



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:34 AM GMT

PDB ID : 2NXZ
Title : HIV-1 gp120 Envelope Glycoprotein (T257S, S334A, S375W) Complexed with CD4 and Antibody 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 : 2.04 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

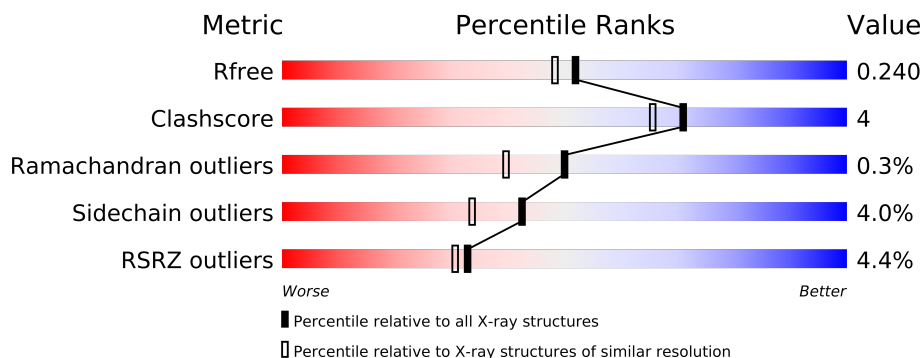
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.04 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}	66092	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	317	
2	B	184	
3	C	214	
4	D	229	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	A	730	-	X
5	NAG	A	734	-	X
5	NAG	A	741	-	X
5	NAG	A	789	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	A	839	-	X
5	NAG	A	892	-	X
7	EDO	A	4003	-	X
7	EDO	C	4002	-	X
8	HEZ	A	4005	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7913 atoms, of which 0 are hydrogen and 0 are deuterium.

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	306	Total	C	N	O	S	0	1	0
			2375	1492	413	450	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	1	0
			1418	889	249	276	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.

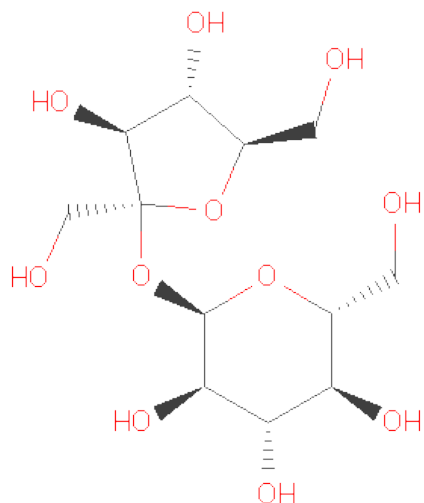
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	222	Total	C	N	O	S	0	1	0
			1682	1065	283	329	5			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



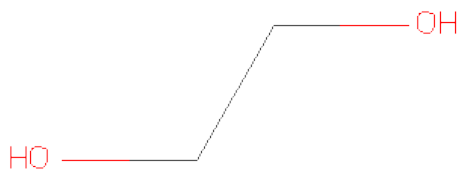
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	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 SUGAR (SUCROSE) (three-letter code: SUC) (formula: C₁₂H₂₂O₁₁).



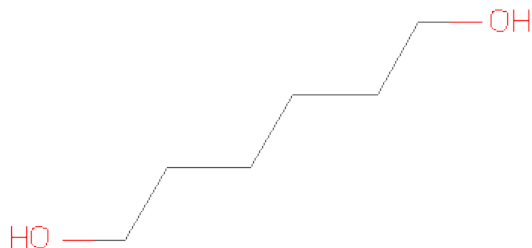
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



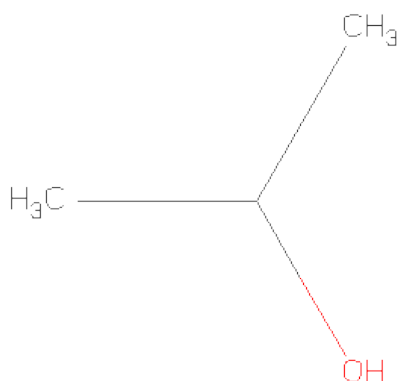
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



