



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 05:18 AM BST

PDB ID : 2NXY
Title : HIV-1 gp120 Envelope Glycoprotein(S334A) Complexed with CD4 and Anti-body 17b
Authors : Zhou, T.; Xu, L.; Dey, B.; Hessel, A.J.; Van Ryk, D.; Xiang, S.H.; Yang, X.; Zhang, M.Y.; Zwick, M.B.; Arthos, J.; Burton, D.R.; Dimitrov, D.S.; Sodroski, J.; Wyatt, R.; Nabel, G.J.; Kwong, P.D.
Deposited on : 2006-11-20
Resolution : 2.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

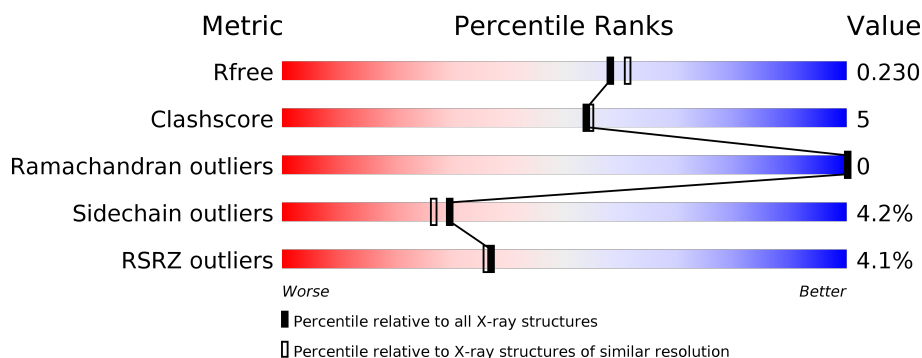
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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 $\leq 5\%$. 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	317	<div> <div>7%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div></div> </div> <div>.</div> </div>
2	B	184	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div></div> </div> <div>..</div> </div>
3	C	214	<div> <div></div> <div> <div></div> <div>88%</div> <div>10%</div> <div></div> </div> <div>.</div> </div>
4	D	229	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div></div> </div> <div>..</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	588	-	-	-	X
5	NAG	A	697	-	-	-	X
5	NAG	A	741	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8158 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 ENVELOPE GLYCOPROTEIN GP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	4	0
			2363	1479	415	449	20			

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	3	0
			1420	888	248	280	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1000	MET	-	initiating methionine	UNP P01730

- Molecule 3 is a protein called ANTIBODY 17B, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1646	1028	282	331	5			

- Molecule 4 is a protein called ANTIBODY 17B, HEAVY CHAIN.

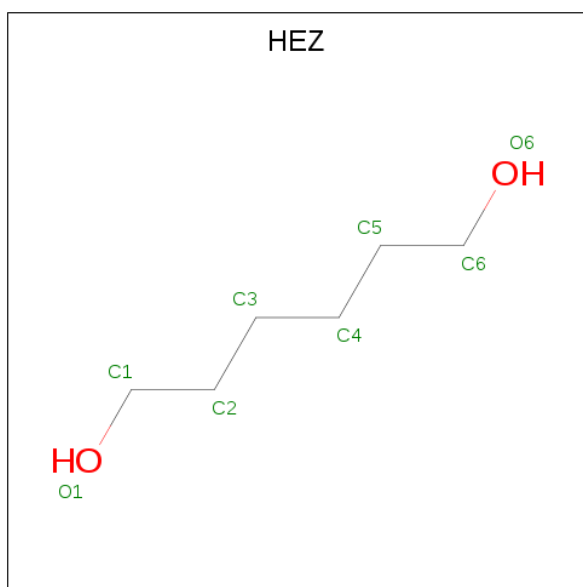
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	227	Total	C	N	O	S	0	1	0
			1709	1078	287	339	5			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		

