wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:35 PM GMT

PDB ID	:	3U4E
Title	:	Crystal Structure of PG9 Fab in Complex with V1V2 Region from HIV-1 strain CAP45
Authors	:	Gorman, J.; McLellan, J.; Pancera, M.; Kwong, P.D.
Deposited on	:	2011-10-07
Resolution	:	2.19 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

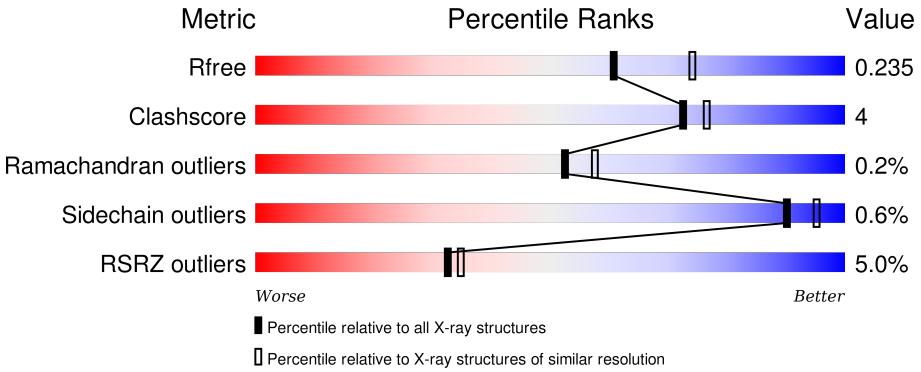
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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	G	124	9%, 74%, 12%, 13%
1	J	124	11%, 79%, 9%, 12%
2	A	248	6%, 88%, 7%
2	H	248	2%, 89%, 8%
3	B	216	5%, 89%, 9%

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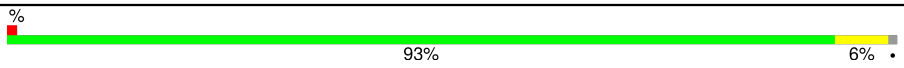
Mol	Chain	Length	Quality of chain
3	L	216	

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	MAN	G	659	-	-	-	X
6	SO4	B	216	-	-	-	X
6	SO4	G	15	-	-	-	X
6	SO4	L	218	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17692 atoms, of which 8372 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 V1V2 region of HIV-1 on 1FD6 scaffold.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	G	108	Total	C	H	N	O	S	0	0	0
			1647	529	805	136	172	5			
1	J	109	Total	C	H	N	O	S	0	0	0
			1659	537	806	137	175	4			

- Molecule 2 is a protein called PG9 Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	239	Total	C	H	N	O	S	0	0	0
			3577	1155	1738	309	365	10			
2	A	230	Total	C	H	N	O	S	0	1	0
			3476	1127	1688	301	351	9			

- Molecule 3 is a protein called PG9 Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	214	Total	C	H	N	O	S	0	0	0
			3138	988	1547	271	328	4			
3	B	212	Total	C	H	N	O	S	0	0	0
			3114	978	1541	268	323	4			

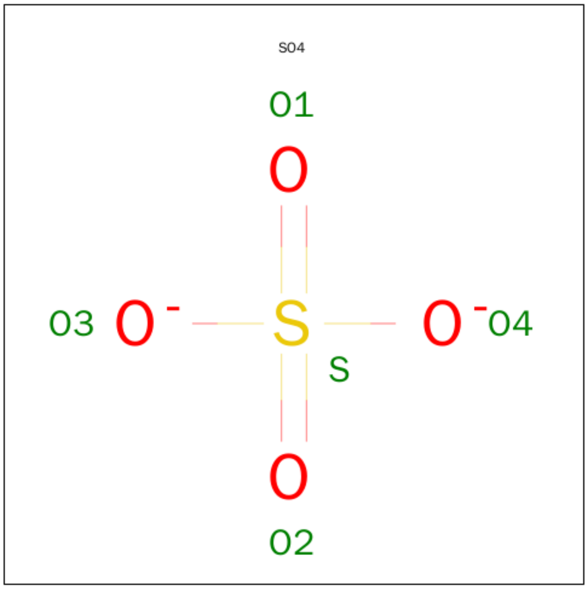
- Molecule 4 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	7	Total	C	H	N	O	0	0
			154	46	71	2	35		
4	J	7	Total	C	H	N	O	0	0
			154	46	71	2	35		

