Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:22 PM GMT

PDB ID	:	4C9F
Title	:	Structure of SIGN-R1 in complex with Sulfodextran
Authors	:	Silva-Martin, N.; Bartual, S.G.; Rodriguez, A.; Ramirez, E.; Chacon, P.; Anthony, R.M.; Park, C.G.; Hermoso, J.A.
Deposited on	:	2013-10-02
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

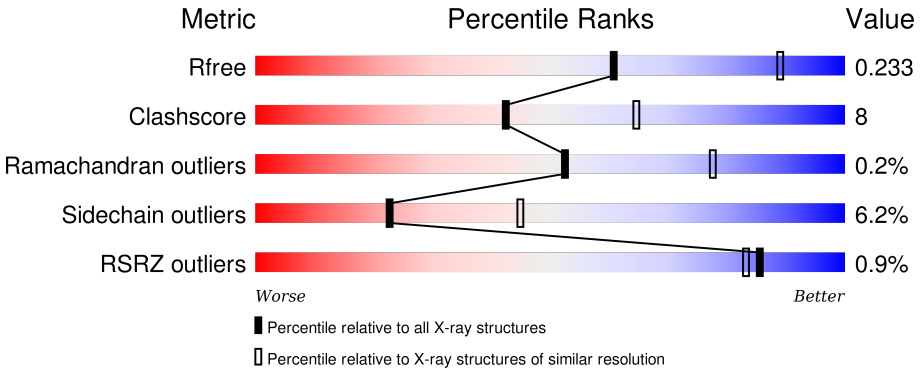
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	134	% 82% 13%
1	B	134	% 77% 21%
1	C	134	% 80% 16%
1	D	134	% 79% 19%

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
4	GQ2	A	1324	-	-	-	X
4	GQ2	B	1329	-	-	-	X
5	GQ4	C	1325	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4680 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 CD209 ANTIGEN-LIKE PROTEIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	0	0
			1073	684	180	200	9			
1	B	133	Total	C	N	O	S	0	0	0
			1080	688	181	202	9			
1	C	132	Total	C	N	O	S	0	0	0
			1073	684	180	200	9			
1	D	134	Total	C	N	O	S	0	0	0
			1089	694	183	203	9			

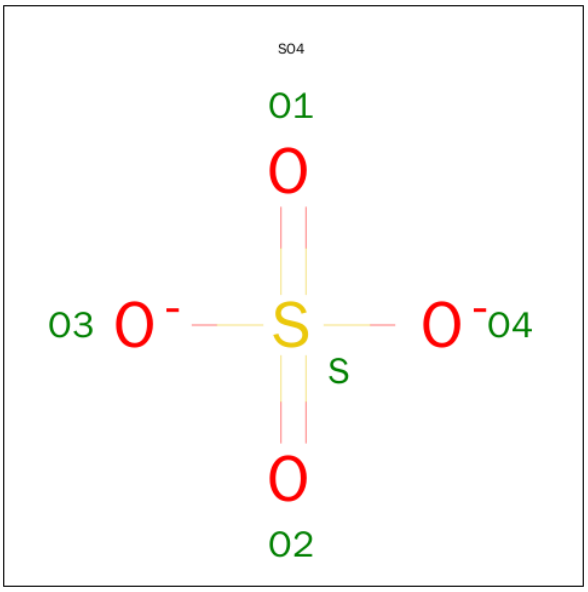
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	LYS	-	EXPRESSION TAG	UNP Q8CJ91
B	190	LYS	-	EXPRESSION TAG	UNP Q8CJ91
C	190	LYS	-	EXPRESSION TAG	UNP Q8CJ91
D	190	LYS	-	EXPRESSION TAG	UNP Q8CJ91

