Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 10:44 AM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

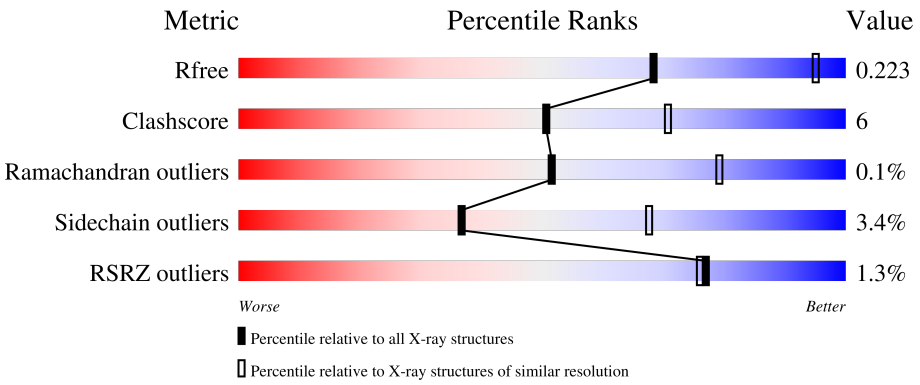
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 86% 11% ••
1	B	670	2% 86% 12% ••
1	C	670	% 85% 13% ••

2 Entry composition (i)

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.

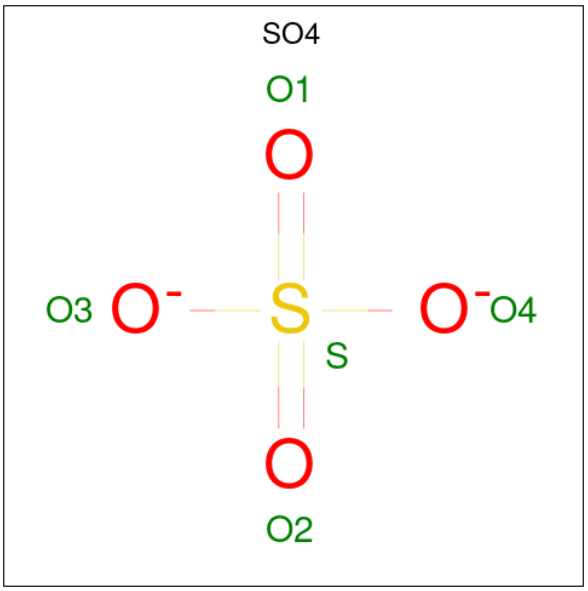
- Molecule 1 is a protein called Non-structural polyprotein.

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

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: O_4S).



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

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

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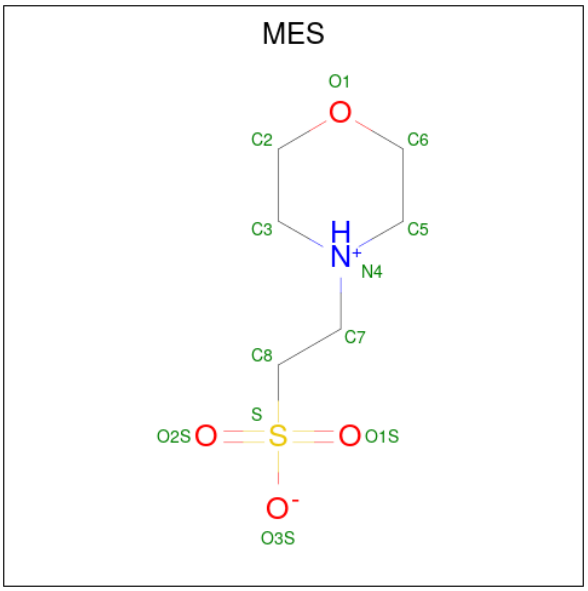
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	C	1	5	4	1		0	0
			Total	O	S			
2	C	1	5	4	1		0	0
			Total	O	S			
2	C	1	5	4	1		0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