- Molecule 5 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
5	G	6	133	40	61	2	30	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	2	Total C H N O 54 16 26 2 10	0	0

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total C H O 40 12 18 10	0	0

- Molecule 9 is water.

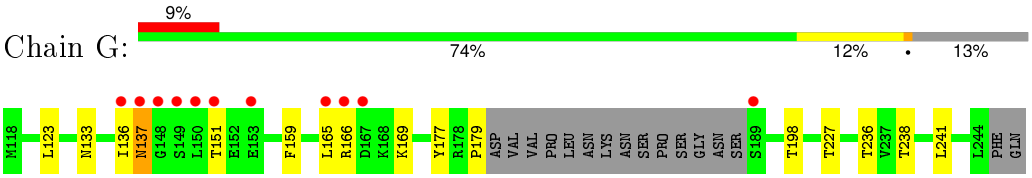
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	21	Total O 21 21	0	0
9	J	19	Total O 19 19	0	0
9	H	123	Total O 123 123	0	0
9	L	135	Total O 135 135	0	0
9	A	109	Total O 109 109	0	0
9	B	79	Total O 79 79	0	0

3 Residue-property plots

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

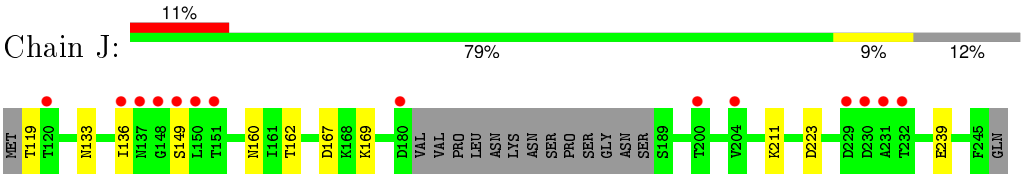
- Molecule 1: V1V2 region of HIV-1 on 1FD6 scaffold

Chain G:



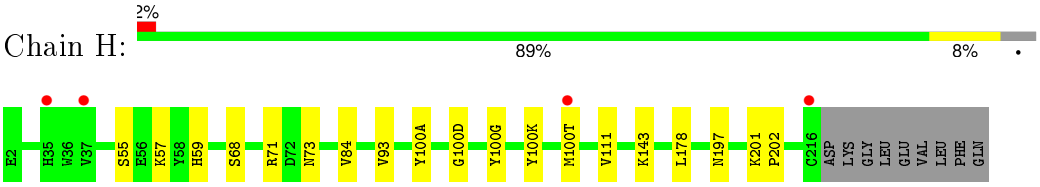
- Molecule 1: V1V2 region of HIV-1 on 1FD6 scaffold

Chain J:



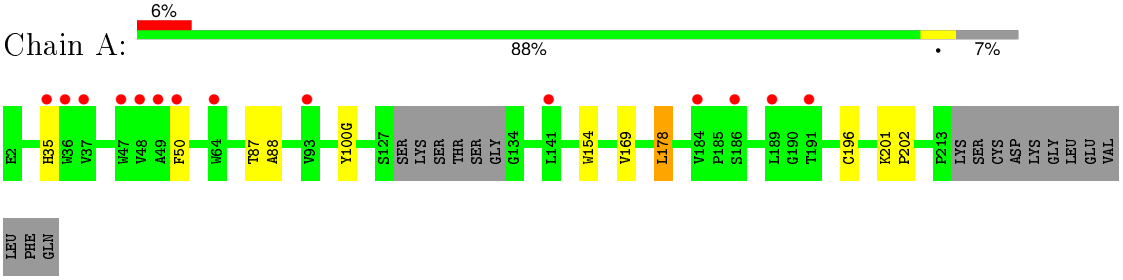
- Molecule 2: PG9 Heavy Chain

Chain H:



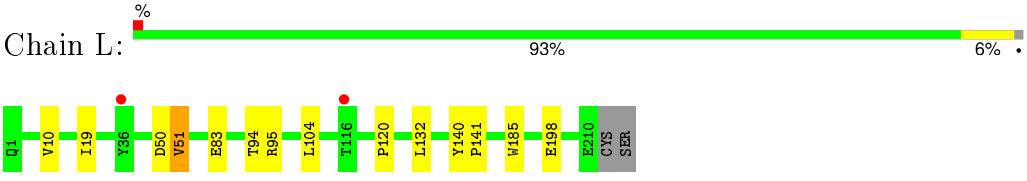
- Molecule 2: PG9 Heavy Chain

Chain A:



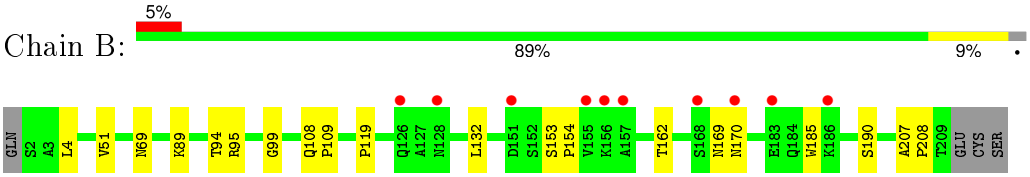
- Molecule 3: PG9 Light Chain

Chain L:



• Molecule 3: PG9 Light Chain

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.03Å 103.55Å 186.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.69 – 2.19 27.69 – 2.18	Depositor EDS
% Data completeness (in resolution range)	91.5 (27.69-2.19) 91.1 (27.69-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.182 , 0.234 0.185 , 0.235	Depositor DCC
R_{free} test set	3454 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	34.9	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 67685 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17692	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.92% 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, 0.375 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: BMA, NAG, TYS, SO4, PCA, MAN

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	G	0.28	0/853	0.50	0/1157
1	J	0.26	0/865	0.48	0/1174
2	A	0.27	0/1798	0.48	0/2446
2	H	0.30	0/1847	0.51	0/2512
3	B	0.29	0/1608	0.50	0/2190
3	L	0.30	0/1626	0.52	0/2214
All	All	0.29	0/8597	0.50	0/11693

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	J	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	136	ILE	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	G	842	805	819	10	0
1	J	853	806	823	8	0
2	A	1788	1688	1690	11	0
2	H	1839	1738	1739	16	0
3	B	1573	1541	1540	17	0
3	L	1591	1547	1557	9	0
4	G	83	71	70	1	0
4	J	83	71	70	3	0
5	G	72	61	61	9	0
6	B	20	0	0	1	0
6	G	5	0	0	0	0
6	L	35	0	0	0	0
7	J	28	26	24	5	0
8	A	22	18	19	5	0
9	A	109	0	0	0	0
9	B	79	0	0	1	0
9	G	21	0	0	1	0
9	H	123	0	0	0	0
9	J	19	0	0	3	0
9	L	135	0	0	1	0
All	All	9320	8372	8412	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 4.