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

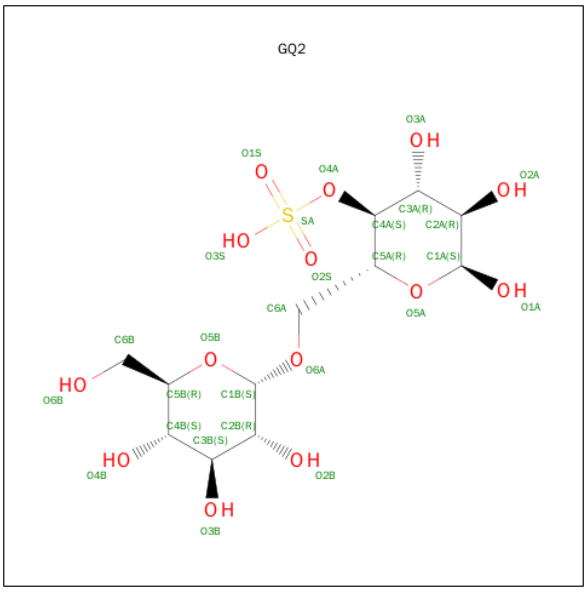
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



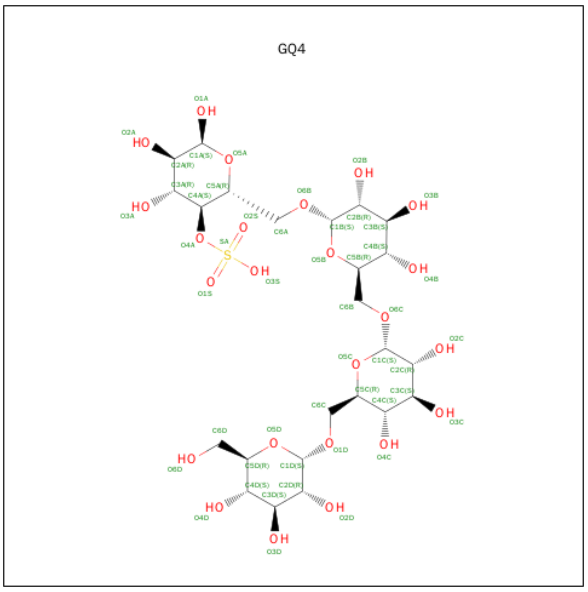
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is SUGAR (6-O-ALPHA-D-GLUCOPYRANOSYL-4-O-SULFO-ALPHA-D-GLUCOPYRANOSE) (three-letter code: GQ2) (formula: $C_{12}H_{22}O_{14}S$).



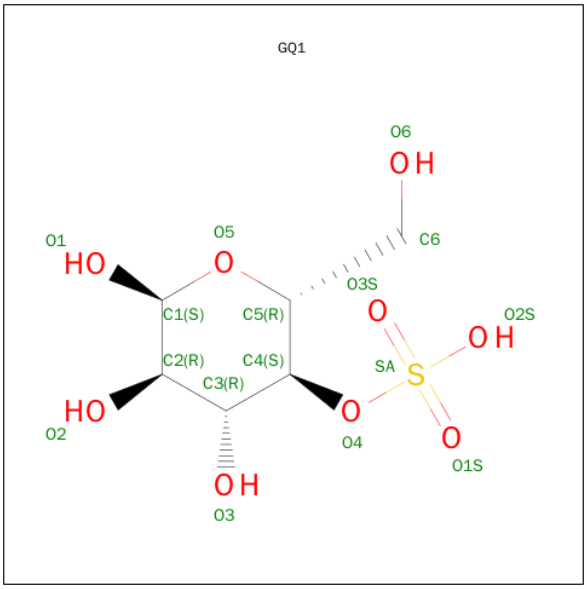
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 27 12 14 1	0	0
4	B	1	Total C O 23 12 11	0	0

- Molecule 5 is SUGAR (ALPHA-D-GLUCOPYRANOSYL-(1->6)-ALPHA-D-GLUCOPYRANOSYL-(1->6)-ALPHA-D-GLUCOPYRANOSYL-(1->6)-4-O-SULFO-ALPHA-D-GLUCOPYRANOSE) (three-letter code: GQ4) (formula: $C_{24}H_{42}O_{24}S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O S 49 24 24 1	0	0

- Molecule 6 is SUGAR (4-O-SULFO-ALPHA-D-GLUCOPYRANOSE) (three-letter code: GQ1) (formula: $C_6H_{12}O_9S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O S 16 6 9 1	0	0
6	D	1	Total C O S 16 6 9 1	0	0
6	D	1	Total C O S 16 6 9 1	0	0

- Molecule 7 is water.

