Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 06:03 AM EDT

PDB ID	:	3IDX
Title	:	Crystal structure of HIV-gp120 core in complex with CD4-binding site antibody b13, space group C222
Authors	:	Chen, L.; Kwon, Y.D.; Zhou, T.; Wu, X.; O'Dell, S.; Cavacini, L.; Hessell, A.J.; Pancera, M.; Tang, M.; Xu, L.; Yang, Z.Y.; Zhang, M.Y.; Arthos, J.; Burton, D.R.; Dimitrov, D.S.; Nabel, G.J.; Posner, M.; Sodroski, J.; Wyatt, R.; Mascola, J.R.; Kwong, P.D.
Deposited on	:	2009-07-22
Resolution	:	2.50 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:

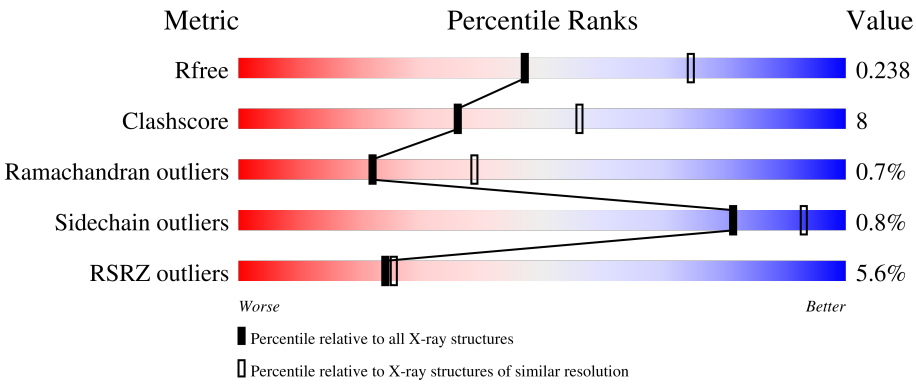
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	G	317	6% 79% 17%
2	H	231	7% 77% 22%
3	L	215	3% 87% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Validation Pipeline (wwPDB-VP) : 2.35

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	NAG	G	897	-	-	-	X
4	NAG	G	963	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6262 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 HIV-1 HxBc2 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	306	2367	1483	412	448	24	0	0	0

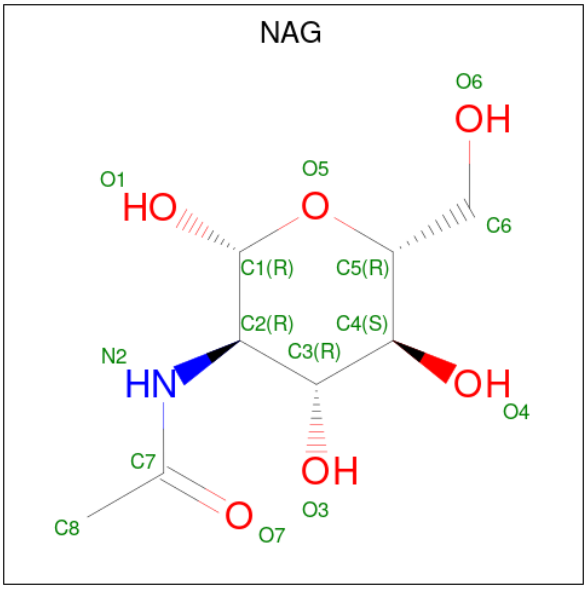
- Molecule 2 is a protein called Fab b13 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	229	1730	1092	297	334	7	0	0	0

- Molecule 3 is a protein called Fab b13 light chain.

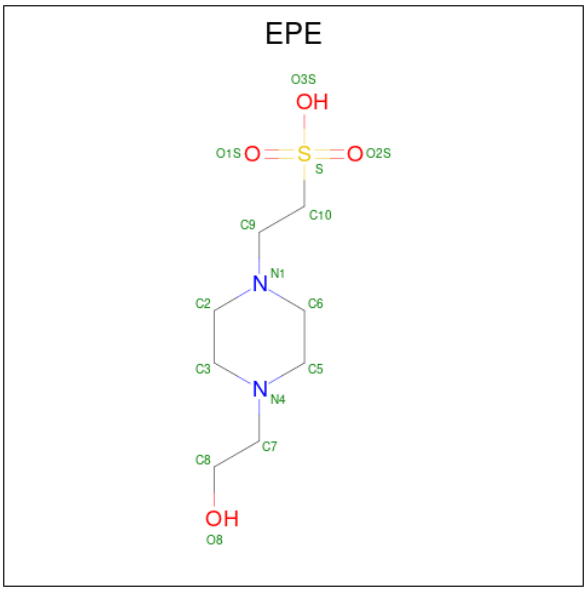
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	214	1654	1028	284	337	5	0	0	0