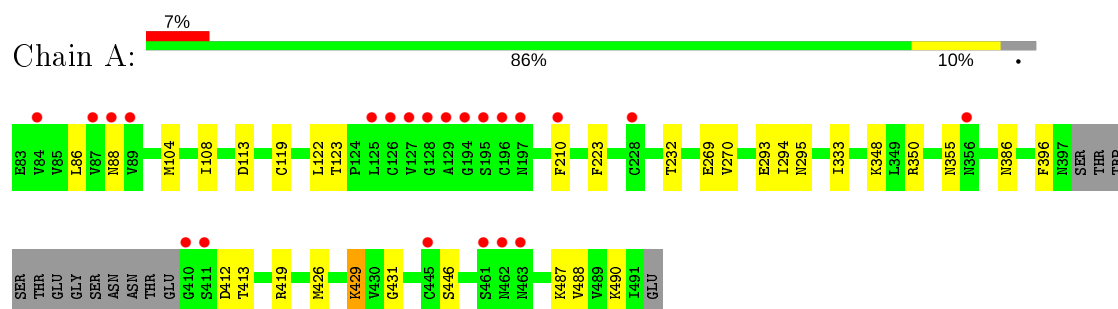
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	259	Total	O	0	0
			259	259		
8	B	137	Total	O	0	0
			137	137		
8	C	188	Total	O	0	0
			188	188		
8	D	222	Total	O	0	0
			222	222		

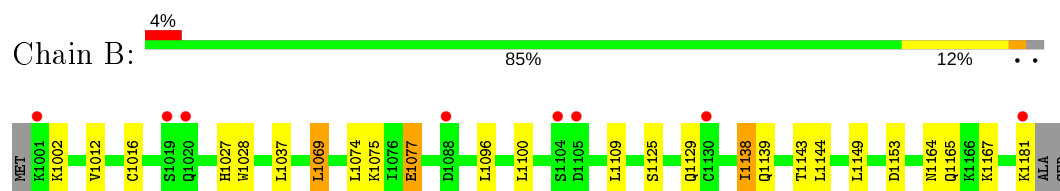
3 Residue-property plots [i](#)

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.

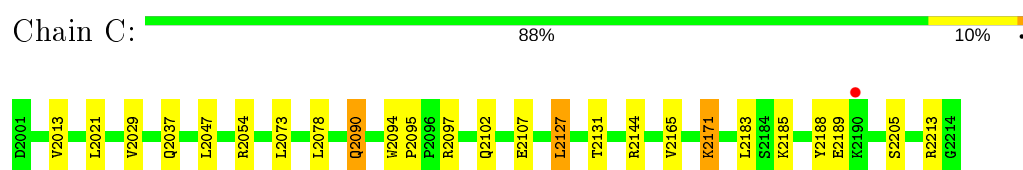
- Molecule 1: ENVELOPE GLYCOPROTEIN GP120



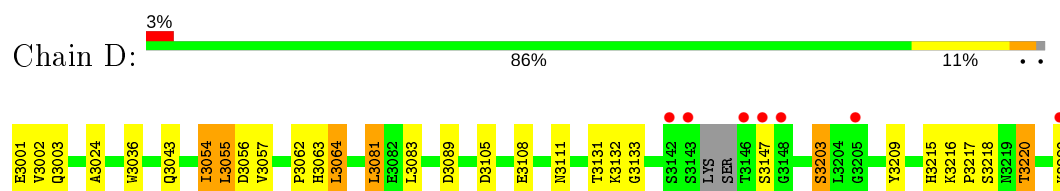
- Molecule 2: T-cell surface glycoprotein CD4



- Molecule 3: ANTIBODY 17B, LIGHT CHAIN



- Molecule 4: ANTIBODY 17B, HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	71.35Å 88.09Å 195.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.01 – 2.00 35.01 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.0 (35.01-2.00) 91.0 (35.01-2.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.181 , 0.231 0.195 , 0.230	Depositor DCC
R_{free} test set	3880 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8158	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: TRS, NAG, HEZ

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	0.30	0/2432	0.46	0/3297
2	B	0.28	0/1454	0.48	0/1960
3	C	0.29	0/1683	0.50	0/2288
4	D	0.31	0/1754	0.49	0/2389
All	All	0.29	0/7323	0.48	0/9934

There are no bond length outliers.

There are no bond angle outliers.

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	A	2363	0	2305	25	0
2	B	1420	0	1444	13	0
3	C	1646	0	1590	16	0
4	D	1709	0	1669	23	1
5	A	182	0	169	4	0
6	A	24	0	42	5	0
7	A	8	0	12	0	0
8	A	259	0	0	7	1
8	B	137	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	188	0	0	2	0
8	D	222	0	0	4	0
All	All	8158	0	7231	77	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 5.