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

- Molecule 9 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			4	3	1		

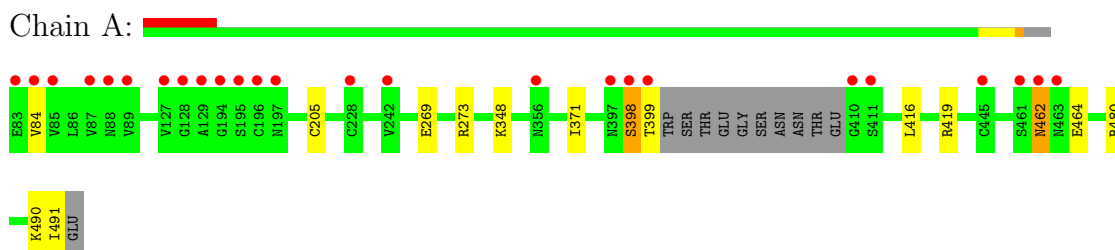
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	190	Total 190	O 190	0	0
10	B	87	Total 87	O 87	0	0
10	C	124	Total 124	O 124	0	0
10	D	162	Total 162	O 162	0	0

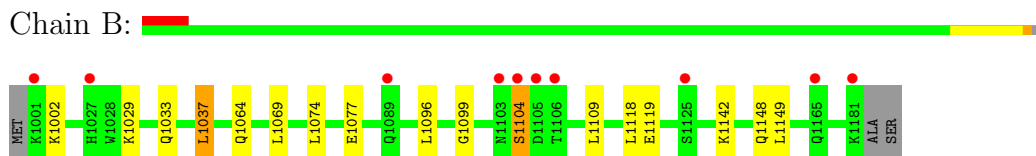
3 Residue-property plots

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.

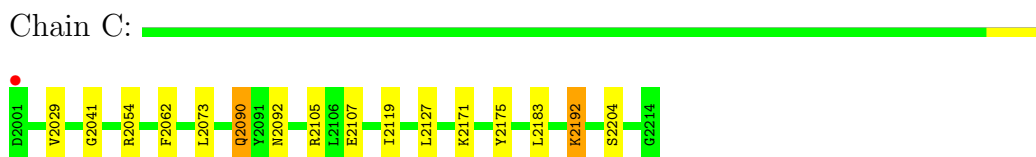
- Molecule 1: ENVELOPE GLYCOPROTEIN GP120



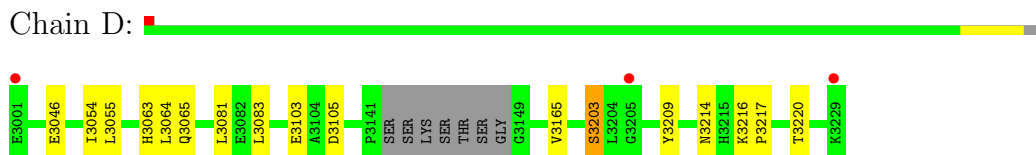
- Molecule 2: T-cell surface glycoprotein CD4



- 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	71.92Å 88.13Å 197.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.38 – 2.04 35.38 – 2.04	Depositor EDS
% Data completeness (in resolution range)	87.1 (35.38-2.04) 87.2 (35.38-2.04)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.206 , 0.244 0.202 , 0.240	Depositor DCC
R_{free} test set	3578 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 28.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 70311 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7913	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, SUC, NAG, HEZ, EDO