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



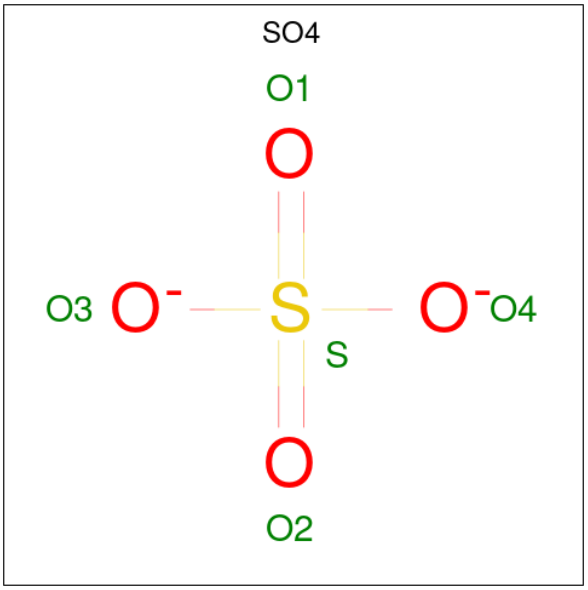
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	G	1	14	8	1	5	0	0
4	G	1	14	8	1	5	0	0
4	G	1	14	8	1	5	0	0
4	G	1	14	8	1	5	0	0
4	G	1	14	8	1	5	0	0
4	G	1	14	8	1	5	0	0
4	G	1	14	8	1	5	0	0
4	G	1	14	8	1	5	0	0
4	G	1	14	8	1	5	0	0
4	G	1	14	8	1	5	0	0
4	G	1	14	8	1	5	0	0
4	G	1	14	8	1	5	0	0
4	G	1	14	8	1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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	G	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
5	H	1	15	8	2	4	1	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	3	2	1			0	0
			Total	O	S				
6	G	1	5	4	1			0	0

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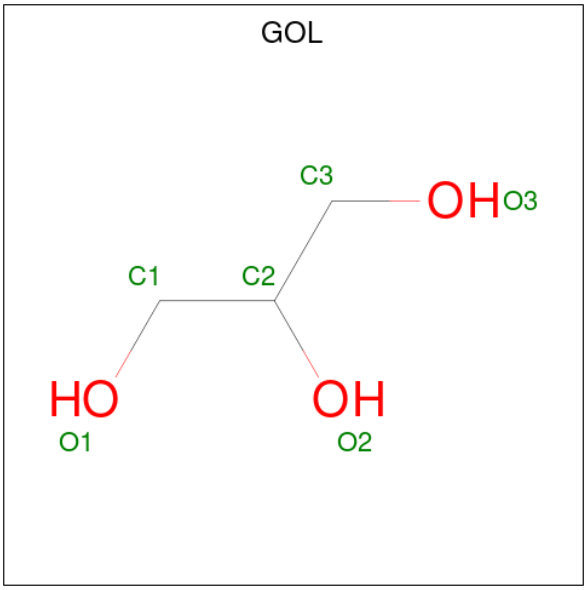
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	G	1	5	4	1	0	0
			Total	O	S		
6	G	1	5	4	1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	G	1	6	3	3	0	0

- Molecule 8 is water.

