Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 01:59 AM EDT

PDB ID	:	5L0Q
Title	:	Crystal structure of the complex between ADAM10 D+C domain and a conformation specific mAb 8C7.
Authors	:	Xu, K.; Saha, N.; Nikolov, D.B.
Deposited on	:	2016-07-28
Resolution	:	2.76 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:

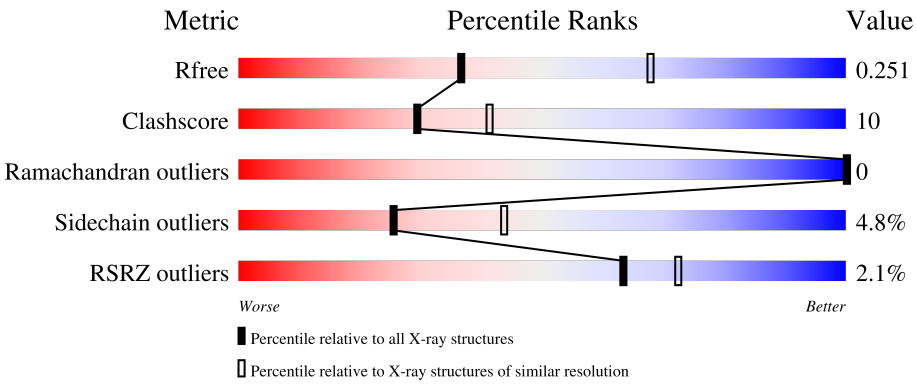
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.76 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	203	3% 68% 27% •
1	D	203	2% 74% 20% •• •
2	B	214	3% 82% 16% •
2	E	214	3% 76% 21% ••
3	C	222	84% 12% •

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Mol	Chain	Length	Quality of chain
3	F	222	% 80% 15% •

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
5	SO4	A	703	-	-	X	-
5	SO4	D	703	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9942 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 Disintegrin and metalloproteinase domain-containing protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	203	1493	893	265	303	32	0	0	0
1	D	195	1440	860	256	292	32	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	450	PRO	-	expression tag	UNP Q10741
A	451	VAL	-	expression tag	UNP Q10741
A	452	GLY	-	expression tag	UNP Q10741
A	453	LEU	-	expression tag	UNP Q10741
A	454	ALA	-	expression tag	UNP Q10741
A	647	GLY	-	expression tag	UNP Q10741
A	648	SER	-	expression tag	UNP Q10741
A	649	ALA	-	expression tag	UNP Q10741
A	650	SER	-	expression tag	UNP Q10741
A	651	GLY	-	expression tag	UNP Q10741
A	652	LEU	-	expression tag	UNP Q10741
D	450	PRO	-	expression tag	UNP Q10741
D	451	VAL	-	expression tag	UNP Q10741
D	452	GLY	-	expression tag	UNP Q10741
D	453	LEU	-	expression tag	UNP Q10741
D	454	ALA	-	expression tag	UNP Q10741
D	647	GLY	-	expression tag	UNP Q10741
D	648	SER	-	expression tag	UNP Q10741
D	649	ALA	-	expression tag	UNP Q10741
D	650	SER	-	expression tag	UNP Q10741
D	651	GLY	-	expression tag	UNP Q10741
D	652	LEU	-	expression tag	UNP Q10741

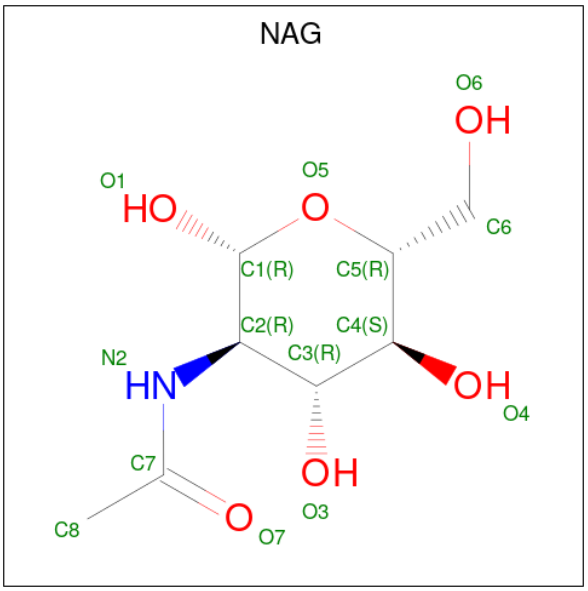
- Molecule 2 is a protein called mAb 8C7 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	212	1645	1024	281	334	6	0	0	0
2	E	212	1651	1027	284	334	6	0	0	0

- Molecule 3 is a protein called mAb 8C7 heavy chain.

