	1707	-	11,12,12	0.76	0	14,16,16	1.87	4 (28%)
2	SO4	C	1701	-	4,4,4	0.15	0	6,6,6	0.15	0
2	SO4	C	1702	-	4,4,4	0.13	0	6,6,6	0.20	0
2	SO4	C	1703	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	C	1704	-	4,4,4	0.21	0	6,6,6	0.18	0
2	SO4	C	1705	-	4,4,4	0.12	0	6,6,6	0.12	0
2	SO4	C	1706	-	4,4,4	0.16	0	6,6,6	0.27	0
2	SO4	C	1707	-	4,4,4	0.19	0	6,6,6	0.09	0
2	SO4	C	1708	-	4,4,4	0.15	0	6,6,6	0.22	0
2	SO4	C	1709	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	C	1710	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	C	1711	-	4,4,4	0.16	0	6,6,6	0.22	0
2	SO4	C	1712	-	4,4,4	0.17	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	1713	-	4,4,4	0.14	0	6,6,6	0.30	0
2	SO4	C	1714	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	C	1715	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	C	1716	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	C	1717	-	4,4,4	0.16	0	6,6,6	0.18	0
2	SO4	C	1718	-	4,4,4	0.09	0	6,6,6	0.21	0
3	MES	C	1719	-	11,12,12	0.56	0	14,16,16	2.08	3 (21%)
3	MES	C	1720	-	11,12,12	0.67	0	14,16,16	1.72	5 (35%)
3	MES	C	1721	-	11,12,12	0.68	0	14,16,16	1.68	3 (21%)

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	1701	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1702	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1703	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1704	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1705	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1706	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1707	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1708	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1709	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1710	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1711	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1712	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1713	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1714	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1715	-	-	0/0/0/0	0/0/0/0
3	MES	A	1716	-	-	0/6/14/14	0/1/1/1
3	MES	A	1717	-	-	0/6/14/14	0/1/1/1
3	MES	A	1718	-	-	0/6/14/14	0/1/1/1
2	SO4	B	1701	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1702	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1703	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1704	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1705	-	-	0/0/0/0	0/0/0/0
3	MES	B	1706	-	-	0/6/14/14	0/1/1/1
3	MES	B	1707	-	-	0/6/14/14	0/1/1/1
2	SO4	C	1701	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	C	1702	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1703	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1704	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1705	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1706	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1707	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1708	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1709	