The worst 5 of 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)
7:J:1657:NAG:O4	8:A:1658:BMA:C1	1.68	1.39
7:J:1657:NAG:O4	8:A:1658:BMA:C2	1.91	1.18
5:G:658:BMA:H62	5:G:660:MAN:H5	1.42	1.00
7:J:1657:NAG:C4	8:A:1658:BMA:C1	2.44	0.94
7:J:1657:NAG:O4	8:A:1658:BMA:H2	1.71	0.91

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	G	104/124 (84%)	99 (95%)	5 (5%)	0	100	100
1	J	105/124 (85%)	103 (98%)	2 (2%)	0	100	100
2	A	225/248 (91%)	220 (98%)	5 (2%)	0	100	100
2	H	235/248 (95%)	229 (97%)	6 (3%)	0	100	100
3	B	210/216 (97%)	203 (97%)	6 (3%)	1 (0%)	34	33
3	L	212/216 (98%)	206 (97%)	5 (2%)	1 (0%)	34	33
All	All	1091/1176 (93%)	1060 (97%)	29 (3%)	2 (0%)	52	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	51	VAL
3	B	51	VAL

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	G	92/107 (86%)	90 (98%)	2 (2%)	60	70
1	J	93/107 (87%)	92 (99%)	1 (1%)	80	88
2	A	192/207 (93%)	191 (100%)	1 (0%)	92	96
2	H	199/207 (96%)	197 (99%)	2 (1%)	82	90
3	B	179/183 (98%)	179 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	L	181/183 (99%)	181 (100%)	0	100 100
All	All	936/994 (94%)	930 (99%)	6 (1%)	90 95

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	149	SER
2	A	178	LEU
2	H	143	LYS
1	G	151	THR
2	H	197	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TYS	A	100(G)	-	15,16,17	2.17	1 (6%)	16,22,24	1.11	2 (12%)
2	TYS	A	100(H)	2	15,16,17	2.15	2 (13%)	16,22,24	1.05	1 (6%)
2	PCA	A	2	2	7,8,9	1.83	2 (28%)	9,10,12	1.67	3 (33%)
2	TYS	H	100(G)	-	15,16,17	2.17	1 (6%)	16,22,24	1.27	2 (12%)
2	TYS	H	100(H)	2	15,16,17	2.13	2 (13%)	16,22,24	1.08	1 (6%)
2	PCA	H	2	2	7,8,9	1.82	2 (28%)	9,10,12	1.67	3 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TYS	A	100(G)	-	-	0/9/11/13	0/1/1/1
2	TYS	A	100(H)	2	-	0/9/11/13	0/1/1/1
2	PCA	A	2	2	-	0/0/11/13	0/1/1/1
2	TYS	H	100(G)	-	-	0/9/11/13	0/1/1/1
2	TYS	H	100(H)	2	-	0/9/11/13	0/1/1/1
2	PCA	H	2	2	-	0/0/11/13	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	100(G)	TYS	OH-S	-8.00	1.48	1.63
2	H	100(G)	TYS	OH-S	-8.00	1.48	1.63
2	A	100(H)	TYS	OH-S	-7.79	1.49	1.63
2	H	100(H)	TYS	OH-S	-7.74	1.49	1.63
2	A	100(H)	TYS	OH-CZ	-2.05	1.39	1.42

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	100(H)	TYS	O2-S-O1	-2.80	100.26	112.46
2	A	2	PCA	CA-N-CD	-2.76	104.55	113.81
2	H	2	PCA	CA-N-CD	-2.76	104.55	113.81
2	A	100(G)	TYS	O2-S-O1	-2.67	100.84	112.46
2	H	100(G)	TYS	O2-S-O1	-2.58	101.24	112.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	100(G)	TYS	1	0
2	H	100(G)	TYS	1	0