All (77) 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)
4:D:3001:GLU:N	8:D:698:HOH:O	1.98	0.97
4:D:3218:SER:OG	4:D:3220:THR:HG22	1.71	0.90
2:B:1153:ASP:HA	8:B:397:HOH:O	1.74	0.85
4:D:3215:HIS:HB3	4:D:3220:THR:HG23	1.58	0.85
1:A:350:ARG:NH1	1:A:355:ASN:O	2.16	0.78
1:A:113:ASP:OD1	8:A:5234:HOH:O	2.01	0.77
2:B:1138:ILE:HD12	2:B:1144:LEU:HB3	1.71	0.72
4:D:3056:ASP:OD2	8:D:34:HOH:O	2.07	0.72
3:C:2144:ARG:NH2	3:C:2165:VAL:HG11	2.05	0.70
1:A:350:ARG:HD2	1:A:396:PHE:CD1	2.26	0.70
1:A:232:THR:HG22	1:A:232:THR:O	1.94	0.67
4:D:3218:SER:OG	4:D:3220:THR:CG2	2.43	0.67
2:B:1077:GLU:OE1	8:B:726:HOH:O	2.14	0.63
1:A:386:ASN:HB2	6:A:5000:HEZ:H52	1.80	0.62
4:D:3215:HIS:HB3	4:D:3220:THR:CG2	2.30	0.61
1:A:88:ASN:HB2	5:A:588:NAG:H83	1.82	0.60
4:D:3043[B]:GLN:NE2	8:D:785:HOH:O	2.36	0.58
3:C:2171:LYS:HA	3:C:2171:LYS:HE3	1.85	0.58
2:B:1125:SER:HB3	8:B:525:HOH:O	2.03	0.57
3:C:2013:VAL:CG1	3:C:2078:LEU:HD12	2.34	0.57
3:C:2188:TYR:CZ	3:C:2213:ARG:HG3	2.41	0.55
1:A:426:MET:HE2	1:A:431:GLY:HA3	1.89	0.55
8:A:5145:HOH:O	4:D:3108:GLU:HB2	2.08	0.54
2:B:1012:VAL:HB	2:B:1074:LEU:HD11	1.90	0.54
1:A:295:ASN:HD22	5:A:795:NAG:H83	1.74	0.53
3:C:2094:TRP:HA	3:C:2095:PRO:C	2.29	0.53
3:C:2029:VAL:HG11	3:C:2090:GLN:CG	2.39	0.53
3:C:2029:VAL:HG11	3:C:2090:GLN:HG3	1.91	0.52
3:C:2185:LYS:HE2	3:C:2189:GLU:OE2	2.10	0.52
3:C:2013:VAL:HG11	3:C:2078:LEU:HD12	1.91	0.51
4:D:3131:THR:OG1	8:D:777:HOH:O	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:CYS:SG	6:A:5002:HEZ:H62	2.51	0.51
5:A:795:NAG:H83	8:A:5029:HOH:O	2.12	0.50
3:C:2037:GLN:HB2	3:C:2047:LEU:HD11	1.92	0.49
2:B:1077:GLU:CD	2:B:1077:GLU:H	2.16	0.49
1:A:104:MET:O	1:A:108:ILE:HG12	2.13	0.48
1:A:223:PHE:HB3	1:A:488:VAL:HG13	1.96	0.47
3:C:2054:ARG:NE	8:C:668:HOH:O	2.47	0.47
1:A:294:ILE:HD12	1:A:333:ILE:HD11	1.95	0.46
1:A:210:PHE:HB3	8:A:5151:HOH:O	2.15	0.46
4:D:3036:TRP:CE2	4:D:3081:LEU:HB2	2.50	0.46
4:D:3133:GLY:HA3	4:D:3220:THR:HG21	1.97	0.46
4:D:3054:ILE:HG23	4:D:3055:LEU:HD13	1.97	0.46
2:B:1129:GLN:HG3	2:B:1139:GLN:HG2	1.97	0.45
4:D:3229:LYS:HD3	4:D:3229:LYS:C	2.36	0.45
4:D:3216:LYS:N	4:D:3217:PRO:CD	2.80	0.45
1:A:123:THR:HG21	1:A:429:LYS:HE3	1.98	0.45
3:C:2102:GLN:NE2	8:C:509:HOH:O	2.48	0.45
4:D:3203:SER:HG	4:D:3209:TYR:HH	1.64	0.45
1:A:270:VAL:O	1:A:348:LYS:HE3	2.17	0.45
4:D:3063:HIS:CD2	4:D:3064:LEU:HD13	2.52	0.44
3:C:2021:LEU:HD12	3:C:2021:LEU:N	2.32	0.44
1:A:232:THR:CG2	1:A:232:THR:O	2.65	0.44
4:D:3203:SER:OG	4:D:3209:TYR:OH	2.32	0.44
6:A:5002:HEZ:C6	4:D:3111:ASN:HD22	2.32	0.43
2:B:1075:LYS:HB3	2:B:1077:GLU:OE2	2.18	0.43
2:B:1016:CYS:HB2	2:B:1028:TRP:CZ2	2.54	0.43
3:C:2097:ARG:HG2	4:D:3062:PRO:HD3	2.01	0.42
4:D:3105:ASP:OD1	4:D:3105:ASP:N	2.47	0.42
1:A:122:LEU:HD21	4:D:3057:VAL:HG21	2.00	0.42
2:B:1164:ASN:O	2:B:1165:GLN:HB2	2.19	0.42
4:D:3132:LYS:HE3	4:D:3132:LYS:HB2	1.88	0.42
1:A:419:ARG:HB2	6:A:5000:HEZ:H31	2.02	0.42
1:A:487:LYS:HE3	6:A:5001:HEZ:H21	2.02	0.42
1:A:269:GLU:HB2	8:A:5190:HOH:O	2.19	0.42
2:B:1028:TRP:CE2	2:B:1069:LEU:HB2	2.55	0.42
3:C:2127:LEU:HA	3:C:2127:LEU:HD12	1.84	0.41
2:B:1167:LYS:HB3	2:B:1167:LYS:HE2	1.70	0.41
1:A:426:MET:CE	1:A:431:GLY:HA3	2.50	0.41
1:A:446:SER:HB2	8:A:5153:HOH:O	2.20	0.41
4:D:3002:VAL:HG21	4:D:3024:ALA:HB1	2.02	0.41
3:C:2188:TYR:CE2	3:C:2213:ARG:HG3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ASN:CB	5:A:588:NAG:H83	2.49	0.40
2:B:1138:ILE:HD13	2:B:1139:GLN:N	2.37	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)
4:D:3147:SER:OG	8:A:5227:HOH:O[1_465]	2.14	0.06