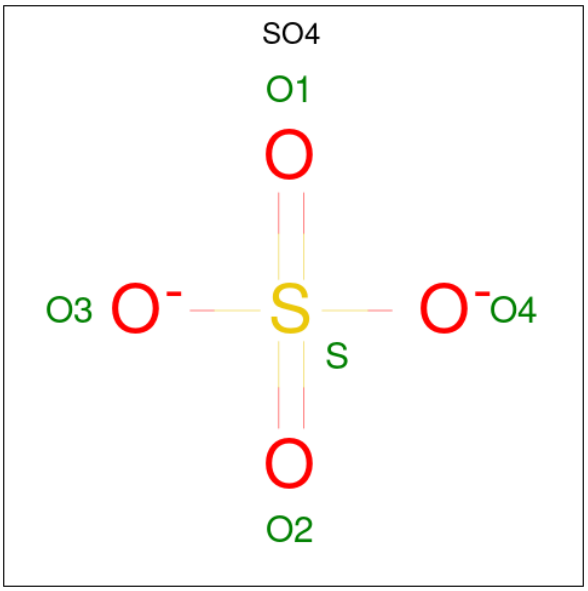
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	213	1624	1031	268	318	7	0	0	0
3	F	214	1632	1035	269	321	7	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
4	C	1	14	8	1	5	0	0
4	D	1	14	8	1	5	0	0
4	F	1	14	8	1	5	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	1	1	1	0	0
			Total	Mg		
6	D	1	1	1	0	0

- Molecule 7 is water.

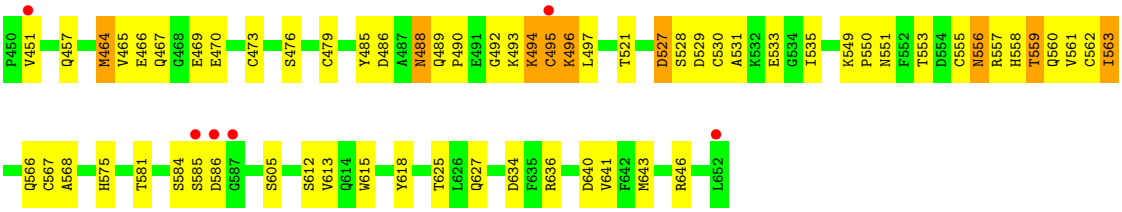
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	40	40	40	0	0
			Total	O		
7	B	51	51	51	0	0
			Total	O		
7	C	66	66	66	0	0
			Total	O		
7	D	44	44	44	0	0
			Total	O		
7	E	56	56	56	0	0
			Total	O		
7	F	77	77	77	0	0

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.

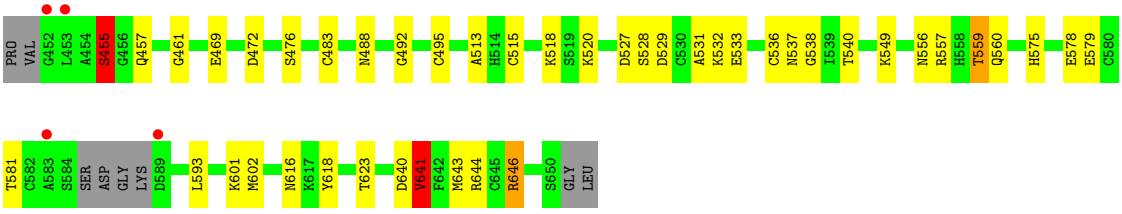
• Molecule 1: Disintegrin and metalloproteinase domain-containing protein 10

Chain A:



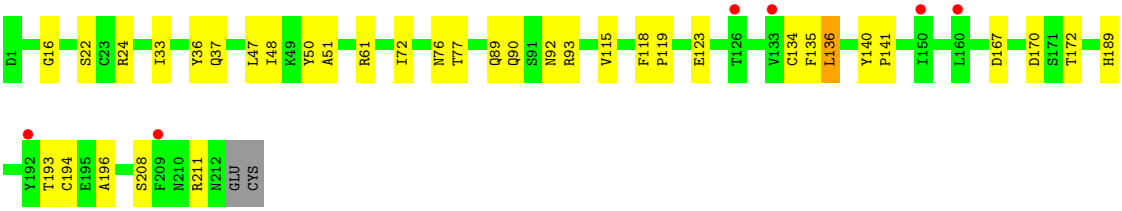
• Molecule 1: Disintegrin and metalloproteinase domain-containing protein 10

Chain D:



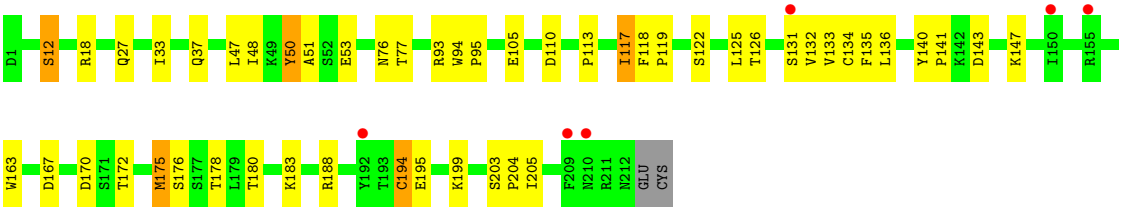
• Molecule 2: mAb 8C7 light chain

Chain B:



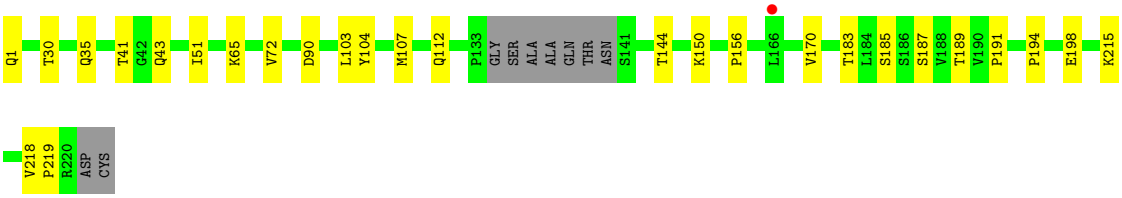
• Molecule 2: mAb 8C7 light chain

Chain E:



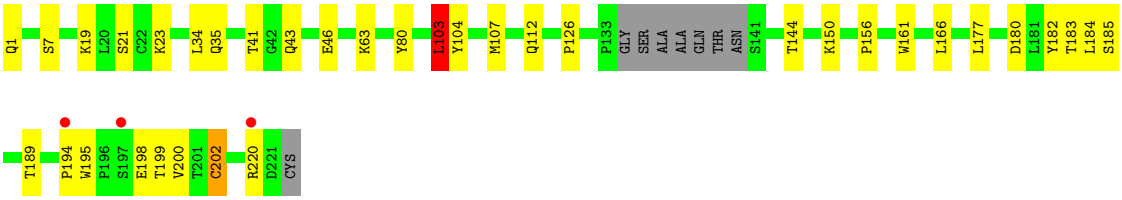
• Molecule 3: mAb 8C7 heavy chain

Chain C:



• Molecule 3: mAb 8C7 heavy chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.33Å 141.68Å 268.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	125.26 – 2.76 125.26 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.5 (125.26-2.76) 98.6 (125.26-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.203 , 0.251 0.205 , 0.251	Depositor DCC
R_{free} test set	2690 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.992	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9942	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.1058e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: SO4, MG, NAG

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	0.83	2/1519 (0.1%)	0.77	3/2040 (0.1%)
1	D	0.45	0/1464	0.65	1/1965 (0.1%)
2	B	0.58	0/1683	0.63	0/2286
2	E	0.61	0/1689	0.64	0/2293
3	C	0.48	0/1668	0.61	0/2278
3	F	0.62	0/1676	0.67	3/2289 (0.1%)
All	All	0.61	2/9699 (0.0%)	0.66	7/13151 (0.1%)

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	3
1	D	0	2
2	B	0	1
2	E	0	1
3	C	0	3
3	F	0	5
All	All	0	15

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	495	CYS	CB-SG	5.28	1.91	1.82
1	A	550	PRO	N-CD	5.17	1.55	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	494	LYS	N-CA-C	-6.51	93.41	111.00
3	F	34	LEU	CA-CB-CG	-5.45	102.76	115.30
1	A	457	GLN	C-N-CD	5.44	139.82	128.40
1	D	641	VAL	CB-CA-C	-5.43	101.09	111.40
3	F	103	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	549	LYS	C-N-CD	5.20	139.33	128.40
3	F	184	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	490	PRO	Peptide
1	A	584	SER	Peptide
1	A	585	SER	Peptide
2	B	50	TYR	Peptide
3	C	104	TYR	Peptide
3	C	156	PRO	Peptide
3	C	41	THR	Peptide
1	D	455	SER	Peptide
1	D	492	GLY	Peptide
2	E	50	TYR	Peptide
3	F	104	TYR	Peptide
3	F	126	PRO	Peptide
3	F	156	PRO	Peptide
3	F	220	ARG	Peptide
3	F	41	THR	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	1493	0	1381	54	0
1	D	1440	0	1324	28	0
2	B	1645	0	1564	31	0
2	E	1651	0	1575	35	0
3	C	1624	0	1581	14	0
3	F	1632	0	1585	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	13	5	0
4	C	14	0	13	1	0
4	D	14	0	13	0	0
4	F	14	0	13	2	0
5	A	15	0	0	4	0
5	B	10	0	0	1	0
5	C	15	0	0	0	0
5	D	10	0	0	2	0
5	E	10	0	0	0	0
5	F	5	0	0	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	40	0	0	12	0
7	B	51	0	0	3	0
7	C	66	0	0	3	0
7	D	44	0	0	5	0
7	E	56	0	0	4	0
7	F	77	0	0	6	0
All	All	9942	0	9062	178	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 10.