5.5 Carbohydrates (i)

24 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	BMA	A	1658	8	11,11,12	0.72	0	14,15,17	1.11	0
8	MAN	A	1659	8	11,11,12	0.67	0	14,15,17	1.13	0
4	NAG	G	560	1,4	14,14,15	1.69	5 (35%)	15,19,21	1.60	4 (26%)
4	NAG	G	561	4	14,14,15	1.67	4 (28%)	15,19,21	1.41	2 (13%)
4	BMA	G	562	4	11,11,12	2.15	4 (36%)	14,15,17	1.51	3 (21%)
4	MAN	G	563	4	11,11,12	2.13	4 (36%)	14,15,17	1.40	2 (14%)
4	MAN	G	564	4	11,11,12	2.20	4 (36%)	14,15,17	1.17	1 (7%)
4	MAN	G	565	4	11,11,12	2.32	4 (36%)	14,15,17	1.16	0
4	MAN	G	566	4	11,11,12	2.03	3 (27%)	14,15,17	1.27	3 (21%)
5	NAG	G	656	1,5	14,14,15	1.74	5 (35%)	15,19,21	1.43	3 (20%)
5	NAG	G	657	5	14,14,15	1.76	4 (28%)	15,19,21	1.65	4 (26%)
5	BMA	G	658	5	11,11,12	0.72	0	14,15,17	1.11	0
5	MAN	G	659	5	11,11,12	0.66	0	14,15,17	1.14	0
5	MAN	G	660	5	11,11,12	0.52	0	14,15,17	0.79	0
5	MAN	G	662	5	11,11,12	0.81	0	14,15,17	1.13	1 (7%)
4	NAG	J	1560	1,4	14,14,15	1.70	4 (28%)	15,19,21	1.55	3 (20%)
4	NAG	J	1561	4	14,14,15	1.78	5 (35%)	15,19,21	1.73	4 (26%)
4	BMA	J	1562	4	11,11,12	2.14	4 (36%)	14,15,17	1.52	3 (21%)
4	MAN	J	1563	4	11,11,12	2.13	4 (36%)	14,15,17	2.22	5 (35%)
4	MAN	J	1564	4	11,11,12	1.98	4 (36%)	14,15,17	1.19	1 (7%)
4	MAN	J	1565	4	11,11,12	2.13	4 (36%)	14,15,17	1.19	1 (7%)
4	MAN	J	1566	4	11,11,12	2.05	3 (27%)	14,15,17	1.31	1 (7%)
7	NAG	J	1656	1,7	14,14,15	1.78	4 (28%)	15,19,21	1.54	3 (20%)
7	NAG	J	1657	7	14,14,15	1.88	5 (35%)	15,19,21	1.67	2 (13%)

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
8	BMA	A	1658	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1659	8	-	0/2/19/22	0/1/1/1
4	NAG	G	560	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	561	4	-	0/6/23/26	0/1/1/1
4	BMA	G	562	4	-	0/2/19/22	0/1/1/1
4	MAN	G	563	4	-	0/2/19/22	0/1/1/1
4	MAN	G	564	4	-	0/2/19/22	0/1/1/1
4	MAN	G	565	4	-	0/2/19/22	0/1/1/1
4	MAN	G	566	4	-	0/2/19/22	0/1/1/1
5	NAG	G	656	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	657	5	-	0/6/23/26	0/1/1/1
5	BMA	G	658	5	-	0/2/19/22	0/1/1/1
5	MAN	G	659	5	-	0/2/19/22	0/1/1/1
5	MAN	G	660	5	-	0/2/19/22	0/1/1/1
5	MAN	G	662	5	-	0/2/19/22	0/1/1/1
4	NAG	J	1560	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	1561	4	-	0/6/23/26	0/1/1/1
4	BMA	J	1562	4	-	0/2/19/22	0/1/1/1
4	MAN	J	1563	4	-	0/2/19/22	0/1/1/1
4	MAN	J	1564	4	-	0/2/19/22	0/1/1/1
4	MAN	J	1565	4	-	0/2/19/22	0/1/1/1
4	MAN	J	1566	4	-	0/2/19/22	0/1/1/1
7	NAG	J	1656	1,7	-	0/6/23/26	0/1/1/1
7	NAG	J	1657	7	-	0/6/23/26	0/1/1/1