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	304/317 (96%)	292 (96%)	12 (4%)	0	100	100
2	B	182/184 (99%)	177 (97%)	5 (3%)	0	100	100
3	C	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
4	D	224/229 (98%)	221 (99%)	3 (1%)	0	100	100
All	All	922/944 (98%)	896 (97%)	26 (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	272/280 (97%)	267 (98%)	5 (2%)	59	63
2	B	167/166 (101%)	155 (93%)	12 (7%)	14	9
3	C	184/184 (100%)	176 (96%)	8 (4%)	29	26
4	D	192/193 (100%)	183 (95%)	9 (5%)	26	22
All	All	815/823 (99%)	781 (96%)	34 (4%)	30	27

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	412	ASP
1	A	413	THR
1	A	429	LYS
1	A	490	LYS
2	B	1002	LYS
2	B	1027	HIS
2	B	1037	LEU
2	B	1069	LEU
2	B	1077	GLU
2	B	1096	LEU
2	B	1100	LEU
2	B	1109	LEU
2	B	1138	ILE
2	B	1143	THR
2	B	1149	LEU
2	B	1181	LYS
3	C	2073	LEU
3	C	2090	GLN
3	C	2107	GLU
3	C	2127	LEU
3	C	2131	THR
3	C	2171	LYS
3	C	2183	LEU
3	C	2205	SER
4	D	3003	GLN
4	D	3054	ILE
4	D	3055	LEU
4	D	3064	LEU
4	D	3081	LEU
4	D	3083	LEU
4	D	3089	ASP
4	D	3203	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	3220	THR

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

Mol	Chain	Res	Type
1	A	114	GLN
2	B	1040	GLN
2	B	1066	ASN
2	B	1129	GLN
3	C	2102	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](#)