All (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:SER:OG	1:A:488:ASN:ND2	1.88	1.06
1:A:470:GLU:OE2	1:A:497:LEU:N	1.88	1.05
2:B:193:THR:OG1	2:B:208:SER:OG	1.73	1.04
2:B:135:PHE:C	2:B:136:LEU:HD23	1.84	0.98
4:A:701:NAG:O6	7:A:801:HOH:O	1.84	0.95
4:F:301:NAG:O6	7:F:401:HOH:O	1.87	0.91
1:D:483:CYS:SG	7:D:801:HOH:O	2.32	0.88
1:A:533:GLU:O	7:A:803:HOH:O	1.93	0.86
1:A:561:VAL:HA	7:A:807:HOH:O	1.75	0.86
1:D:559:THR:HG22	1:D:560:GLN:HG3	1.56	0.85
2:B:193:THR:OG1	2:B:208:SER:CB	2.24	0.85
1:A:492:GLY:O	7:A:804:HOH:O	1.97	0.81
3:F:35:GLN:HE22	3:F:107:MET:HG2	1.45	0.81
5:B:301:SO4:O3	7:B:401:HOH:O	2.00	0.80
1:A:551:ASN:HA	1:A:562:CYS:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:163:TRP:CD1	2:E:175:MET:HG3	2.18	0.79
1:D:513:ALA:O	7:D:801:HOH:O	2.01	0.79
3:C:90:ASP:OD1	7:C:401:HOH:O	2.02	0.78
1:A:466:GLU:N	1:A:469:GLU:OE2	2.20	0.74
1:D:515:CYS:SG	7:D:801:HOH:O	2.45	0.74
1:A:559:THR:HG23	1:A:560:GLN:HG3	1.71	0.73
2:E:135:PHE:O	2:E:136:LEU:HD23	1.88	0.73
1:A:563:ILE:CD1	4:A:701:NAG:H62	2.19	0.72
2:E:18:ARG:NH2	7:E:402:HOH:O	2.23	0.71
1:A:494:LYS:HB3	1:A:495:CYS:SG	2.30	0.71
1:A:627:GLN:NE2	7:A:809:HOH:O	2.24	0.70
2:B:189:HIS:O	2:B:211:ARG:NH1	2.24	0.69
2:B:170:ASP:OD2	2:B:172:THR:OG1	2.08	0.69
1:A:495:CYS:O	1:A:496:LYS:HD2	1.93	0.69
2:B:136:LEU:HD23	2:B:136:LEU:N	2.06	0.69
2:E:105:GLU:OE2	7:E:401:HOH:O	2.10	0.69
2:E:135:PHE:C	2:E:136:LEU:HD23	2.13	0.67
3:F:194:PRO:O	3:F:198:GLU:N	2.21	0.65
2:E:110:ASP:OD2	2:E:199:LYS:NZ	2.29	0.65
1:D:518:LYS:O	7:D:802:HOH:O	2.14	0.65
3:F:161:TRP:CZ3	3:F:202:CYS:HB3	2.31	0.65
1:A:563:ILE:HD12	4:A:701:NAG:O5	1.97	0.65
3:F:35:GLN:NE2	3:F:107:MET:HG2	2.13	0.64
3:C:194:PRO:O	3:C:198:GLU:N	2.19	0.64
1:A:646:ARG:NH1	5:A:704:SO4:O4	2.27	0.63
1:A:555:CYS:N	7:A:807:HOH:O	2.31	0.63
2:B:51:ALA:HB1	7:B:419:HOH:O	1.98	0.63
1:A:527:ASP:N	1:A:527:ASP:OD1	2.32	0.61
4:C:301:NAG:O4	7:C:402:HOH:O	2.16	0.61
2:E:163:TRP:HE1	2:E:175:MET:HE3	1.64	0.61
2:E:51:ALA:HB1	7:E:421:HOH:O	2.01	0.61
1:A:563:ILE:HD11	4:A:701:NAG:H62	1.81	0.61
3:C:191:PRO:HB2	3:C:194:PRO:HD2	1.82	0.60
2:E:12:SER:HB2	2:E:105:GLU:HB3	1.83	0.59
1:A:466:GLU:HB2	1:A:469:GLU:OE2	2.04	0.58
1:A:558:HIS:NE2	7:A:805:HOH:O	2.10	0.57
2:B:136:LEU:HD13	2:B:196:ALA:HB2	1.86	0.57
2:B:135:PHE:O	2:B:136:LEU:HD23	2.04	0.57
2:B:16:GLY:HA2	2:B:77:THR:HG23	1.86	0.57
3:F:46:GLU:OE1	3:F:63:LYS:NZ	2.27	0.57
1:A:486:ASP:HB2	1:A:489:GLN:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:SER:OG	1:A:529:ASP:N	2.38	0.56
3:F:199:THR:HA	7:F:419:HOH:O	2.06	0.56
2:E:117:ILE:HD12	2:E:194:CYS:HB3	1.88	0.56
1:A:636:ARG:NH1	5:A:702:SO4:O2	2.32	0.56
1:D:556:ASN:O	1:D:559:THR:HB	2.05	0.56
2:E:170:ASP:OD2	2:E:172:THR:OG1	2.13	0.56
2:E:163:TRP:NE1	2:E:175:MET:CE	2.69	0.55
3:F:150:LYS:HA	3:F:183:THR:HG23	1.88	0.55