The worst 5 of 74 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	565	MAN	C2-C3	-4.90	1.45	1.52
4	G	564	MAN	C2-C3	-4.35	1.46	1.52
4	J	1563	MAN	C2-C3	-4.29	1.46	1.52
4	J	1565	MAN	C2-C3	-4.16	1.46	1.52
4	G	563	MAN	C2-C3	-4.15	1.46	1.52

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	J	1656	NAG	C2-N2-C7	-2.93	119.27	123.04
5	G	662	MAN	C1-O5-C5	-2.74	108.77	112.25
4	J	1563	MAN	O4-C4-C5	-2.60	102.35	109.24
4	G	560	NAG	C3-C2-N2	-2.47	104.65	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	1566	MAN	C1-O5-C5	-2.46	109.12	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1658	BMA	5	0
4	G	560	NAG	1	0
5	G	657	NAG	1	0
5	G	658	BMA	5	0
5	G	659	MAN	3	0
5	G	660	MAN	4	0
4	J	1560	NAG	1	0
4	J	1564	MAN	2	0
4	J	1565	MAN	2	0
7	J	1657	NAG	5	0

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SO4	B	213	-	4,4,4	0.22	0	6,6,6	0.07	0
6	SO4	B	214	-	4,4,4	0.19	0	6,6,6	0.12	0
6	SO4	B	215	-	4,4,4	0.20	0	6,6,6	0.10	0
6	SO4	B	216	-	4,4,4	0.20	0	6,6,6	0.14	0
6	SO4	G	15	-	4,4,4	0.18	0	6,6,6	0.07	0
6	SO4	L	12	-	4,4,4	0.19	0	6,6,6	0.11	0
6	SO4	L	213	-	4,4,4	0.19	0	6,6,6	0.08	0
6	SO4	L	214	-	4,4,4	0.15	0	6,6,6	0.11	0
6	SO4	L	215	-	4,4,4	0.24	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SO4	L	216	-	4,4,4	0.22	0	6,6,6	0.15	0
6	SO4	L	217	-	4,4,4	0.15	0	6,6,6	0.11	0
6	SO4	L	218	-	4,4,4	0.20	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
6	SO4	B	213	-	-	0/0/0/0	0/0/0/0
6	SO4	B	214	-	-	0/0/0/0	0/0/0/0
6	SO4	B	215	-	-	0/0/0/0	0/0/0/0
6	SO4	B	216	-	-	0/0/0/0	0/0/0/0
6	SO4	G	15	-	-	0/0/0/0	0/0/0/0
6	SO4	L	12	-	-	0/0/0/0	0/0/0/0
6	SO4	L	213	-	-	0/0/0/0	0/0/0/0
6	SO4	L	214	-	-	0/0/0/0	0/0/0/0
6	SO4	L	215	-	-	0/0/0/0	0/0/0/0
6	SO4	L	216	-	-	0/0/0/0	0/0/0/0
6	SO4	L	217	-	-	0/0/0/0	0/0/0/0
6	SO4	L	218	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	213	SO4	1	0

5.7 Other polymers (i)

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	G	108/124 (87%)	0.43	11 (10%) 9 10	29, 46, 96, 124	0
1	J	109/124 (87%)	0.59	14 (12%) 5 5	31, 58, 103, 116	0
2	A	227/248 (91%)	0.16	14 (6%) 24 26	21, 42, 82, 112	0
2	H	236/248 (95%)	0.01	4 (1%) 73 74	21, 33, 68, 106	0
3	B	212/216 (98%)	0.15	10 (4%) 35 37	24, 44, 80, 102	0
3	L	214/216 (99%)	-0.08	2 (0%) 85 86	19, 33, 55, 109	0
All	All	1106/1176 (94%)	0.15	55 (4%) 32 35	19, 40, 82, 124	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	191	THR	5.4
2	A	189	LEU	4.8
1	J	136	ILE	4.8
1	J	150	LEU	4.8
1	G	137	ASN	4.7