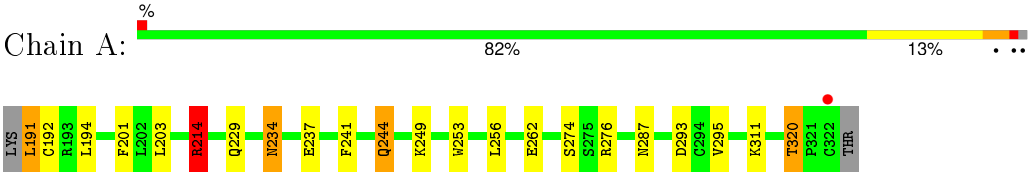
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	43	Total O 43 43	0	0
7	B	44	Total O 44 44	0	0
7	C	40	Total O 40 40	0	0
7	D	37	Total O 37 37	0	0

3 Residue-property plots (i)

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

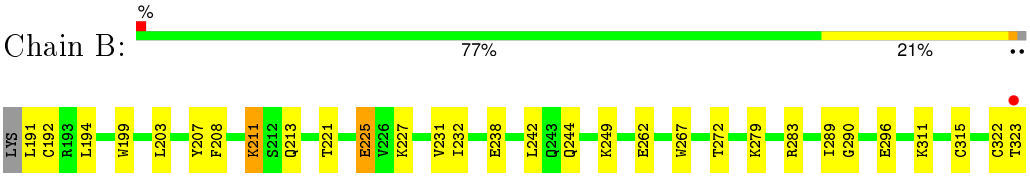
- Molecule 1: CD209 ANTIGEN-LIKE PROTEIN B

Chain A:



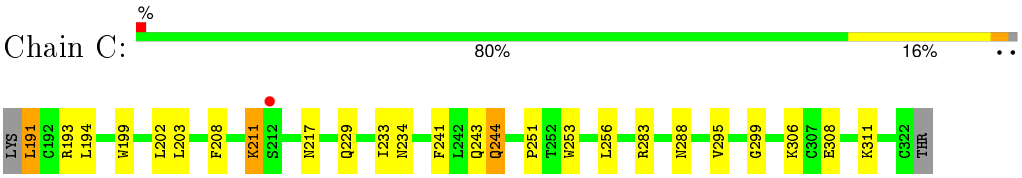
- Molecule 1: CD209 ANTIGEN-LIKE PROTEIN B

Chain B:



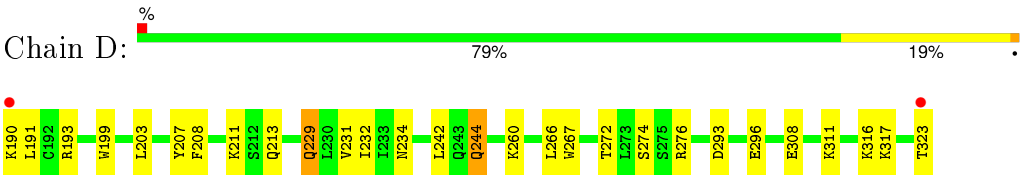
- Molecule 1: CD209 ANTIGEN-LIKE PROTEIN B

Chain C:



- Molecule 1: CD209 ANTIGEN-LIKE PROTEIN B

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.03Å 97.96Å 73.85Å 90.00° 120.86° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 61.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.00-2.60) 99.0 (61.82-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.191 , 0.233 0.198 , 0.233	Depositor DCC
R_{free} test set	1345 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 13.5	EDS
Estimated twinning fraction	0.468 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	4 of 26958 reflections (0.015%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4680	wwPDB-VP
Average B, all atoms (Å^2)	35.0	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 42.07 % 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 2.1526e-04.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, 0.375 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: CA, GQ4, SO4, GQ1, GQ2