2:B:76:ASN:OD1	2:B:77:THR:N	2.40	0.55
4:F:301:NAG:O4	7:F:403:HOH:O	2.04	0.54
1:A:521:THR:HA	1:A:535:ILE:HB	1.89	0.54
1:A:640:ASP:HA	3:C:103:LEU:HB3	1.90	0.54
1:A:612:SER:HB2	5:A:703:SO4:O1	2.08	0.54
2:B:93:ARG:NH1	7:B:405:HOH:O	2.40	0.53
1:D:528:SER:OG	1:D:529:ASP:N	2.40	0.53
2:E:147:LYS:HB3	2:E:195:GLU:HG2	1.89	0.53
2:E:163:TRP:HE1	2:E:175:MET:CE	2.21	0.53
2:E:113:PRO:HG2	2:E:205:ILE:HD12	1.89	0.53
2:E:18:ARG:NH1	7:E:405:HOH:O	2.32	0.53
3:F:23:LYS:HG3	7:F:434:HOH:O	2.07	0.53
1:A:556:ASN:HB3	1:A:559:THR:HG22	1.91	0.53
2:E:37:GLN:HB2	2:E:47:LEU:HD11	1.91	0.52
3:C:198:GLU:HG2	7:C:408:HOH:O	2.08	0.52
1:D:646:ARG:NH2	5:D:703:SO4:O1	2.43	0.52
1:A:473:CYS:N	7:A:802:HOH:O	1.88	0.52
1:A:560:GLN:HB3	1:A:568:ALA:O	2.10	0.52
3:C:1:GLN:OE1	3:C:1:GLN:N	2.35	0.52
1:A:464:MET:HE2	1:A:466:GLU:OE1	2.10	0.52
1:A:560:GLN:O	7:A:807:HOH:O	2.18	0.52
2:E:133:VAL:HG22	2:E:178:THR:HG23	1.92	0.51
1:A:553:THR:O	7:A:807:HOH:O	2.19	0.51
1:D:641:VAL:HG22	3:F:103:LEU:O	2.11	0.51
1:A:488:ASN:C	1:A:488:ASN:HD22	2.13	0.51
1:D:532:LYS:HE3	1:D:533:GLU:H	1.76	0.51
2:E:33:ILE:CG2	2:E:51:ALA:HB2	2.41	0.50
2:B:136:LEU:N	2:B:136:LEU:CD2	2.75	0.50
3:F:144:THR:HG22	3:F:189:THR:OG1	2.11	0.50
2:B:193:THR:OG1	2:B:208:SER:HB2	2.07	0.50
3:C:35:GLN:NE2	3:C:107:MET:HG2	2.27	0.50
3:F:180:ASP:OD1	7:F:404:HOH:O	2.20	0.50
1:D:578:GLU:HG3	1:D:601:LYS:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:144:THR:HG22	3:C:189:THR:OG1	2.12	0.49
1:D:461:GLY:HA3	1:D:472:ASP:OD1	2.12	0.49
1:A:555:CYS:SG	1:A:556:ASN:N	2.85	0.49
1:A:528:SER:HB3	1:A:531:ALA:HB3	1.95	0.49
2:B:33:ILE:HG22	2:B:51:ALA:HB2	1.95	0.49
2:B:90:GLN:OE1	2:B:92:ASN:N	2.45	0.49
1:A:469:GLU:HB2	1:A:495:CYS:HB3	1.94	0.49
3:F:161:TRP:HB2	3:F:166:LEU:HB2	1.94	0.49
2:E:131:SER:OG	2:E:180:THR:HG23	2.13	0.49
2:B:167:ASP:HB3	2:B:170:ASP:HB3	1.94	0.48
2:B:33:ILE:CG2	2:B:51:ALA:HB2	2.44	0.48
1:D:640:ASP:HA	3:F:103:LEU:HB3	1.95	0.48
1:A:530:CYS:SG	1:A:566:GLN:O	2.71	0.48
2:B:123:GLU:OE2	3:C:215:LYS:NZ	2.41	0.48
2:E:163:TRP:NE1	2:E:175:MET:HE2	2.28	0.48
2:B:193:THR:HG1	2:B:208:SER:CB	2.19	0.47
2:E:163:TRP:CE2	2:E:175:MET:HE2	2.49	0.47
1:D:455:SER:OG	1:D:457:GLN:N	2.47	0.47
2:E:76:ASN:HA	2:E:77:THR:HA	1.64	0.47
2:B:33:ILE:HG13	2:B:89:GLN:O	2.14	0.47
2:E:125:LEU:O	2:E:183:LYS:HD2	2.13	0.47
1:A:465:VAL:HG23	1:A:465:VAL:O	2.15	0.47
3:C:150:LYS:HA	3:C:183:THR:HG23	1.97	0.47
2:E:167:ASP:HB3	2:E:170:ASP:HB3	1.96	0.47
1:A:613:VAL:HG12	5:A:703:SO4:S	2.55	0.47
1:D:513:ALA:HB3	7:D:837:HOH:O	2.14	0.47
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.98	0.46
1:D:469:GLU:HB2	1:D:495:CYS:HB3	1.96	0.46
1:D:528:SER:HB3	1:D:531:ALA:HB3	1.96	0.46
1:D:575:HIS:CG	1:D:618:TYR:HB3	2.49	0.46
2:E:118:PHE:HA	2:E:119:PRO:HD3	1.69	0.46
1:A:495:CYS:C	1:A:496:LYS:HD2	2.36	0.46