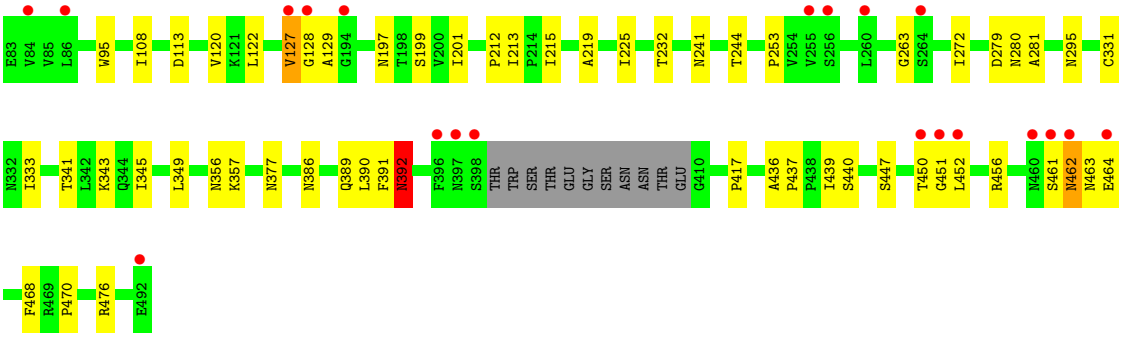
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	G	110	110	110	0	0
			Total	O		
8	H	50	50	50	0	0
			Total	O		
8	L	73	73	73	0	0

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.

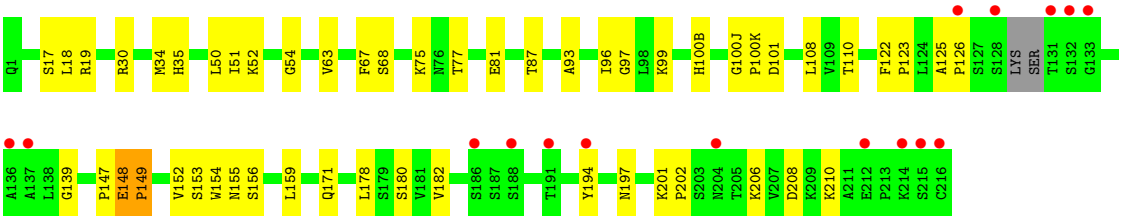
- Molecule 1: HIV-1 HxBc2 gp120 core

Chain G:



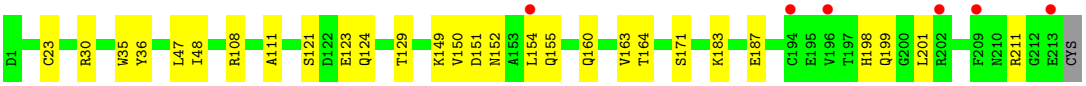
- Molecule 2: Fab b13 heavy chain

Chain H:



- Molecule 3: Fab b13 light chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	112.61Å 203.96Å 109.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.22 – 2.50 39.21 – 2.19	Depositor EDS
% Data completeness (in resolution range)	79.0 (39.22-2.50) 56.3 (39.21-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.18Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.178 , 0.239 0.179 , 0.238	Depositor DCC
R_{free} test set	1870 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	63.1	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 80.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6262	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: EPE, GOL, NAG, 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	G	0.29	0/2415	0.47	0/3274
2	H	0.26	0/1771	0.50	1/2407 (0.0%)
3	L	0.28	0/1688	0.46	0/2291
All	All	0.28	0/5874	0.48	1/7972 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	148	GLU	C-N-CD	-9.56	99.56	120.60

There are no chirality outliers.

There are no planarity outliers.

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	G	2367	0	2296	39	0
2	H	1730	0	1696	37	0
3	L	1654	0	1602	23	0
4	G	224	0	208	5	0
5	G	15	0	17	0	0
5	H	15	0	17	1	0
6	G	18	0	0	1	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	6	0	8	0	0
8	G	110	0	0	4	0
8	H	50	0	0	6	0
8	L	73	0	0	2	0
All	All	6262	0	5844	95	1