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

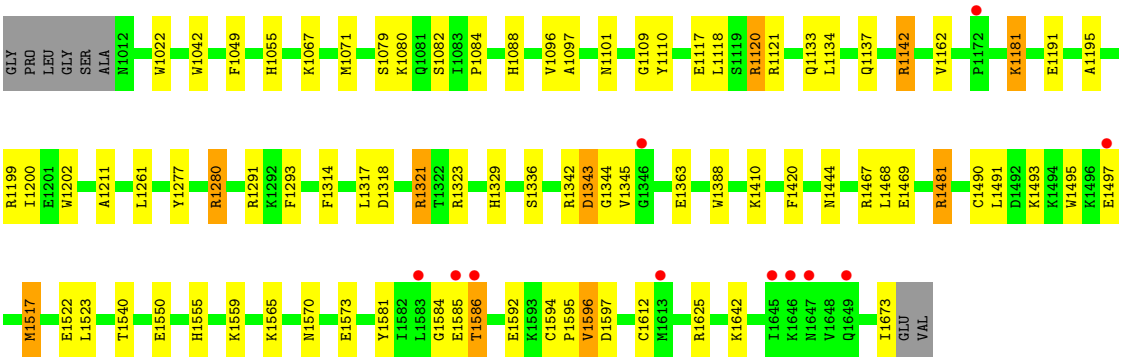
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	C	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

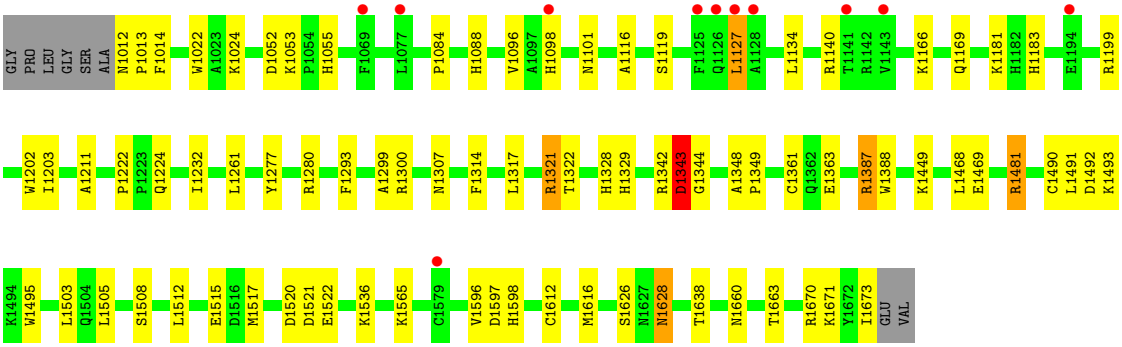
• Molecule 1: Non-structural polyprotein

Chain A:



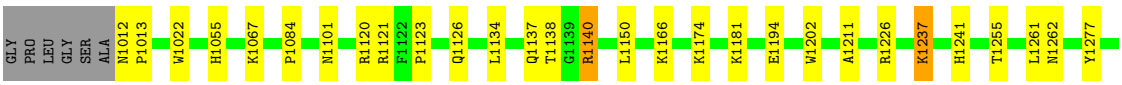
• Molecule 1: Non-structural polyprotein

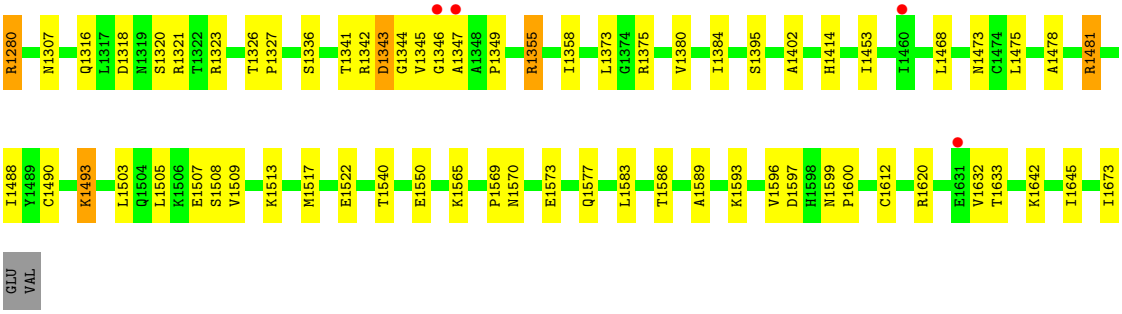
Chain B:



• Molecule 1: Non-structural polyprotein

Chain C:




R1280
N1307
Q1316
L1317
D1318
N1319
S1320
R1321
T1322
R1323
T1326
P1327
S1336
T1341
R1342
D1343
G1344
V1345
G1346
A1347
A1348
P1349
R1355
I1358
L1373
G1374
R1375
V1380
I1384
S1395
A1402
H1414
I1453
I1460
L1468
N1473
C1474
L1475
A1478
R1481
I1488
Y1489
C1490
K1493
L1503
Q1504
L1505
K1506
E1507
S1508
V1509
K1513
M1517
E1522
T1540
E1550
K1565
P1569
N1570
E1573
Q1577
L1583
T1586
A1589
K1593
V1596
D1597
H1598
N1599
P1600
C1612
R1620
E1631
V1632
T1633
K1642
I1645
I1673
GLU
VAL

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.84 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1066)	Depositor
R, R_{free}	0.186 , 0.217 0.192 , 0.223	Depositor DCC
R_{free} test set	5285 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	60.8	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MES, 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	0.32	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 (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	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:O	1:A:1121:ARG:HG3	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:N	1:B:1522:GLU:OE1	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:CZ	1:A:1142:ARG:HB3	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:N	1:A:1469:GLU:OE1	2.36	0.58
1:B:1521:ASP:N	1:B:1522:GLU:OE1	2.36	0.58
1:B:1232:ILE:N	1:B:1232:ILE:HD12	2.19	0.58
1:C:1596:VAL:CG1	1:C:1597:ASP:N	2.67	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:B:1321:ARG:NH1	1:B:1322:THR:OG1	2.42	0.53
1:C:1341:THR:HG22	1:C:1342:ARG:N	2.23	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:O	1:B:1300:ARG:HG3	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:HD13	1:B:1127:LEU:N	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:C	1:B:1468:LEU:HD23	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:A:1318:ASP:OD1	1:A:1323:ARG:NH2	2.45	0.49
1:B:1116:ALA:O	1:B:1119:SER:OG	2.21	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:A:1293:PHE:CE2	1:A:1317:LEU:HB2	2.48	0.48
1:C:1277:TYR:CD1	1:C:1277:TYR:N	2.82	0.48
1:A:1199:ARG:HG3	1:A:1199:ARG:HH11	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:N	1:B:1277:TYR:CD1	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:HD3	1:A:1082:SER:HG	1.82	0.45
1:A:1080:LYS:HB3	1:A:1109:GLY:O	2.16	0.45
1:A:1181:LYS:HD3	1:A:1181:LYS:N	2.30	0.45
1:B:1166:LYS:HG2	1:B:1307:ASN:ND2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1012:ASN:N	1:C:1013:PRO:CD	2.79	0.45