1:A:625:THR:HB	1:A:643:MET:SD	2.56	0.46
1:D:557:ARG:NH1	2:E:93:ARG:HD2	2.31	0.46
2:E:94:TRP:HA	2:E:95:PRO:C	2.36	0.46
3:F:177:LEU:HD13	3:F:182:TYR:CZ	2.51	0.46
1:A:486:ASP:HB2	1:A:489:GLN:CG	2.45	0.45
3:F:195:TRP:O	7:F:405:HOH:O	2.21	0.45
1:D:518:LYS:O	1:D:538:GLY:HA2	2.16	0.45
1:A:557:ARG:NH2	2:B:93:ARG:HD2	2.32	0.45
2:E:163:TRP:NE1	2:E:175:MET:HG3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:ARG:HD2	2:B:77:THR:O	2.17	0.45
3:C:218:VAL:HA	3:C:219:PRO:HD3	1.73	0.45
1:D:528:SER:O	1:D:549:LYS:NZ	2.44	0.45
2:E:122:SER:O	2:E:126:THR:HG23	2.16	0.44
1:A:493:LYS:O	1:A:494:LYS:C	2.53	0.43
2:B:115:VAL:HG13	2:B:136:LEU:HD22	2.01	0.43
1:D:537:ASN:OD1	1:D:540:THR:HG22	2.19	0.43
2:E:136:LEU:HD23	2:E:136:LEU:N	2.33	0.43
2:B:36:TYR:HE2	2:B:89:GLN:HB3	1.84	0.43
1:A:528:SER:O	7:A:808:HOH:O	2.21	0.43
1:D:476:SER:HB2	1:D:488:ASN:HB2	2.01	0.43
2:B:140:TYR:CG	2:B:141:PRO:HA	2.54	0.43
3:C:170:VAL:HA	3:C:187:SER:O	2.18	0.42
1:A:488:ASN:ND2	1:A:488:ASN:O	2.45	0.42
1:A:615:TRP:N	7:A:806:HOH:O	2.15	0.42
1:D:643:MET:HA	1:D:643:MET:HE2	2.00	0.42
1:D:520:LYS:O	1:D:536:CYS:O	2.37	0.42
2:E:140:TYR:CG	2:E:141:PRO:HA	2.54	0.42
1:D:575:HIS:ND1	1:D:618:TYR:HB3	2.35	0.42
1:A:485:TYR:CD2	1:A:493:LYS:HB3	2.54	0.42
3:F:7:SER:HB3	3:F:21:SER:OG	2.19	0.42
3:C:35:GLN:HE22	3:C:107:MET:HG2	1.83	0.42
1:A:451:VAL:HG11	2:B:72:ILE:HD12	2.01	0.42
2:B:118:PHE:HA	2:B:119:PRO:HD3	1.77	0.41
2:B:135:PHE:O	2:B:136:LEU:CD2	2.67	0.41
1:D:646:ARG:NH2	5:D:703:SO4:O4	2.54	0.41
2:E:27:GLN:OE1	2:E:93:ARG:NH1	2.54	0.41
2:B:16:GLY:HA2	2:B:77:THR:CG2	2.51	0.41
3:F:1:GLN:OE1	3:F:1:GLN:N	2.38	0.41
1:A:575:HIS:ND1	1:A:618:TYR:HB3	2.35	0.41
3:C:51:ILE:HD13	3:C:72:VAL:HG13	2.01	0.41
1:D:601:LYS:HD2	1:D:602:MET:N	2.35	0.41
1:A:479:CYS:SG	1:A:486:ASP:OD1	2.79	0.41
2:E:50:TYR:O	2:E:53:GLU:HG3	2.21	0.41
2:E:203:SER:HA	2:E:204:PRO:HD3	1.87	0.41
1:A:563:ILE:HD12	4:A:701:NAG:H62	2.01	0.41
3:F:19:LYS:HE2	3:F:80:TYR:CD1	2.56	0.41
1:A:643:MET:HA	1:A:643:MET:HE2	2.03	0.41
1:A:559:THR:CG2	1:A:560:GLN:HG3	2.47	0.40
1:A:470:GLU:OE1	1:A:496:LYS:HG3	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	201/203 (99%)	196 (98%)	5 (2%)	0	100	100
1	D	191/203 (94%)	190 (100%)	1 (0%)	0	100	100
2	B	210/214 (98%)	204 (97%)	6 (3%)	0	100	100
2	E	210/214 (98%)	206 (98%)	4 (2%)	0	100	100
3	C	209/222 (94%)	200 (96%)	9 (4%)	0	100	100
3	F	210/222 (95%)	203 (97%)	7 (3%)	0	100	100
All	All	1231/1278 (96%)	1199 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	171/171 (100%)	157 (92%)	14 (8%)	11	20
1	D	165/171 (96%)	154 (93%)	11 (7%)	16	28
2	B	189/192 (98%)	183 (97%)	6 (3%)	39	59
2	E	190/192 (99%)	180 (95%)	10 (5%)	22	38
3	C	181/187 (97%)	176 (97%)	5 (3%)	43	63
3	F	182/187 (97%)	176 (97%)	6 (3%)	38	58
All	All	1078/1100 (98%)	1026 (95%)	52 (5%)	25	44