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 (95) 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:G:439:ILE:HG22	1:G:440:SER:H	1.31	0.93
3:L:108:ARG:HH12	3:L:111:ALA:HB2	1.46	0.81
1:G:127:VAL:HG12	1:G:128:GLY:H	1.46	0.79
1:G:439:ILE:HG22	1:G:440:SER:N	2.02	0.73
1:G:391:PHE:CD1	1:G:470:PRO:HG3	2.24	0.72
2:H:52:LYS:HE2	8:H:1134:HOH:O	1.92	0.69
2:H:68:SER:HB3	2:H:81:GLU:HG2	1.75	0.68
2:H:153:SER:OG	2:H:197:ASN:HB2	1.94	0.67
3:L:183:LYS:O	3:L:187:GLU:HG2	1.94	0.67
2:H:96:ILE:HG13	2:H:100(J):GLY:O	1.96	0.66
2:H:139:GLY:HA2	2:H:154:TRP:CH2	2.32	0.64
2:H:139:GLY:HA2	2:H:154:TRP:HH2	1.62	0.64
3:L:198:HIS:CG	3:L:199:GLN:H	2.15	0.64
1:G:377:ASN:HB2	8:G:1078:HOH:O	1.98	0.64
1:G:113:ASP:HB2	1:G:213:ILE:HD11	1.78	0.63
2:H:18:LEU:HD23	2:H:19:ARG:N	2.17	0.59
2:H:96:ILE:HG12	2:H:101:ASP:HB3	1.84	0.59
1:G:439:ILE:CG2	1:G:440:SER:H	2.12	0.58
1:G:356:ASN:OD1	4:G:856:NAG:H2	2.06	0.56
3:L:149:LYS:HG2	3:L:154:LEU:HD23	1.87	0.56
1:G:386:ASN:HB3	1:G:417:PRO:HD2	1.86	0.56
3:L:23:CYS:HB2	3:L:35:TRP:CH2	2.41	0.55
1:G:127:VAL:HG12	1:G:128:GLY:N	2.20	0.55
1:G:122:LEU:HD21	1:G:199:SER:HB3	1.88	0.54
1:G:389:GLN:HG2	4:G:892:NAG:H81	1.89	0.54
3:L:108:ARG:HD2	3:L:171:SER:HB2	1.89	0.54
2:H:108:LEU:HD23	2:H:149:PRO:HD3	1.90	0.53
1:G:343:LYS:HD3	4:G:839:NAG:H81	1.90	0.52
1:G:219:ALA:HB2	1:G:225:ILE:HG13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:156:SER:HA	2:H:197:ASN:ND2	2.25	0.52
3:L:187:GLU:HA	3:L:211:ARG:NH2	2.24	0.52
3:L:198:HIS:CG	3:L:199:GLN:N	2.78	0.52
2:H:178:LEU:C	2:H:178:LEU:HD12	2.30	0.51
2:H:97:GLY:HA3	8:H:1152:HOH:O	2.10	0.51
1:G:341:THR:O	1:G:345:ILE:HG13	2.10	0.51
1:G:462:ASN:C	1:G:464:GLU:H	2.12	0.51
3:L:30:ARG:HB3	3:L:30:ARG:NH2	2.26	0.51
1:G:253:PRO:HA	6:G:1003:SO4:O2	2.11	0.51
2:H:108:LEU:CD2	2:H:149:PRO:HD3	2.42	0.50
3:L:123:GLU:HB2	8:L:1164:HOH:O	2.11	0.50
2:H:100(K):PRO:HD2	3:L:36:TYR:OH	2.13	0.49
2:H:63:VAL:HB	2:H:67:PHE:CG	2.48	0.48
3:L:47:LEU:C	3:L:48:ILE:HD12	2.34	0.48
2:H:87:THR:HG23	2:H:110:THR:HA	1.96	0.48
1:G:120:VAL:HB	1:G:201:ILE:HD11	1.95	0.48
1:G:241:ASN:HA	8:G:1007:HOH:O	2.13	0.48
2:H:17:SER:HB3	8:H:1188:HOH:O	2.13	0.47