1:C:1316:GLN:HB3	1:C:1509:VAL:HG21	1.97	0.45
1:A:1042:TRP:HB3	1:A:1049:PHE:CD2	2.52	0.45
1:C:1355:ARG:HD2	1:C:1493:LYS:HZ3	1.81	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:1222:PRO:CB	1:C:1508:SER:HB3	2.47	0.44
1:B:1387:ARG:O	1:B:1387:ARG:HG3	2.17	0.44
1:C:1121:ARG:O	1:C:1121:ARG:HG3	2.16	0.44
1:C:1565:LYS:NZ	1:C:1569:PRO:O	2.50	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:C	1:C:1468:LEU:HD23	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:N	1:A:1343:ASP:OD1	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:A:1202:TRP:CE3	1:A:1211:ALA:HA	2.53	0.43
1:C:1022:TRP:CE2	1:C:1055:HIS:HB3	2.53	0.43
1:C:1346:GLY:HA3	1:C:1347:ALA:HA	1.80	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:A:1420:PHE:CG	1:A:1467:ARG:NH1	2.87	0.43
1:B:1348:ALA:HA	1:B:1349:PRO:HD3	1.87	0.43
1:C:1138:THR:OG1	1:C:1140:ARG:HG2	2.19	0.43
1:C:1321:ARG:HE	1:C:1513:LYS:CB	2.32	0.43
1:A:1121:ARG:O	1:A:1121:ARG:CG	2.63	0.43
1:B:1638:THR:HG22	1:B:1638:THR:O	2.19	0.43
1:C:1150:LEU:HD13	1:C:1241:HIS:HB2	2.00	0.43
1:C:1402:ALA:HA	1:C:1414:HIS:O	2.18	0.43
1:A:1570:ASN:OD1	1:A:1573:GLU:HG3	2.19	0.43
1:C:1174:LYS:HB3	1:C:1194:GLU:O	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:CD1	1:A:1277:TYR:N	2.86	0.42
1:B:1014:PHE:CZ	1:B:1024:LYS:HA	2.55	0.42
1:B:1293:PHE:CE2	1:B:1317:LEU:HB2	2.55	0.42
1:B:1673:ILE:HD12	1:B:1673:ILE:O	2.20	0.42
1:C:1453:ILE:O	1:C:1488:ILE:HA	2.20	0.42
1:C:1577:GLN:OE1	1:C:1593:LYS:HE2	2.19	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:HE	1:B:1387:ARG:HB2	1.75	0.42
1:A:1162:VAL:O	1:A:1162:VAL:HG23	2.20	0.41
1:A:1293:PHE:CG	1:A:1314:PHE:HB3	2.55	0.41
1:C:1336:SER:HB2	1:C:1342:ARG:CD	2.48	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:C	1:C:1475:LEU:HD23	2.41	0.41
1:A:1344:GLY:C	1:A:1345:VAL:CG2	2.90	0.41
1:A:1540:THR:HB	2:A:1707:SO4:O3	2.21	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: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:A:1096:VAL:HG12	1:A:1097:ALA:N	2.35	0.40
1:C:1336:SER:CB	1:C:1342:ARG:HD3	2.46	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:C:1345:VAL:O	1:C:1346:GLY:C	2.59	0.40
1:A:1067:LYS:O	1:A:1133:GLN:HG3	2.21	0.40
1:B:1293:PHE:CG	1:B:1314:PHE:HB3	2.55	0.40
1:C:1067:LYS:HD3	1:C:1067:LYS:HA	1.91	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 (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	660/670 (98%)	641 (97%)	18 (3%)	1 (0%)	47	75
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%)	51	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1586	THR