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1710	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1711	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1712	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1713	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1714	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1715	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1716	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1717	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1718	-	-	0/0/0/0	0/0/0/0
3	MES	C	1719	-	-	0/6/14/14	0/1/1/1
3	MES	C	1720	-	-	0/6/14/14	0/1/1/1
3	MES	C	1721	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1717	MES	C6-C5-N4	-5.22	102.21	110.12
3	B	1707	MES	C6-C5-N4	-3.47	104.86	110.12
3	A	1716	MES	C2-C3-N4	-3.30	105.12	110.12
3	A	1716	MES	C6-C5-N4	-3.11	105.41	110.12
3	C	1721	MES	C6-C5-N4	-2.83	105.84	110.12
3	B	1707	MES	C2-C3-N4	-2.57	106.24	110.12
3	B	1706	MES	C6-C5-N4	-2.34	106.58	110.12
3	C	1720	MES	C6-C5-N4	-2.32	106.61	110.12
3	C	1720	MES	C7-N4-C5	2.01	116.41	111.27
3	B	1707	MES	O2S-S-C8	2.03	108.64	106.91
3	C	1720	MES	O1S-S-C8	2.07	108.67	106.91
3	A	1718	MES	C5-N4-C3	2.07	113.38	108.90
3	A	1716	MES	C7-N4-C5	2.18	116.86	111.27
3	A	1716	MES	C5-N4-C3	2.29	113.85	108.90
3	C	1719	MES	O2S-S-C8	2.33	108.89	106.91
3	B	1706	MES	C5-N4-C3	2.36	114.01	108.90
3	A	1717	MES	C5-N4-C3	2.41	114.11	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1721	MES	O1S-S-C8	2.50	109.03	106.91
3	A	1717	MES	C7-N4-C5	2.54	117.77	111.27
3	C	1719	MES	C5-N4-C3	2.63	114.59	108.90
3	A	1717	MES	O2S-S-C8	2.69	109.20	106.91
3	C	1720	MES	C5-N4-C3	2.85	115.06	108.90
3	A	1718	MES	O2S-S-C8	3.04	109.50	106.91
3	C	1720	MES	O2S-S-C8	3.06	109.52	106.91
3	A	1718	MES	O1S-S-C8	3.17	109.61	106.91
3	A	1716	MES	O2S-S-C8	3.23	109.66	106.91
3	B	1706	MES	O2S-S-C8	3.34	109.76	106.91
3	C	1721	MES	O2S-S-C8	3.47	109.86	106.91
3	B	1707	MES	O1S-S-C8	3.84	110.18	106.91
3	A	1717	MES	O1S-S-C8	4.14	110.44	106.91
3	B	1706	MES	O1S-S-C8	4.30	110.58	106.91
3	C	1719	MES	O1S-S-C8	6.24	112.23	106.91
3	A	1716	MES	O1S-S-C8	7.19	113.04	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1707	SO4	1	0
2	C	1701	SO4	1	0
2	C	1706	SO4	1	0
2	C	1714	SO4	1	0
2	C	1717	SO4	1	0
3	C	1720	MES	1	0
3	C	1721	MES	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	662/670 (98%)	0.15	13 (1%) 68 64	45, 68, 103, 154	0
1	B	662/670 (98%)	0.15	18 (2%) 58 52	43, 71, 107, 158	0
1	C	662/670 (98%)	0.02	4 (0%) 90 89	37, 55, 87, 134	0
All	All	1986/2010 (98%)	0.11	35 (1%) 71 68	37, 65, 102, 158	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1126	GLN	4.3
1	B	1125	PHE	3.9
1	B	1127	LEU	3.7
1	A	1346	GLY	3.6
1	B	1128	ALA	3.1
1	A	1586	THR	3.0
1	C	1347	ALA	2.9
1	B	1194	GLU	2.6
1	C	1346	GLY	2.6
1	A	1497	GLU	2.5
1	B	1143	VAL	2.5
1	B	1069	PHE	2.5
1	A	1645	ILE	2.5
1	A	1613	MET	2.5
1	A	1583	LEU	2.4
1	A	1649	GLN	2.4
1	A	1585	GLU	2.4
1	A	1172	PRO	2.4
1	A	1647	ASN	2.4
1	B	1077	LEU	2.3