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	464	MET
1	A	467	GLN
1	A	488	ASN
1	A	496	LYS
1	A	527	ASP
1	A	556	ASN
1	A	559	THR
1	A	563	ILE
1	A	567	CYS
1	A	581	THR
1	A	586	ASP
1	A	605	SER
1	A	634	ASP
1	A	641	VAL
2	B	22	SER
2	B	24	ARG
2	B	48	ILE
2	B	134	CYS
2	B	136	LEU
2	B	194	CYS
3	C	30	THR
3	C	43	GLN
3	C	65	LYS
3	C	112	GLN
3	C	185	SER
1	D	455	SER
1	D	527	ASP
1	D	559	THR
1	D	579	GLU
1	D	581	THR
1	D	593	LEU
1	D	616	ASN
1	D	623	THR
1	D	641	VAL
1	D	644	ARG
1	D	646	ARG
2	E	12	SER
2	E	48	ILE
2	E	117	ILE
2	E	132	VAL
2	E	134	CYS
2	E	143	ASP

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Mol	Chain	Res	Type
2	E	175	MET
2	E	176	SER
2	E	188	ARG
2	E	194	CYS
3	F	43	GLN
3	F	103	LEU
3	F	112	GLN
3	F	185	SER
3	F	200	VAL
3	F	202	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	488	ASN
1	A	556	ASN
1	A	560	GLN
1	A	627	GLN
3	F	62	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
5	SO4	A	703	-	4,4,4	0.23	0	6,6,6	0.36	0
5	SO4	A	704	-	4,4,4	0.17	0	6,6,6	0.43	0
5	SO4	B	302	-	4,4,4	0.23	0	6,6,6	0.21	0
5	SO4	C	303	-	4,4,4	0.24	0	6,6,6	0.17	0
4	NAG	A	701	1	14,14,15	0.93	0	17,19,21	3.32	5 (29%)
4	NAG	C	301	3	14,14,15	0.51	0	17,19,21	0.66	0
5	SO4	E	301	-	4,4,4	0.19	0	6,6,6	0.13	0
5	SO4	F	302	-	4,4,4	0.24	0	6,6,6	0.28	0
5	SO4	C	302	-	4,4,4	0.11	0	6,6,6	0.29	0
5	SO4	A	702	-	4,4,4	0.16	0	6,6,6	0.19	0
5	SO4	D	702	-	4,4,4	0.16	0	6,6,6	0.12	0
5	SO4	C	304	-	4,4,4	0.22	0	6,6,6	0.35	0
5	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.07	0
4	NAG	F	301	3	14,14,15	0.33	0	17,19,21	0.88	1 (5%)
4	NAG	D	701	1	14,14,15	0.29	0	17,19,21	0.50	0
5	SO4	E	302	-	4,4,4	0.17	0	6,6,6	0.25	0
5	SO4	D	703	-	4,4,4	0.14	0	6,6,6	0.17	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
4	NAG	D	701	1	-	0/6/23/26	0/1/1/1
4	NAG	A	701	1	-	5/6/23/26	0/1/1/1
4	NAG	F	301	3	-	2/6/23/26	0/1/1/1
4	NAG	C	301	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	701	NAG	C1-O5-C5	9.49	125.05	112.19
4	A	701	NAG	C4-C3-C2	-6.24	101.88	111.02
4	A	701	NAG	C3-C4-C5	-4.41	102.38	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	701	NAG	C2-N2-C7	-4.28	116.81	122.90
4	F	301	NAG	C1-O5-C5	2.95	116.19	112.19
4	A	701	NAG	O5-C5-C6	2.80	111.60	107.20