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	551/574 (96%)	533 (97%)	18 (3%)	38	68
1	B	548/574 (96%)	526 (96%)	22 (4%)	31	62
1	C	566/574 (99%)	549 (97%)	17 (3%)	41	72
All	All	1665/1722 (97%)	1608 (97%)	57 (3%)	37	67

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

Sometimes 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 monosaccharides 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	0.13	0	6,6,6	0.28	0
2	SO4	A	1714	-	4,4,4	0.15	0	6,6,6	0.27	0
2	SO4	C	1705	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	C	1701	-	4,4,4	0.14	0	6,6,6	0.19	0
2	SO4	C	1706	-	4,4,4	0.13	0	6,6,6	0.24	0
2	SO4	A	1703	-	4,4,4	0.12	0	6,6,6	0.14	0
3	MES	A	1717	-	12,12,12	2.21	1 (8%)	14,16,16	2.22	5 (35%)
2	SO4	C	1707	-	4,4,4	0.14	0	6,6,6	0.08	0
3	MES	A	1716	-	12,12,12	2.18	1 (8%)	14,16,16	2.27	6 (42%)
3	MES	B	1706	-	12,12,12	2.16	1 (8%)	14,16,16	1.64	5 (35%)
2	SO4	A	1705	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	C	1710	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	C	1712	-	4,4,4	0.17	0	6,6,6	0.08	0
3	MES	A	1718	-	12,12,12	2.16	1 (8%)	14,16,16	1.54	4 (28%)
3	MES	C	1719	-	12,12,12	2.19	1 (8%)	14,16,16	1.69	3 (21%)
3	MES	C	1720	-	12,12,12	2.18	1 (8%)	14,16,16	1.74	5 (35%)
3	MES	C	1721	-	12,12,12	2.14	1 (8%)	14,16,16	1.59	3 (21%)
2	SO4	A	1708	-	4,4,4	0.12	0	6,6,6	0.19	0
2	SO4	A	1704	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	1702	-	4,4,4	0.15	0	6,6,6	0.23	0
2	SO4	B	1701	-	4,4,4	0.17	0	6,6,6	0.06	0
2	SO4	A	1713	-	4,4,4	0.13	0	6,6,6	0.16	0
2	SO4	C	1708	-	4,4,4	0.13	0	6,6,6	0.19	0
2	SO4	C	1714	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	A	1709	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	B	1703	-	4,4,4	0.16	0	6,6,6	0.09	0
2	SO4	A	1711	-	4,4,4	0.19	0	6,6,6	0.18	0
2	SO4	B	1705	-	4,4,4	0.10	0	6,6,6	0.22	0
2	SO4	A	1706	-	4,4,4	0.13	0	6,6,6	0.09	0
2	SO4	C	1716	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	C	1709	-	4,4,4	0.16	0	6,6,6	0.15	0
2	SO4	C	1717	-	4,4,4	0.15	0	6,6,6	0.28	0
2	SO4	A	1715	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	A	1710	-	4,4,4	0.16	0	6,6,6	0.12	0
3	MES	B	1707	-	12,12,12	2.10	1 (8%)	14,16,16	1.77	4 (28%)
2	SO4	A	1712	-	4,4,4	0.12	0	6,6,6	0.08	0
2	SO4	A	1707	-	4,4,4	0.15	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	C	1715	-	4,4,4	0.19	0	6,6,6	0.08	0
2	SO4	C	1703	-	4,4,4	0.13	0	6,6,6	0.12	0
2	SO4	B	1702	-	4,4,4	0.11	0	6,6,6	0.19	0
2	SO4	C	1718	-	4,4,4	0.16	0	6,6,6	0.20	0
2	SO4	B	1704	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	C	1704	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	A	1702	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	C	1711	-	4,4,4	0.17	0	6,6,6	0.17	0
2	SO4	C	1713	-	4,4,4	0.09	0	6,6,6	0.21	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	MES	C	1719	-	-	1/6/14/14	0/1/1/1
3	MES	A	1717	-	-	4/6/14/14	0/1/1/1
3	MES	B	1706	-	-	0/6/14/14	0/1/1/1
3	MES	C	1720	-	-	2/6/14/14	0/1/1/1
3	MES	C	1721	-	-	4/6/14/14	0/1/1/1
3	MES	A	1716	-	-	3/6/14/14	0/1/1/1
3	MES	B	1707	-	-	0/6/14/14	0/1/1/1
3	MES	A	1718	-	-	2/6/14/14	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1719	MES	C8-S	-7.35	1.67	1.77
3	A	1717	MES	C8-S	-7.32	1.67	1.77
3	A	1716	MES	C8-S	-7.24	1.67	1.77
3	C	1720	MES	C8-S	-7.22	1.67	1.77
3	B	1706	MES	C8-S	-7.19	1.67	1.77
3	A	1718	MES	C8-S	-7.17	1.67	1.77
3	C	1721	MES	C8-S	-7.06	1.67	1.77
3	B	1707	MES	C8-S	-6.86	1.67	1.77