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	0.81	0/1103	0.88	2/1493 (0.1%)
1	B	0.82	0/1110	0.90	1/1503 (0.1%)
1	C	0.86	1/1103 (0.1%)	0.90	1/1493 (0.1%)
1	D	0.84	1/1119 (0.1%)	0.88	1/1514 (0.1%)
All	All	0.83	2/4435 (0.0%)	0.89	5/6003 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	308	GLU	CG-CD	5.44	1.60	1.51
1	D	308	GLU	CG-CD	5.30	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	D	293	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	293	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	283	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	283	ARG	NE-CZ-NH1	5.11	122.86	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	290	GLY	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	1073	0	1017	17	0
1	B	1080	0	1024	21	0
1	C	1073	0	1017	21	0
1	D	1089	0	1037	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0
3	B	25	0	0	1	0
3	C	15	0	0	0	0
3	D	5	0	0	0	0
4	A	27	0	22	2	0
4	B	23	0	21	2	0
5	C	49	0	42	4	0
6	D	48	0	35	4	0
7	A	43	0	0	5	0
7	B	44	0	0	3	0
7	C	40	0	0	4	0
7	D	37	0	0	0	0
All	All	4680	0	4215	72	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 8.

All (72) 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:191:LEU:HD11	1:D:213:GLN:HE21	1.29	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1326:GQ1:H3A	6:D:1326:GQ1:O2S	1.77	0.85
1:B:296:GLU:OE2	4:B:1329:GQ2:O2B	2.01	0.76
1:A:320:THR:O	1:A:320:THR:HG22	1.93	0.68
1:A:234:ASN:ND2	7:A:2016:HOH:O	2.26	0.68
6:D:1326:GQ1:C3	6:D:1326:GQ1:O2S	2.39	0.67
1:C:234:ASN:OD1	7:C:2015:HOH:O	2.12	0.67
1:C:202:LEU:HD12	1:D:244:GLN:OE1	1.94	0.67
1:D:207:TYR:CE2	1:D:316:LYS:HD3	2.31	0.64
1:B:262:GLU:CG	1:B:289:ILE:HG22	2.32	0.59
1:B:227:LYS:O	1:B:227:LYS:HD3	2.03	0.59
1:C:311:LYS:NZ	5:C:1325:GQ4:H2B	2.17	0.58
1:C:251:PRO:HD3	5:C:1325:GQ4:H1D	1.86	0.57
1:C:217:ASN:ND2	7:C:2011:HOH:O	2.11	0.57
1:D:260:LYS:HD2	1:D:266:LEU:HD12	1.87	0.57
1:D:232:ILE:HG23	1:D:267:TRP:CD2	2.40	0.56
1:D:234:ASN:HB2	6:D:1327:GQ1:O1S	2.06	0.55
4:A:1324:GQ2:O2B	4:A:1324:GQ2:H6AA	2.06	0.55
1:B:221:THR:O	1:B:225:GLU:HG2	2.07	0.54
1:C:211:LYS:HG2	1:D:193:ARG:HG3	1.89	0.54
1:B:323:THR:HG22	1:B:323:THR:O	2.07	0.54
1:A:287:ASN:C	1:A:287:ASN:OD1	2.46	0.54
1:A:256:LEU:HD23	1:A:295:VAL:HG21	1.90	0.53
4:B:1329:GQ2:H6AA	4:B:1329:GQ2:O2B	2.09	0.52
1:C:311:LYS:HZ2	5:C:1325:GQ4:H2B	1.73	0.52
1:A:253:TRP:CE2	1:A:311:LYS:HG3	2.45	0.51