1	A	1631	GLU	2.3
1	B	1040	CYS	2.3
1	B	1141	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1647	ASN	2.3
1	A	1614	TYR	2.2
1	A	1646	LYS	2.2
1	B	1579	CYS	2.2
1	B	1124	VAL	2.2
1	B	1134	LEU	2.2
1	C	1631	GLU	2.1
1	B	1098	HIS	2.1
1	C	1460	ILE	2.0
1	B	1129	GLY	2.0
1	B	1302	ASP	2.0
1	B	1623	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 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
2	SO4	C	1710	5/5	0.96	0.40	8.01	101,104,109,112	0
2	SO4	A	1703	5/5	0.90	0.44	7.74	114,115,117,119	0
3	MES	C	1721	12/12	0.93	0.31	4.93	82,96,116,116	0
2	SO4	C	1706	5/5	0.82	0.27	4.30	116,118,122,125	0
3	MES	C	1720	12/12	0.95	0.26	4.25	76,93,103,104	0
2	SO4	C	1705	5/5	0.86	0.30	3.83	104,109,117,131	0
2	SO4	A	1709	5/5	0.79	0.26	3.27	121,124,126,129	0
3	MES	A	1718	12/12	0.86	0.44	2.48	107,116,124,129	0
2	SO4	C	1713	5/5	0.61	0.33	2.43	114,118,130,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	1704	5/5	0.90	0.33	1.71	140,140,142,144	0
2	SO4	B	1705	5/5	0.70	0.28	1.38	116,122,128,134	0
2	SO4	B	1702	5/5	0.84	0.23	1.38	118,125,128,134	0
2	SO4	C	1712	5/5	0.87	0.32	1.22	127,128,131,131	0
2	SO4	A	1714	5/5	0.63	0.28	1.08	124,125,130,133	0
3	MES	A	1717	12/12	0.96	0.23	1.07	62,77,80,85	0
2	SO4	A	1701	5/5	0.91	0.24	0.89	102,103,109,113	0
2	SO4	C	1702	5/5	0.80	0.23	0.81	112,114,122,128	0
2	SO4	C	1703	5/5	0.92	0.24	0.75	106,108,118,121	0
2	SO4	A	1710	5/5	0.87	0.24	0.65	106,116,120,126	0
2	SO4	A	1707	5/5	0.92	0.24	0.16	119,120,122,124	0
3	MES	C	1719	12/12	0.99	0.20	0.12	36,47,54,64	0
3	MES	B	1706	12/12	0.94	0.20	0.10	63,81,92,94	0
2	SO4	C	1716	5/5	0.89	0.20	-0.05	108,112,119,123	0
2	SO4	C	1714	5/5	0.88	0.23	-0.24	105,109,114,118	0
3	MES	B	1707	12/12	0.96	0.18	-0.27	49,67,77,77	0
2	SO4	C	1708	5/5	0.91	0.19	-0.31	99,109,111,116	0
2	SO4	A	1702	5/5	0.94	0.19	-0.62	105,109,114,120	0
3	MES	A	1716	12/12	0.96	0.18	-0.72	67,91,97,98	0
2	SO4	B	1701	5/5	0.91	0.16	-0.94	112,117,122,125	0
2	SO4	C	1701	5/5	0.93	0.14	-1.19	95,100,105,110	0
2	SO4	C	1711	5/5	0.80	0.17	-1.27	113,116,130,130	0
4	ZN	B	1708	1/1	0.99	0.11	-1.37	96,96,96,96	0
4	ZN	A	1719	1/1	0.99	0.09	-1.62	91,91,91,91	0
4	ZN	C	1722	1/1	0.99	0.12	-1.73	70,70,70,70	0
2	SO4	A	1705	5/5	0.94	0.16	-	119,121,126,128	0
2	SO4	A	1712	5/5	0.80	0.28	-	154,156,157,157	0
2	SO4	C	1718	5/5	0.88	0.32	-	99,102,114,115	0
2	SO4	C	1715	5/5	0.92	0.15	-	90,95,98,100	0
2	SO4	C	1717	5/5	0.89	0.27	-	99,105,107,109	0
2	SO4	A	1711	5/5	0.66	0.32	-	113,131,134,135	0
2	SO4	A	1706	5/5	0.90	0.34	-	119,121,124,126	0
2	SO4	A	1708	5/5	0.84	0.34	-	117,121,126,132	0
2	SO4	C	1707	5/5	0.74	0.29	-	134,141,142,143	0
2	SO4	A	1713	5/5	0.80	0.23	-	128,129,132,136	0
2	SO4	B	1704	5/5	0.87	0.39	-	141,142,145,146	0
2	SO4	A	1715	5/5	0.83	0.31	-	120,125,128,133	0
2	SO4	C	1709	5/5	0.74	0.35	-	124,128,139,143	0
2	SO4	C	1704	5/5	0.84	0.24	-	123,125,130,131	0
2	SO4	B	1703	5/5	0.86	0.25	-	123,125,127,133	0

6.5 Other polymers [i](#)

There are no such residues in this entry.