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1717	MES	C6-C5-N4	-5.20	102.21	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1716	MES	O1S-S-C8	5.09	113.04	106.92
3	C	1719	MES	O1S-S-C8	4.41	112.23	106.92
3	B	1707	MES	C6-C5-N4	-3.45	104.86	110.10
3	A	1716	MES	C2-C3-N4	-3.29	105.12	110.10
3	A	1716	MES	C6-C5-N4	-3.09	105.41	110.10
3	B	1706	MES	O1S-S-C8	3.04	110.58	106.92
3	C	1720	MES	O3S-S-C8	3.03	110.67	105.77
3	A	1717	MES	O1S-S-C8	2.92	110.44	106.92
3	C	1721	MES	C6-C5-N4	-2.81	105.84	110.10
3	C	1720	MES	C5-N4-C3	2.77	115.06	108.83
3	A	1718	MES	O3S-S-C8	2.75	110.21	105.77
3	B	1707	MES	O1S-S-C8	2.71	110.18	106.92
3	C	1719	MES	C5-N4-C3	2.56	114.59	108.83
3	A	1717	MES	C7-N4-C5	2.56	117.77	111.23
3	B	1707	MES	C2-C3-N4	-2.55	106.24	110.10
3	A	1717	MES	O3S-S-C8	2.55	109.89	105.77
3	C	1721	MES	O2S-S-C8	2.45	109.86	106.92
3	C	1721	MES	O3S-S-C8	2.43	109.70	105.77
3	B	1706	MES	O3S-S-C8	2.37	109.60	105.77
3	B	1706	MES	O2S-S-C8	2.36	109.76	106.92
3	A	1717	MES	C5-N4-C3	2.35	114.11	108.83
3	B	1706	MES	C6-C5-N4	-2.32	106.58	110.10
3	B	1706	MES	C5-N4-C3	2.30	114.01	108.83
3	C	1720	MES	C6-C5-N4	-2.30	106.61	110.10
3	A	1716	MES	O2S-S-C8	2.28	109.66	106.92
3	A	1718	MES	O1S-S-C8	2.24	109.61	106.92
3	A	1716	MES	C5-N4-C3	2.23	113.85	108.83
3	C	1719	MES	O2S-S-O1S	-2.22	106.27	113.95
3	A	1716	MES	C7-N4-C5	2.20	116.86	111.23
3	C	1720	MES	O2S-S-C8	2.16	109.52	106.92
3	A	1718	MES	O2S-S-C8	2.14	109.50	106.92
3	B	1707	MES	O3S-S-C8	2.04	109.07	105.77
3	C	1720	MES	C7-N4-C5	2.02	116.41	111.23
3	A	1718	MES	C5-N4-C3	2.02	113.38	108.83

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1717	MES	C8-C7-N4-C5
3	A	1718	MES	C8-C7-N4-C3
3	C	1720	MES	C8-C7-N4-C3

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Mol	Chain	Res	Type	Atoms
3	C	1720	MES	C8-C7-N4-C5
3	C	1721	MES	C8-C7-N4-C3
3	A	1716	MES	C7-C8-S-O3S
3	A	1717	MES	C7-C8-S-O3S
3	C	1721	MES	C7-C8-S-O3S
3	A	1718	MES	C8-C7-N4-C5
3	A	1716	MES	C7-C8-S-O1S
3	A	1716	MES	C7-C8-S-O2S
3	A	1717	MES	C7-C8-S-O1S
3	A	1717	MES	C7-C8-S-O2S
3	C	1721	MES	C7-C8-S-O1S
3	C	1721	MES	C7-C8-S-O2S
3	C	1719	MES	C8-C7-N4-C5