17 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	$\# Z > 2$
7	TRS	A	5003	-	7,7,7	0.30	0	9,9,9	0.40	0
6	HEZ	A	5000	-	7,7,7	0.24	0	6,6,6	0.60	0
5	NAG	A	886	1	14,14,15	0.47	0	17,19,21	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	762	1	14,14,15	0.58	0	17,19,21	0.97	1 (5%)
5	NAG	A	795	1	14,14,15	0.51	0	17,19,21	1.03	1 (5%)
5	NAG	A	741	1	14,14,15	0.59	0	17,19,21	0.93	1 (5%)
5	NAG	A	948	1	14,14,15	0.50	0	17,19,21	0.71	0
5	NAG	A	789	1	14,14,15	0.55	0	17,19,21	0.75	0
6	HEZ	A	5001	-	7,7,7	0.32	0	6,6,6	0.45	0
5	NAG	A	892	1	14,14,15	0.51	0	17,19,21	0.71	0
5	NAG	A	697	1	14,14,15	0.55	0	17,19,21	0.90	1 (5%)
5	NAG	A	776	1	14,14,15	0.51	0	17,19,21	0.87	0
5	NAG	A	588	1	14,14,15	0.52	0	17,19,21	0.75	0
5	NAG	A	734	1	14,14,15	0.48	0	17,19,21	0.85	0
6	HEZ	A	5002	-	7,7,7	0.29	0	6,6,6	0.52	0
5	NAG	A	730	1	14,14,15	0.55	0	17,19,21	0.82	1 (5%)
5	NAG	A	839	1	14,14,15	0.65	0	17,19,21	1.30	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
7	TRS	A	5003	-	-	3/9/9/9	-
6	HEZ	A	5000	-	-	3/5/5/5	-
5	NAG	A	886	1	-	0/6/23/26	0/1/1/1
5	NAG	A	762	1	-	2/6/23/26	0/1/1/1
5	NAG	A	795	1	-	2/6/23/26	0/1/1/1
5	NAG	A	741	1	-	4/6/23/26	0/1/1/1
5	NAG	A	948	1	-	2/6/23/26	0/1/1/1
5	NAG	A	789	1	-	0/6/23/26	0/1/1/1
6	HEZ	A	5001	-	-	2/5/5/5	-
5	NAG	A	892	1	-	2/6/23/26	0/1/1/1
5	NAG	A	697	1	-	3/6/23/26	0/1/1/1
5	NAG	A	776	1	-	0/6/23/26	0/1/1/1
5	NAG	A	588	1	-	4/6/23/26	0/1/1/1
5	NAG	A	734	1	-	0/6/23/26	0/1/1/1
6	HEZ	A	5002	-	-	2/5/5/5	-
5	NAG	A	730	1	-	0/6/23/26	0/1/1/1
5	NAG	A	839	1	-	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($^{\circ}$)	Ideal($^{\circ}$)
5	A	839	NAG	C4-C3-C2	3.61	116.31	111.02
5	A	762	NAG	O5-C5-C6	2.93	111.79	107.20
5	A	741	NAG	C4-C3-C2	2.56	114.78	111.02
5	A	730	NAG	O5-C5-C6	2.40	110.96	107.20
5	A	795	NAG	O5-C5-C6	2.20	110.65	107.20
5	A	697	NAG	O5-C5-C6	2.15	110.58	107.20