1:C:203:LEU:N	1:D:244:GLN:OE1	2.40	0.51
1:A:214:ARG:NE	7:A:2011:HOH:O	2.44	0.51
1:C:203:LEU:HD23	1:D:244:GLN:HG3	1.94	0.49
1:C:234:ASN:ND2	7:C:2017:HOH:O	2.45	0.49
1:A:234:ASN:HD22	1:A:234:ASN:C	2.15	0.48
1:A:214:ARG:CD	7:A:2011:HOH:O	2.61	0.48
1:C:306:LYS:NZ	7:C:2035:HOH:O	2.46	0.48
1:B:191:LEU:C	1:B:191:LEU:HD23	2.34	0.48
1:A:244:GLN:NE2	1:B:203:LEU:H	2.12	0.47
1:A:203:LEU:HD11	1:A:237:GLU:OE1	2.14	0.47
1:D:296:GLU:OE1	1:D:311:LYS:HE3	2.15	0.47
4:A:1324:GQ2:O2B	4:A:1324:GQ2:C6A	2.64	0.46
1:A:192:CYS:O	1:B:249:LYS:NZ	2.49	0.46
1:A:191:LEU:N	7:A:2001:HOH:O	2.48	0.46
1:C:233:ILE:HD12	1:C:233:ILE:N	2.30	0.46
1:B:262:GLU:OE2	1:B:289:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:THR:N	7:B:2042:HOH:O	2.40	0.45
1:C:243:GLN:NE2	1:C:299:GLY:O	2.50	0.45
1:B:211:LYS:HD2	3:B:1328:SO4:O2	2.17	0.45
1:A:249:LYS:HD3	1:B:192:CYS:SG	2.57	0.44
1:B:199:TRP:CE2	1:B:208:PHE:HB2	2.53	0.44
1:D:229:GLN:HB2	1:D:229:GLN:HE21	1.57	0.44
1:D:276:ARG:HB2	6:D:1326:GQ1:H2A	2.00	0.44
1:B:231:VAL:HG21	1:B:242:LEU:HD11	2.00	0.44
1:A:214:ARG:HD2	7:A:2011:HOH:O	2.17	0.44
1:D:231:VAL:HG21	1:D:242:LEU:CD1	2.48	0.44
5:C:1325:GQ4:O2B	5:C:1325:GQ4:H6AA	2.18	0.43
1:B:322:CYS:HA	7:B:2042:HOH:O	2.18	0.43
1:C:253:TRP:CE2	1:C:311:LYS:HG3	2.53	0.43
1:A:194:LEU:HD13	1:A:201:PHE:CD1	2.53	0.43
1:B:238:GLU:O	1:B:242:LEU:HG	2.19	0.43
1:A:241:PHE:O	1:A:244:GLN:HG3	2.19	0.42
1:B:311:LYS:NZ	7:B:2037:HOH:O	2.51	0.42
1:D:199:TRP:CD2	1:D:208:PHE:HB2	2.54	0.42
1:B:213:GLN:HA	1:B:311:LYS:O	2.19	0.42
1:D:231:VAL:HG21	1:D:242:LEU:HD11	2.00	0.42
1:C:199:TRP:CE2	1:C:208:PHE:HB2	2.55	0.42
1:C:256:LEU:HD23	1:C:295:VAL:HG21	2.01	0.42
1:A:191:LEU:HA	1:B:211:LYS:O	2.20	0.41
1:C:244:GLN:NE2	1:D:203:LEU:H	2.18	0.41
1:B:232:ILE:HG23	1:B:267:TRP:CD2	2.55	0.41
1:C:199:TRP:CD2	1:C:208:PHE:HB2	2.56	0.41
1:B:207:TYR:HA	1:B:315:CYS:O	2.21	0.40
1:C:191:LEU:HD13	1:C:191:LEU:N	2.36	0.40
1:C:241:PHE:O	1:C:244:GLN:HG3	2.22	0.40
1:D:323:THR:O	1:D:323:THR:HG22	2.20	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	130/134 (97%)	121 (93%)	9 (7%)	0	100 100
1	B	131/134 (98%)	128 (98%)	3 (2%)	0	100 100
1	C	130/134 (97%)	126 (97%)	3 (2%)	1 (1%)	24 46
1	D	132/134 (98%)	124 (94%)	8 (6%)	0	100 100
All	All	523/536 (98%)	499 (95%)	23 (4%)	1 (0%)	52 77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	288	ASN