3:L:30:ARG:HB3	3:L:30:ARG:HH21	1.78	0.47
1:G:197:ASN:HB2	4:G:697:NAG:H82	1.97	0.46
3:L:151:ASP:O	3:L:152:ASN:HB2	2.16	0.46
1:G:128:GLY:HA2	1:G:129:ALA:HA	1.55	0.46
2:H:206:LYS:HE2	8:H:1171:HOH:O	2.16	0.45
3:L:150:VAL:HG22	3:L:155:GLN:NE2	2.32	0.45
1:G:476:ARG:NH2	5:H:1001:EPE:H51	2.32	0.45
2:H:201:LYS:N	2:H:202:PRO:CD	2.80	0.45
1:G:295:ASN:O	1:G:331:CYS:HA	2.17	0.45
3:L:124:GLN:HG2	3:L:129:THR:O	2.16	0.45
1:G:108:ILE:HD12	1:G:215:ILE:HG21	1.98	0.45
1:G:392:ASN:O	1:G:392:ASN:CG	2.55	0.45
2:H:51:ILE:HD11	2:H:54:GLY:HA2	1.99	0.44
2:H:93:ALA:HB1	2:H:100(K):PRO:HB3	1.98	0.44
2:H:125:ALA:HA	2:H:126:PRO:HD3	1.77	0.44
2:H:152:VAL:HG11	2:H:180:SER:CB	2.47	0.44
1:G:333:ILE:HD12	1:G:390:LEU:HD21	1.99	0.44
3:L:201:LEU:HB2	8:L:1225:HOH:O	2.16	0.44
1:G:447:SER:HB3	4:G:762:NAG:HN2	1.82	0.44
2:H:159:LEU:HD21	2:H:182:VAL:HG21	1.99	0.44
2:H:75:LYS:O	2:H:77:THR:HG23	2.17	0.44
1:G:212:PRO:HB3	8:G:1181:HOH:O	2.16	0.44
1:G:456:ARG:HB2	1:G:468:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:461:SER:C	1:G:463:ASN:H	2.21	0.43
1:G:232:THR:HG22	1:G:232:THR:O	2.18	0.43
3:L:183:LYS:HE2	3:L:187:GLU:OE2	2.18	0.43
1:G:272:ILE:CD1	1:G:349:LEU:HD23	2.49	0.42
2:H:99:LYS:HB2	2:H:100(B):HIS:CE1	2.54	0.42
2:H:35:HIS:CE1	2:H:50:LEU:HD13	2.54	0.42
2:H:122:PHE:HA	2:H:123:PRO:HD3	1.85	0.42
1:G:462:ASN:C	1:G:464:GLU:N	2.73	0.42
1:G:263:GLY:O	1:G:450:THR:HG21	2.20	0.42
2:H:155:ASN:OD1	2:H:194:TYR:HA	2.20	0.42
8:G:1039:HOH:O	2:H:52:LYS:HE3	2.20	0.41
2:H:30:ARG:HD2	8:H:1135:HOH:O	2.20	0.41
1:G:451:GLY:C	1:G:452:LEU:HD12	2.40	0.41
1:G:279:ASP:C	1:G:281:ALA:H	2.24	0.41
2:H:123:PRO:HD2	3:L:121:SER:CB	2.51	0.41
2:H:210:LYS:HG3	8:H:1196:HOH:O	2.19	0.41
3:L:108:ARG:NH1	3:L:111:ALA:HB2	2.25	0.41
1:G:357:LYS:HE2	1:G:464:GLU:HA	2.02	0.41
1:G:122:LEU:CD2	1:G:199:SER:HB3	2.51	0.41
2:H:34:MET:O	2:H:50:LEU:HD12	2.21	0.41
3:L:163:VAL:HG12	3:L:164:THR:O	2.20	0.40
2:H:122:PHE:HB3	3:L:121:SER:OG	2.20	0.40
1:G:436:ALA:HA	1:G:437:PRO:HD3	1.86	0.40
2:H:108:LEU:HD23	2:H:148:GLU:O	2.22	0.40
2:H:171:GLN:HA	3:L:160:GLN:HE22	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:1002:SO4:O1	6:G:1002:SO4:O1[4_557]	2.02	0.18