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	5003	TRS	C1-C-C3-O3
7	A	5003	TRS	C2-C-C3-O3
7	A	5003	TRS	N-C-C3-O3
5	A	741	NAG	C8-C7-N2-C2
5	A	741	NAG	O7-C7-N2-C2
5	A	588	NAG	C8-C7-N2-C2
5	A	588	NAG	O7-C7-N2-C2
5	A	839	NAG	C8-C7-N2-C2
5	A	697	NAG	C8-C7-N2-C2
5	A	697	NAG	O7-C7-N2-C2
5	A	839	NAG	O7-C7-N2-C2
5	A	588	NAG	C1-C2-N2-C7
5	A	892	NAG	O5-C5-C6-O6
5	A	892	NAG	C4-C5-C6-O6
5	A	795	NAG	C8-C7-N2-C2
5	A	795	NAG	O7-C7-N2-C2
5	A	697	NAG	C1-C2-N2-C7
5	A	741	NAG	C4-C5-C6-O6
6	A	5001	HEZ	C2-C3-C4-C5
6	A	5000	HEZ	C3-C4-C5-C6
5	A	762	NAG	C4-C5-C6-O6
5	A	762	NAG	O5-C5-C6-O6
5	A	741	NAG	O5-C5-C6-O6
6	A	5002	HEZ	C3-C4-C5-C6
6	A	5000	HEZ	O1-C1-C2-C3
6	A	5001	HEZ	C1-C2-C3-C4
5	A	948	NAG	C4-C5-C6-O6
6	A	5000	HEZ	C4-C5-C6-O6
5	A	948	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	5002	HEZ	C2-C3-C4-C5
5	A	588	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	5000	HEZ	2	0
5	A	795	NAG	2	0
6	A	5001	HEZ	1	0
5	A	588	NAG	2	0
6	A	5002	HEZ	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 ⓘ

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, 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	304/317 (95%)	0.30	22 (7%) 15 14	14, 27, 55, 96	0
2	B	181/184 (98%)	0.14	8 (4%) 34 33	15, 32, 52, 61	0
3	C	214/214 (100%)	-0.17	1 (0%) 91 90	13, 26, 51, 63	0
4	D	227/229 (99%)	-0.08	7 (3%) 49 48	13, 22, 60, 78	0
All	All	926/944 (98%)	0.07	38 (4%) 37 36	13, 27, 54, 96	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	GLY	8.6
4	D	3146	THR	6.6
4	D	3147	SER	6.4
1	A	129	ALA	6.3
1	A	128	GLY	6.0
1	A	462	ASN	5.3
1	A	210	PHE	5.0
4	D	3143	SER	4.9
1	A	195	SER	4.7
1	A	197	ASN	4.7
1	A	410	GLY	4.3
1	A	88	ASN	4.0
1	A	125	LEU	3.8
2	B	1001	LYS	3.8
1	A	127	VAL	3.7
1	A	445	CYS	3.7
1	A	87	VAL	3.6
1	A	126	CYS	3.5
1	A	196	CYS	3.5
2	B	1104	SER	3.4
4	D	3148	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	84	VAL	3.2
1	A	89	VAL	3.1
4	D	3142	SER	2.9
2	B	1088	ASP	2.7
4	D	3229	LYS	2.7
2	B	1019	SER	2.6
4	D	3205	GLY	2.6
1	A	463	ASN	2.6
2	B	1020	GLN	2.6
1	A	411	SER	2.5
1	A	356	ASN	2.3
2	B	1105[A]	ASP	2.3
2	B	1181	LYS	2.2
2	B	1130	CYS	2.1
1	A	461	SER	2.1
3	C	2190	LYS	2.0
1	A	228	CYS	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 monosaccharides 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. 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
5	NAG	A	588	14/15	0.48	0.51	57,58,59,60	0
5	NAG	A	697	14/15	0.62	0.59	53,55,56,56	0
5	NAG	A	839	14/15	0.65	0.40	49,51,52,52	0
6	HEZ	A	5002	8/8	0.68	0.31	66,66,66,66	0
5	NAG	A	892	14/15	0.69	0.40	45,47,47,48	0
6	HEZ	A	5001	8/8	0.73	0.39	58,58,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	A	741	14/15	0.78	0.41	50,51,53,53	0
5	NAG	A	948	14/15	0.81	0.18	38,39,41,41	0
5	NAG	A	734	14/15	0.81	0.18	42,44,44,44	0
5	NAG	A	730	14/15	0.82	0.30	47,48,49,49	0
7	TRS	A	5003	8/8	0.88	0.19	36,37,37,37	0
5	NAG	A	886	14/15	0.89	0.12	33,34,34,34	0
5	NAG	A	795	14/15	0.90	0.16	34,35,35,36	0
5	NAG	A	776	14/15	0.91	0.13	36,37,39,39	0
5	NAG	A	789	14/15	0.91	0.18	36,37,38,38	0
6	HEZ	A	5000	8/8	0.92	0.16	30,31,32,33	0
5	NAG	A	762	14/15	0.92	0.13	30,32,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.