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	117/119 (98%)	108 (92%)	9 (8%)	16 31
1	B	118/119 (99%)	112 (95%)	6 (5%)	29 55
1	C	117/119 (98%)	111 (95%)	6 (5%)	29 55
1	D	119/119 (100%)	111 (93%)	8 (7%)	20 40
All	All	471/476 (99%)	442 (94%)	29 (6%)	23 45

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	LEU
1	A	214	ARG
1	A	229	GLN
1	A	234	ASN
1	A	244	GLN
1	A	262	GLU
1	A	274	SER

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Mol	Chain	Res	Type
1	A	276	ARG
1	A	320	THR
1	B	194	LEU
1	B	211	LYS
1	B	225	GLU
1	B	244	GLN
1	B	272	THR
1	B	279	LYS
1	C	191	LEU
1	C	193	ARG
1	C	194	LEU
1	C	211	LYS
1	C	229	GLN
1	C	244	GLN
1	D	190	LYS
1	D	191	LEU
1	D	211	LYS
1	D	229	GLN
1	D	244	GLN
1	D	272	THR
1	D	274	SER
1	D	317	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	244	GLN
1	B	213	GLN
1	C	234	ASN
1	C	244	GLN
1	D	213	GLN
1	D	229	GLN

5.3.3 RNA

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 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
3	SO4	A	1323	-	4,4,4	0.35	0	6,6,6	0.23	0
4	GQ2	A	1324	2	28,28,28	0.85	0	40,42,42	1.53	7 (17%)
3	SO4	B	1324	-	4,4,4	0.20	0	6,6,6	0.57	0
3	SO4	B	1325	-	4,4,4	0.59	0	6,6,6	0.58	0
3	SO4	B	1326	-	4,4,4	0.72	0	6,6,6	0.48	0
3	SO4	B	1327	-	4,4,4	0.53	0	6,6,6	0.27	0
3	SO4	B	1328	-	4,4,4	0.73	0	6,6,6	1.27	1 (16%)
4	GQ2	B	1329	2	24,24,28	0.98	1 (4%)	35,35,42	2.04	10 (28%)
3	SO4	C	1323	-	4,4,4	0.73	0	6,6,6	0.48	0
3	SO4	C	1324	-	4,4,4	0.74	0	6,6,6	0.22	0
5	GQ4	C	1325	-	52,52,52	1.07	3 (5%)	76,78,78	1.76	16 (21%)
3	SO4	C	1326	-	4,4,4	0.48	0	6,6,6	0.20	0
3	SO4	D	1324	-	4,4,4	0.28	0	6,6,6	0.87	0
6	GQ1	D	1325	-	16,16,16	1.40	3 (18%)	22,24,24	2.88	6 (27%)
6	GQ1	D	1326	-	16,16,16	1.20	2 (12%)	22,24,24	1.79	5 (22%)
6	GQ1	D	1327	-	16,16,16	1.05	1 (6%)	22,24,24	2.53	11 (50%)

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	SO4	A	1323	-	-	0/0/0/0	0/0/0/0
4	GQ2	A	1324	2	-	0/12/52/52	0/2/2/2
3	SO4	B	1324	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1325	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1326	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1327	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1328	-	-	0/0/0/0	0/0/0/0
4	GQ2	B	1329	2	-	0/7/47/52	0/2/2/2
3	SO4	C	1323	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1324	-	-	0/0/0/0	0/0/0/0
5	GQ4	C	1325	-	-	0/22/102/102	0/4/4/4
3	SO4	C	1326	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1324	-	-	0/0/0/0	0/0/0/0
6	GQ1	D	1325	-	-	0/7/27/27	0/1/1/1
6	GQ1	D	1326	-	-	0/7/27/27	0/1/1/1
6	GQ1	D	1327	-	-	0/7/27/27	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1325	GQ1	C3-C2	-2.51	1.45	1.52
6	D	1327	GQ1	C1-C2	-2.48	1.48	1.52
5	C	1325	GQ4	O6B-C1B	2.21	1.44	1.40
6	D	1325	GQ1	O5-C1	2.25	1.47	1.43
6	D	1325	GQ1	C1-C2	2.29	1.57	1.52
6	D	1326	GQ1	C1-C2	2.33	1.57	1.52
4	B	1329	GQ2	O6A-C1B	2.55	1.44	1.40
6	D	1326	GQ1	O5-C1	2.71	1.48	1.43
5	C	1325	GQ4	O6C-C1C	3.23	1.46	1.40
5	C	1325	GQ4	O1D-C1D	3.83	1.47	1.40