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	302/317 (95%)	270 (89%)	28 (9%)	4 (1%)	12	21
2	H	225/231 (97%)	209 (93%)	15 (7%)	1 (0%)	34	54
3	L	212/215 (99%)	199 (94%)	13 (6%)	0	100	100
All	All	739/763 (97%)	678 (92%)	56 (8%)	5 (1%)	22	39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	127	VAL
1	G	462	ASN
2	H	149	PRO
1	G	280	ASN
1	G	392	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	G	271/281 (96%)	268 (99%)	3 (1%)	73	89
2	H	189/191 (99%)	187 (99%)	2 (1%)	73	89
3	L	189/190 (100%)	189 (100%)	0	100	100
All	All	649/662 (98%)	644 (99%)	5 (1%)	81	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	95	TRP
1	G	244	THR
1	G	392	ASN
2	H	147	PRO
2	H	208	ASP

Sometimes 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)

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)

23 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	$\#\|Z\| > 2$
5	EPE	H	1001	-	15,15,15	0.86	1 (6%)	18,20,20	1.80	6 (33%)
4	NAG	G	741	1	14,14,15	0.53	0	17,19,21	0.84	1 (5%)
4	NAG	G	776	1	14,14,15	0.54	0	17,19,21	0.87	0
6	SO4	G	1002	6	2,2,4	0.95	0	1,1,6	0.92	0
6	SO4	G	1005	-	4,4,4	0.12	0	6,6,6	0.10	0
4	NAG	G	697	1	14,14,15	0.53	0	17,19,21	0.80	1 (5%)
4	NAG	G	856	1	14,14,15	0.56	0	17,19,21	1.22	3 (17%)
4	NAG	G	839	1	14,14,15	0.55	0	17,19,21	1.13	2 (11%)
4	NAG	G	734	1	14,14,15	0.57	0	17,19,21	0.99	1 (5%)
6	SO4	G	1004	-	4,4,4	0.14	0	6,6,6	0.06	0
4	NAG	G	789	1	14,14,15	0.56	0	17,19,21	0.93	1 (5%)
5	EPE	G	1000	-	15,15,15	0.87	1 (6%)	18,20,20	1.65	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	G	588	1	14,14,15	0.46	0	17,19,21	0.88	0
6	SO4	G	1003	-	4,4,4	0.13	0	6,6,6	0.10	0
4	NAG	G	886	1	14,14,15	0.63	0	17,19,21	0.96	0
4	NAG	G	897	1	14,14,15	0.43	0	17,19,21	0.95	1 (5%)
4	NAG	G	730	1	14,14,15	0.43	0	17,19,21	0.87	1 (5%)
4	NAG	G	892	1	14,14,15	0.55	0	17,19,21	0.66	0
4	NAG	G	948	1	14,14,15	0.56	0	17,19,21	0.99	1 (5%)
7	GOL	G	1006	-	5,5,5	0.34	0	5,5,5	0.34	0
4	NAG	G	762	1	14,14,15	0.62	0	17,19,21	1.65	4 (23%)
4	NAG	G	963	1	14,14,15	0.46	0	17,19,21	0.94	2 (11%)
4	NAG	G	795	1	14,14,15	0.45	0	17,19,21	0.92	1 (5%)

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
5	EPE	H	1001	-	-	7/9/19/19	0/1/1/1
4	NAG	G	741	1	-	5/6/23/26	0/1/1/1
4	NAG	G	776	1	-	0/6/23/26	0/1/1/1
4	NAG	G	697	1	-	4/6/23/26	0/1/1/1
4	NAG	G	856	1	-	2/6/23/26	0/1/1/1
4	NAG	G	839	1	-	2/6/23/26	0/1/1/1
4	NAG	G	734	1	-	2/6/23/26	0/1/1/1
4	NAG	G	789	1	-	0/6/23/26	0/1/1/1
5	EPE	G	1000	-	-	5/9/19/19	0/1/1/1
4	NAG	G	588	1	-	3/6/23/26	0/1/1/1
4	NAG	G	886	1	-	0/6/23/26	0/1/1/1
4	NAG	G	897	1	-	3/6/23/26	0/1/1/1
4	NAG	G	730	1	-	2/6/23/26	0/1/1/1
4	NAG	G	892	1	-	2/6/23/26	0/1/1/1
4	NAG	G	948	1	-	2/6/23/26	0/1/1/1
7	GOL	G	1006	-	-	2/4/4/4	-
4	NAG	G	762	1	-	2/6/23/26	0/1/1/1
4	NAG	G	963	1	-	2/6/23/26	0/1/1/1
4	NAG	G	795	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1001	EPE	C10-S	2.95	1.81	1.77
5	G	1000	EPE	C10-S	2.88	1.81	1.77