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	NAG	C8-C7-N2-C2
4	A	701	NAG	O7-C7-N2-C2
4	F	301	NAG	O5-C5-C6-O6
4	C	301	NAG	O5-C5-C6-O6
4	C	301	NAG	C4-C5-C6-O6
4	F	301	NAG	C4-C5-C6-O6
4	A	701	NAG	C4-C5-C6-O6
4	A	701	NAG	O5-C5-C6-O6
4	A	701	NAG	C3-C2-N2-C7

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	703	SO4	2	0
5	A	704	SO4	1	0
4	A	701	NAG	5	0
4	C	301	NAG	1	0
5	A	702	SO4	1	0
5	B	301	SO4	1	0
4	F	301	NAG	2	0
5	D	703	SO4	2	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	203/203 (100%)	0.35	6 (2%)	50	59	13, 40, 64, 80	0
1	D	195/203 (96%)	0.28	4 (2%)	63	72	13, 40, 58, 79	0
2	B	212/214 (99%)	0.32	6 (2%)	53	62	11, 25, 68, 74	0
2	E	212/214 (99%)	0.34	6 (2%)	53	62	9, 24, 67, 73	0
3	C	213/222 (95%)	0.30	1 (0%)	91	94	12, 25, 48, 65	0
3	F	214/222 (96%)	0.27	3 (1%)	75	82	11, 25, 47, 83	0
All	All	1249/1278 (97%)	0.31	26 (2%)	63	72	9, 29, 62, 83	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	585	SER	3.7
2	B	209	PHE	3.6
1	A	652	LEU	3.4
3	F	220	ARG	3.2
1	A	586	ASP	3.0
2	B	160	LEU	2.9
1	A	587	GLY	2.8
2	B	192	TYR	2.6
2	B	150	ILE	2.5
1	D	589	ASP	2.5
2	E	155	ARG	2.5
2	E	150	ILE	2.4
1	D	453	LEU	2.4
1	A	495	CYS	2.3
1	D	452	GLY	2.3
2	B	133	VAL	2.3
3	F	197	SER	2.2
2	E	209	PHE	2.2
2	E	210	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	583	ALA	2.1
1	A	451	VAL	2.1
2	E	192	TYR	2.1
2	B	126	THR	2.1
2	E	131	SER	2.0
3	C	166	LEU	2.0
3	F	194	PRO	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
4	NAG	A	701	14/15	0.79	0.23	66,74,80,81	0
4	NAG	D	701	14/15	0.82	0.18	52,60,65,67	0
6	MG	A	705	1/1	0.84	0.33	28,28,28,28	0
4	NAG	F	301	14/15	0.86	0.17	42,48,54,57	0
5	SO4	A	703	5/5	0.89	0.16	43,44,63,71	0
4	NAG	C	301	14/15	0.90	0.13	39,48,58,59	0
5	SO4	D	702	5/5	0.92	0.19	57,59,64,78	0
5	SO4	B	301	5/5	0.92	0.14	44,54,63,75	0
6	MG	D	704	1/1	0.92	0.23	33,33,33,33	0
5	SO4	C	302	5/5	0.93	0.13	39,40,47,53	0
5	SO4	E	302	5/5	0.94	0.19	39,39,47,59	0
5	SO4	C	303	5/5	0.94	0.20	32,34,47,55	0
5	SO4	B	302	5/5	0.94	0.19	39,40,49,66	0
5	SO4	A	704	5/5	0.96	0.16	37,40,44,45	0
5	SO4	F	302	5/5	0.96	0.17	33,34,46,65	0
5	SO4	A	702	5/5	0.96	0.21	45,54,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	D	703	5/5	0.96	0.12	45,47,56,57	0
5	SO4	E	301	5/5	0.97	0.17	37,37,46,53	0
5	SO4	C	304	5/5	0.99	0.17	21,21,22,26	0

6.5 Other polymers (i)

There are no such residues in this entry.