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1325	GQ1	O2-C2-C3	-7.50	93.45	110.34
6	D	1325	GQ1	O3-C3-C2	-6.24	96.28	110.34
4	B	1329	GQ2	O4A-C4A-C5A	-5.15	95.59	109.24
6	D	1327	GQ1	O3-C3-C2	-3.99	101.35	110.34
6	D	1327	GQ1	O1-C1-C2	-3.60	99.56	109.21
6	D	1327	GQ1	O2-C2-C3	-3.34	102.81	110.34
4	B	1329	GQ2	C1A-C2A-C3A	-2.97	106.01	110.43
6	D	1327	GQ1	O2-C2-C1	-2.79	103.67	109.82
4	A	1324	GQ2	O5A-C1A-C2A	-2.56	105.72	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1325	GQ1	C1-C2-C3	-2.40	106.86	110.43
5	C	1325	GQ4	C3D-C4D-C5D	-2.18	106.39	110.20
4	A	1324	GQ2	O3B-C3B-C4B	-2.10	105.60	110.34
4	B	1329	GQ2	O3A-C3A-C2A	-2.04	105.74	110.34
5	C	1325	GQ4	C3C-C4C-C5C	2.04	113.76	110.20
4	B	1329	GQ2	C1A-O5A-C5A	2.07	117.30	113.47
6	D	1327	GQ1	C3-C4-C5	2.13	115.65	110.84
6	D	1326	GQ1	O3-C3-C4	2.16	114.98	109.87
5	C	1325	GQ4	O4D-C4D-C5D	2.16	114.97	109.24
3	B	1328	SO4	O4-S-O3	2.17	117.82	108.98
4	B	1329	GQ2	C6A-O6A-C1B	2.19	118.41	113.82
6	D	1326	GQ1	O5-C1-C2	2.20	113.31	109.80
4	A	1324	GQ2	C1B-C2B-C3B	2.23	114.37	109.97
5	C	1325	GQ4	C6A-C5A-C4A	2.25	119.04	113.35
4	A	1324	GQ2	O6A-C1B-C2B	2.29	110.93	108.04
5	C	1325	GQ4	C1D-O5D-C5D	2.35	118.31	113.75
4	B	1329	GQ2	O5A-C5A-C4A	2.36	114.12	109.68
4	A	1324	GQ2	O5A-C5A-C6A	2.43	111.57	106.61
6	D	1327	GQ1	O4-SA-O3S	2.54	115.09	106.86
5	C	1325	GQ4	O1D-C6C-C5C	2.59	113.77	109.08
5	C	1325	GQ4	O5B-C5B-C6B	2.60	111.91	106.61
6	D	1326	GQ1	O5-C5-C6	2.61	112.96	106.36
6	D	1327	GQ1	O5-C1-C2	2.91	114.43	109.80
6	D	1327	GQ1	C4-O4-SA	3.03	124.54	118.77
4	A	1324	GQ2	C2A-C3A-C4A	3.09	116.39	109.60
5	C	1325	GQ4	O6B-C6A-C5A	3.09	114.68	109.08
6	D	1325	GQ1	O5-C5-C4	3.15	116.41	109.75
4	B	1329	GQ2	O6A-C6A-C5A	3.21	114.90	109.08
5	C	1325	GQ4	C2A-C3A-C4A	3.32	116.88	109.60
4	B	1329	GQ2	O5B-C5B-C6B	3.34	114.79	106.36
6	D	1326	GQ1	O2-C2-C1	3.38	117.25	109.82
5	C	1325	GQ4	C6C-O1D-C1D	3.38	120.91	113.82
6	D	1327	GQ1	O5-C5-C4	3.53	117.20	109.75
5	C	1325	GQ4	O6C-C1C-C2C	3.67	112.68	108.04
6	D	1325	GQ1	O3-C3-C4	3.72	118.67	109.87
5	C	1325	GQ4	C1A-C2A-C3A	3.84	116.13	110.43
6	D	1327	GQ1	C2-C3-C4	4.17	118.75	109.60
4	A	1324	GQ2	C4A-O4A-SA	4.24	126.84	118.77