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

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
2	TYS	A	100(G)	16/17	0.95	0.10	-	28,38,92,103	0
2	PCA	A	2	8/9	0.98	0.11	-	31,45,55,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	TYS	H	100(H)	16/17	0.94	0.14	-	25,35,102,112	0
2	TYS	H	100(G)	16/17	0.92	0.14	-	27,35,105,119	0
2	TYS	A	100(H)	16/17	0.93	0.11	-	21,33,94,107	0
2	PCA	H	2	8/9	0.97	0.09	-	27,35,48,61	0

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
5	MAN	G	659	11/12	0.70	0.34	7.96	111,144,176,190	0
7	NAG	J	1657	14/15	0.94	0.13	0.79	48,63,77,82	0
5	NAG	G	657	14/15	0.93	0.12	0.29	49,68,88,100	0
4	MAN	G	566	11/12	0.96	0.14	-0.45	23,37,50,50	0
7	NAG	J	1656	14/15	0.94	0.09	-0.60	38,47,62,66	0
4	NAG	J	1560	14/15	0.96	0.09	-0.83	27,41,55,58	0
5	NAG	G	656	14/15	0.95	0.08	-0.95	32,51,61,69	0
4	NAG	G	560	14/15	0.97	0.10	-0.95	27,40,50,58	0
4	MAN	G	565	11/12	0.96	0.09	-1.17	27,37,49,53	0
4	MAN	J	1566	11/12	0.97	0.10	-1.30	24,38,58,58	0
4	MAN	J	1565	11/12	0.96	0.10	-1.33	32,42,52,60	0
4	MAN	G	564	11/12	0.98	0.09	-2.01	29,37,47,48	0
8	MAN	A	1659	11/12	0.74	0.28	-	118,143,167,174	0
4	NAG	G	561	14/15	0.95	0.12	-	33,47,84,101	0
4	MAN	J	1563	11/12	0.89	0.32	-	108,114,138,138	0
4	NAG	J	1561	14/15	0.96	0.10	-	22,46,74,85	0
5	MAN	G	660	11/12	0.60	0.43	-	130,148,176,178	0
8	BMA	A	1658	11/12	0.84	0.14	-	136,144,171,173	0
4	MAN	G	563	11/12	0.80	0.36	-	93,110,131,132	0
5	MAN	G	662	11/12	0.54	0.38	-	112,142,167,171	0
5	BMA	G	658	11/12	0.83	0.14	-	116,141,169,171	0
4	BMA	J	1562	11/12	0.95	0.12	-	45,61,91,96	0
4	MAN	J	1564	11/12	0.94	0.07	-	32,39,46,54	0
4	BMA	G	562	11/12	0.89	0.13	-	41,67,96,100	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
6	SO4	G	15	5/5	0.85	0.24	6.17	116,116,122,132	0
6	SO4	B	216	5/5	0.83	0.21	4.56	107,121,125,126	0
6	SO4	L	218	5/5	0.85	0.23	4.50	115,120,123,129	0
6	SO4	L	214	5/5	0.95	0.12	1.05	44,52,82,91	0
6	SO4	B	214	5/5	0.91	0.15	1.02	85,93,99,103	0
6	SO4	L	217	5/5	0.98	0.10	0.31	40,50,55,65	0
6	SO4	B	213	5/5	0.95	0.12	-0.34	70,83,90,92	0
6	SO4	L	215	5/5	0.96	0.12	-0.76	68,72,79,83	0
6	SO4	L	216	5/5	0.99	0.08	-1.01	35,38,45,53	0
6	SO4	L	12	5/5	0.93	0.18	-	85,89,96,100	0
6	SO4	B	215	5/5	0.94	0.19	-	94,98,103,108	0
6	SO4	L	213	5/5	0.94	0.11	-	80,89,94,99	0

6.5 Other polymers (i)

There are no such residues in this entry.