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	762	NAG	C1-O5-C5	4.78	118.67	112.19
5	H	1001	EPE	C5-N4-C3	4.46	118.88	108.83
5	G	1000	EPE	C5-N4-C3	3.26	116.17	108.83
4	G	839	NAG	O5-C1-C2	3.02	116.05	111.29
4	G	897	NAG	C1-O5-C5	2.97	116.22	112.19
4	G	856	NAG	C1-O5-C5	2.95	116.19	112.19
5	H	1001	EPE	C7-N4-C5	2.88	118.61	111.23
4	G	789	NAG	C1-O5-C5	2.88	116.09	112.19
4	G	856	NAG	O5-C1-C2	2.84	115.77	111.29
5	G	1000	EPE	C7-N4-C5	2.70	118.14	111.23
5	G	1000	EPE	C7-N4-C3	2.67	118.07	111.23
4	G	839	NAG	C1-O5-C5	2.64	115.77	112.19
5	H	1001	EPE	C7-N4-C3	2.62	117.93	111.23
4	G	697	NAG	C1-O5-C5	2.54	115.63	112.19
4	G	948	NAG	C1-O5-C5	2.52	115.61	112.19
4	G	762	NAG	C6-C5-C4	-2.51	107.12	113.00
4	G	762	NAG	O5-C1-C2	2.47	115.19	111.29
5	G	1000	EPE	O1S-S-C10	2.46	109.88	106.92
5	H	1001	EPE	O2S-S-C10	2.46	109.88	106.92
4	G	963	NAG	C1-O5-C5	2.43	115.49	112.19
5	G	1000	EPE	O3S-S-C10	2.41	109.67	105.77
5	H	1001	EPE	O3S-S-C10	2.41	109.66	105.77
4	G	730	NAG	C1-O5-C5	2.33	115.34	112.19
4	G	762	NAG	C2-N2-C7	-2.30	119.62	122.90
4	G	734	NAG	O5-C1-C2	2.25	114.84	111.29
4	G	741	NAG	C1-O5-C5	2.23	115.21	112.19
4	G	795	NAG	C1-O5-C5	2.22	115.20	112.19
5	H	1001	EPE	O1S-S-C10	2.17	109.53	106.92
4	G	856	NAG	O5-C5-C6	2.12	110.53	107.20
4	G	963	NAG	O5-C5-C6	2.07	110.45	107.20

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	588	NAG	C3-C2-N2-C7
4	G	588	NAG	C8-C7-N2-C2
4	G	588	NAG	O7-C7-N2-C2
4	G	697	NAG	O7-C7-N2-C2
4	G	730	NAG	C8-C7-N2-C2
4	G	730	NAG	O7-C7-N2-C2
4	G	741	NAG	C3-C2-N2-C7
4	G	741	NAG	C8-C7-N2-C2
4	G	741	NAG	O7-C7-N2-C2
4	G	839	NAG	C8-C7-N2-C2
4	G	839	NAG	O7-C7-N2-C2
4	G	856	NAG	C8-C7-N2-C2
4	G	856	NAG	O7-C7-N2-C2
4	G	897	NAG	C8-C7-N2-C2
4	G	897	NAG	O7-C7-N2-C2
4	G	963	NAG	C8-C7-N2-C2
4	G	963	NAG	O7-C7-N2-C2
5	G	1000	EPE	C9-C10-S-O1S
5	G	1000	EPE	C9-C10-S-O3S
5	H	1001	EPE	C10-C9-N1-C2
5	H	1001	EPE	C8-C7-N4-C3
5	H	1001	EPE	C9-C10-S-O1S
5	H	1001	EPE	C9-C10-S-O3S
7	G	1006	GOL	O1-C1-C2-C3
4	G	697	NAG	C8-C7-N2-C2
4	G	795	NAG	C8-C7-N2-C2
4	G	795	NAG	O7-C7-N2-C2
4	G	734	NAG	C8-C7-N2-C2
4	G	734	NAG	O7-C7-N2-C2
4	G	762	NAG	O5-C5-C6-O6
4	G	762	NAG	C4-C5-C6-O6
4	G	892	NAG	C8-C7-N2-C2
4	G	892	NAG	O7-C7-N2-C2
4	G	948	NAG	C8-C7-N2-C2
4	G	741	NAG	O5-C5-C6-O6
4	G	948	NAG	O7-C7-N2-C2
4	G	897	NAG	O5-C5-C6-O6
7	G	1006	GOL	O1-C1-C2-O2
5	H	1001	EPE	C8-C7-N4-C5
5	G	1000	EPE	C10-C9-N1-C2
4	G	741	NAG	C4-C5-C6-O6
5	G	1000	EPE	C9-C10-S-O2S
5	H	1001	EPE	C9-C10-S-O2S