5	C	1325	GQ4	C1D-C2D-C3D	4.25	118.35	109.97
4	B	1329	GQ2	O5A-C5A-C6A	4.37	115.55	106.61
4	B	1329	GQ2	C3A-C4A-C5A	4.46	117.97	110.20
5	C	1325	GQ4	O1D-C1D-C2D	4.63	113.89	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1326	GQ1	C1-O5-C5	4.65	122.06	113.47
5	C	1325	GQ4	C1C-O5C-C5C	4.67	122.82	113.75
6	D	1327	GQ1	C1-O5-C5	4.73	122.22	113.47
5	C	1325	GQ4	C4A-O4A-SA	4.95	128.19	118.77
6	D	1325	GQ1	O2-C2-C1	6.09	123.23	109.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1324	GQ2	2	0
3	B	1328	SO4	1	0
4	B	1329	GQ2	2	0
5	C	1325	GQ4	4	0
6	D	1326	GQ1	3	0
6	D	1327	GQ1	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	132/134 (98%)	-0.21	1 (0%)	87	85	20, 33, 54, 77	0
1	B	133/134 (99%)	-0.23	1 (0%)	87	85	20, 30, 52, 69	0
1	C	132/134 (98%)	-0.19	1 (0%)	87	85	20, 31, 54, 69	0
1	D	134/134 (100%)	-0.21	2 (1%)	76	71	22, 30, 52, 78	0
All	All	531/536 (99%)	-0.21	5 (0%)	85	83	20, 31, 54, 78	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	322	CYS	4.3
1	D	190	LYS	3.6
1	D	323	THR	2.3
1	C	212	SER	2.1
1	B	323	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GQ2	A	1324	27/27	0.72	0.35	5.11	68,85,129,142	0
5	GQ4	C	1325	49/49	0.73	0.44	4.48	73,102,132,145	0
4	GQ2	B	1329	23/27	0.81	0.26	3.58	56,73,86,89	0
3	SO4	B	1325	5/5	0.96	0.17	1.26	63,67,76,77	0
6	GQ1	D	1326	16/16	0.83	0.24	0.81	51,72,104,110	0
3	SO4	C	1324	5/5	0.98	0.14	0.78	61,62,70,74	0
3	SO4	A	1323	5/5	0.99	0.15	0.40	42,44,50,51	0
6	GQ1	D	1325	16/16	0.91	0.19	0.36	38,61,69,73	0
6	GQ1	D	1327	16/16	0.90	0.15	0.19	54,71,87,100	0
3	SO4	C	1323	5/5	0.98	0.19	0.17	53,61,65,68	0
3	SO4	D	1324	5/5	0.99	0.15	0.05	32,33,35,39	0
3	SO4	B	1324	5/5	0.99	0.13	-0.67	32,34,37,42	0
3	SO4	B	1327	5/5	0.99	0.14	-1.00	45,45,48,49	0
2	CA	C	401	1/1	0.91	0.11	-1.63	54,54,54,54	0
2	CA	B	401	1/1	0.96	0.10	-2.29	50,50,50,50	0
2	CA	D	401	1/1	0.92	0.09	-3.33	53,53,53,53	0
2	CA	A	401	1/1	0.97	0.04	-4.24	56,56,56,56	0
3	SO4	B	1328	5/5	0.97	0.11	-	43,46,50,50	0
3	SO4	B	1326	5/5	0.94	0.28	-	66,74,78,80	0
3	SO4	C	1326	5/5	0.85	0.43	-	117,120,127,128	0

6.5 Other polymers (i)

There are no such residues in this entry.