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1701	SO4	1	0
2	C	1706	SO4	1	0
3	C	1720	MES	1	0
3	C	1721	MES	1	0
2	C	1714	SO4	1	0
2	C	1717	SO4	1	0
2	A	1707	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.10	11 (1%)	70	68	45, 68, 103, 154	0
1	B	662/670 (98%)	0.11	11 (1%)	70	68	43, 71, 107, 158	0
1	C	662/670 (98%)	-0.02	4 (0%)	89	89	37, 55, 87, 134	0
All	All	1986/2010 (98%)	0.07	26 (1%)	77	76	37, 65, 102, 158	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1126	GLN	3.7
1	A	1346	GLY	3.7
1	B	1125	PHE	3.5
1	B	1127	LEU	3.4
1	A	1586	THR	2.9
1	C	1347	ALA	2.9
1	B	1128	ALA	2.8
1	C	1346	GLY	2.5
1	B	1194	GLU	2.5
1	A	1497	GLU	2.4
1	B	1143	VAL	2.3
1	A	1585	GLU	2.3
1	A	1645	ILE	2.3
1	A	1172	PRO	2.2
1	A	1583	LEU	2.2
1	B	1069	PHE	2.2
1	B	1077	LEU	2.1
1	A	1649	GLN	2.1
1	B	1098	HIS	2.1
1	C	1631	GLU	2.1
1	B	1141	THR	2.1
1	A	1647	ASN	2.1
1	B	1579	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1613	MET	2.1
1	A	1646	LYS	2.0
1	C	1460	ILE	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	C	1713	5/5	0.62	0.32	114,118,130,135	0
2	SO4	A	1714	5/5	0.63	0.28	124,125,130,133	0
2	SO4	A	1711	5/5	0.66	0.31	113,131,134,135	0
2	SO4	B	1705	5/5	0.70	0.27	116,122,128,134	0
2	SO4	C	1709	5/5	0.74	0.35	124,128,139,143	0
2	SO4	C	1707	5/5	0.74	0.29	134,141,142,143	0
2	SO4	A	1709	5/5	0.79	0.25	121,124,126,129	0
2	SO4	A	1712	5/5	0.80	0.25	154,156,157,157	0
2	SO4	A	1713	5/5	0.80	0.23	128,129,132,136	0
2	SO4	C	1711	5/5	0.80	0.16	113,116,130,130	0
2	SO4	C	1702	5/5	0.80	0.23	112,114,122,128	0
2	SO4	C	1706	5/5	0.82	0.26	116,118,122,125	0
2	SO4	A	1715	5/5	0.83	0.32	120,125,128,133	0
2	SO4	C	1704	5/5	0.84	0.23	123,125,130,131	0
2	SO4	A	1708	5/5	0.84	0.32	117,121,126,132	0
2	SO4	B	1702	5/5	0.84	0.23	118,125,128,134	0
2	SO4	C	1705	5/5	0.86	0.30	104,109,117,131	0
2	SO4	B	1703	5/5	0.86	0.25	123,125,127,133	0
3	MES	A	1718	12/12	0.86	0.43	107,116,124,129	0
2	SO4	C	1712	5/5	0.87	0.32	127,128,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	1710	5/5	0.87	0.24	106,116,120,126	0
2	SO4	B	1704	5/5	0.87	0.37	141,142,145,146	0
2	SO4	C	1718	5/5	0.88	0.32	99,102,114,115	0
2	SO4	C	1714	5/5	0.88	0.23	105,109,114,118	0
2	SO4	C	1716	5/5	0.89	0.20	108,112,119,123	0
2	SO4	C	1717	5/5	0.89	0.26	99,105,107,109	0
2	SO4	A	1706	5/5	0.90	0.35	119,121,124,126	0
2	SO4	A	1703	5/5	0.90	0.42	114,115,117,119	0
2	SO4	A	1704	5/5	0.90	0.33	140,140,142,144	0
2	SO4	B	1701	5/5	0.91	0.16	112,117,122,125	0
2	SO4	A	1701	5/5	0.91	0.23	102,103,109,113	0
2	SO4	C	1708	5/5	0.91	0.20	99,109,111,116	0
2	SO4	A	1707	5/5	0.92	0.25	119,120,122,124	0
2	SO4	C	1703	5/5	0.92	0.23	106,108,118,121	0
2	SO4	C	1701	5/5	0.93	0.14	95,100,105,110	0
2	SO4	C	1715	5/5	0.93	0.15	90,95,98,100	0
3	MES	C	1721	12/12	0.93	0.29	82,96,116,116	0
2	SO4	A	1702	5/5	0.94	0.18	105,109,114,120	0
3	MES	B	1706	12/12	0.94	0.20	63,81,92,94	0
2	SO4	A	1705	5/5	0.94	0.16	119,121,126,128	0
3	MES	C	1720	12/12	0.95	0.24	76,93,103,104	0
3	MES	A	1716	12/12	0.96	0.18	67,91,97,98	0
3	MES	B	1707	12/12	0.96	0.18	49,67,77,77	0
3	MES	A	1717	12/12	0.96	0.21	62,77,80,85	0
2	SO4	C	1710	5/5	0.96	0.38	101,104,109,112	0
3	MES	C	1719	12/12	0.99	0.20	36,47,54,64	0
4	ZN	A	1719	1/1	0.99	0.10	91,91,91,91	0
4	ZN	B	1708	1/1	0.99	0.11	96,96,96,96	0
4	ZN	C	1722	1/1	0.99	0.12	70,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.