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Mol	Chain	Res	Type	Atoms
4	G	697	NAG	C4-C5-C6-O6
5	G	1000	EPE	C10-C9-N1-C6
4	G	697	NAG	O5-C5-C6-O6
5	H	1001	EPE	C10-C9-N1-C6

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1001	EPE	1	0
6	G	1002	SO4	0	1
4	G	697	NAG	1	0
4	G	856	NAG	1	0
4	G	839	NAG	1	0
6	G	1003	SO4	1	0
4	G	892	NAG	1	0
4	G	762	NAG	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	G	306/317 (96%)	0.16	20 (6%)	18	19	73, 96, 167, 225	0
2	H	229/231 (99%)	0.20	16 (6%)	16	16	78, 114, 179, 200	0
3	L	214/215 (99%)	-0.14	6 (2%)	53	56	78, 107, 152, 194	0
All	All	749/763 (98%)	0.09	42 (5%)	24	25	73, 104, 169, 225	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	131	THR	6.7
2	H	216	CYS	6.3
2	H	132	SER	4.8
1	G	460	ASN	4.4
2	H	212	GLU	4.3
3	L	202	ARG	4.3
1	G	398	SER	4.0
2	H	128	SER	3.9
2	H	215	SER	3.8
2	H	214	LYS	3.7
1	G	464	GLU	3.4
2	H	126	PRO	3.4
1	G	127	VAL	3.3
1	G	194	GLY	3.3
2	H	136	ALA	3.2
1	G	396	PHE	3.1
2	H	133	GLY	2.9
2	H	191	THR	2.9
3	L	154	LEU	2.9
2	H	137	ALA	2.8
1	G	492	GLU	2.8
3	L	209	PHE	2.8
1	G	260	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	L	194	CYS	2.6
2	H	188	SER	2.6
2	H	194	TYR	2.6
1	G	84	VAL	2.6
3	L	196	VAL	2.6
2	H	186	SER	2.5
1	G	451	GLY	2.3
1	G	256	SER	2.3
1	G	86	LEU	2.3
1	G	128	GLY	2.3
1	G	462	ASN	2.2
1	G	452	LEU	2.1
1	G	450	THR	2.1
1	G	264	SER	2.1
1	G	461	SER	2.1
2	H	204	ASN	2.1
1	G	255	VAL	2.0
1	G	397	ASN	2.0
3	L	213	GLU	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	G	963	14/15	0.55	0.81	205,210,215,217	0
4	NAG	G	697	14/15	0.71	0.28	154,168,169,170	0
4	NAG	G	730	14/15	0.73	0.26	140,160,166,167	0
6	SO4	G	1005	5/5	0.77	0.19	179,181,183,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	G	897	14/15	0.78	0.54	167,183,186,187	0
5	EPE	H	1001	15/15	0.81	0.21	139,149,230,231	0
6	SO4	G	1004	5/5	0.83	0.25	179,182,183,187	0
4	NAG	G	856	14/15	0.84	0.44	190,200,205,205	0
7	GOL	G	1006	6/6	0.86	0.33	112,115,125,127	0
6	SO4	G	1003	5/5	0.87	0.27	158,160,164,166	0
6	SO4	G	1002	3/5	0.89	0.07	125,125,131,131	1
4	NAG	G	741	14/15	0.90	0.28	132,147,156,161	0
4	NAG	G	839	14/15	0.91	0.31	141,152,158,163	0
5	EPE	G	1000	15/15	0.92	0.14	112,126,145,145	0
4	NAG	G	948	14/15	0.93	0.25	100,112,117,118	0
4	NAG	G	588	14/15	0.93	0.20	132,139,141,142	0
4	NAG	G	734	14/15	0.93	0.12	131,144,152,152	0
4	NAG	G	776	14/15	0.94	0.14	107,119,124,126	0
4	NAG	G	892	14/15	0.94	0.29	121,136,137,139	0
4	NAG	G	795	14/15	0.96	0.13	99,112,115,119	0
4	NAG	G	886	14/15	0.97	0.09	90,111,118,119	0
4	NAG	G	789	14/15	0.97	0.15	78,94,105,115	0
4	NAG	G	762	14/15	0.98	0.24	72,81,86,88	0

6.5 Other polymers (i)

There are no such residues in this entry.