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	0.34	0/2427	0.48	0/3292
2	B	0.29	0/1443	0.51	1/1945 (0.1%)
3	C	0.61	3/1683 (0.2%)	0.53	1/2288 (0.0%)
4	D	0.33	0/1727	0.51	0/2353
All	All	0.41	3/7280 (0.0%)	0.51	2/9878 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2192	LYS	CE-NZ	18.08	1.94	1.49
3	C	2192	LYS	CG-CD	9.19	1.83	1.52
3	C	2192	LYS	CD-CE	6.69	1.68	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2192	LYS	CB-CG-CD	-5.49	97.33	111.60
2	B	1037	LEU	CA-CB-CG	5.45	127.84	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2375	0	0	8	0
2	B	1418	0	0	6	0
3	C	1646	0	0	9	0
4	D	1682	0	0	10	0
5	A	182	0	169	0	0
6	D	23	0	22	4	0
7	A	8	0	12	0	0
7	C	4	0	6	1	0
8	A	8	0	14	3	0
9	B	4	0	6	1	0
10	A	190	0	0	2	1
10	B	87	0	0	5	0
10	C	124	0	0	0	0
10	D	162	0	0	3	0
All	All	7913	0	229	34	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (34) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:2192:LYS:CG	3:C:2192:LYS:CD	1.83	1.52
3:C:2192:LYS:CE	3:C:2192:LYS:NZ	1.94	1.29
4:D:3046:GLU:OE2	4:D:3063[B]:HIS:CE1	2.23	0.91
2:B:1148:GLN:NE2	10:B:195:HOH:O	2.04	0.90
4:D:3065:GLN:NE2	10:D:36:HOH:O	2.11	0.83
3:C:2192:LYS:CD	3:C:2192:LYS:CB	2.59	0.81
3:C:2192:LYS:CG	3:C:2192:LYS:CE	2.68	0.72
4:D:3214:ASN:ND2	10:D:248:HOH:O	2.27	0.68
4:D:3063[B]:HIS:CD2	6:D:4000:SUC:O6'	2.48	0.66
4:D:3063[B]:HIS:NE2	6:D:4000:SUC:O6'	2.29	0.65
2:B:1104:SER:O	10:B:545:HOH:O	2.16	0.61
4:D:3203:SER:OG	4:D:3209:TYR:OH	2.19	0.60
2:B:1033:GLN:NE2	10:B:207:HOH:O	2.33	0.60
9:B:4004:IPA:H12	10:B:71:HOH:O	2.00	0.60
2:B:1118:LEU:O	2:B:1142:LYS:CD	2.53	0.56
6:D:4000:SUC:O1'	10:D:470:HOH:O	2.18	0.55
1:A:480:ARG:NE	10:A:4050:HOH:O	2.39	0.54
1:A:205:CYS:SG	8:A:4005:HEZ:H32	2.48	0.54
1:A:205:CYS:N	8:A:4005:HEZ:HO1	2.07	0.53
1:A:273:ARG:NH1	10:A:4187:HOH:O	2.42	0.52
1:A:205:CYS:N	8:A:4005:HEZ:O1	2.45	0.50
4:D:3063[B]:HIS:CE1	6:D:4000:SUC:HO6'	2.30	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1099:GLY:O	2:B:1119:GLU:N	2.49	0.45
1:A:398:SER:OG	1:A:399:THR:N	2.50	0.45
3:C:2054:ARG:NH1	3:C:2062:PHE:O	2.50	0.45
3:C:2105:ARG:NH2	3:C:2175:TYR:OH	2.50	0.44
3:C:2090:GLN:OE1	3:C:2092:ASN:N	2.50	0.44
4:D:3216:LYS:N	4:D:3217:PRO:CD	2.81	0.44
3:C:2041:GLY:N	7:C:4002:EDO:HO1	2.16	0.43
2:B:1029:LYS:NZ	10:B:207:HOH:O	2.52	0.42
3:C:2029:VAL:CG1	3:C:2090:GLN:CG	2.98	0.41
1:A:419:ARG:NH2	4:D:3103:GLU:OE2	2.54	0.41
4:D:3105:ASP:N	4:D:3105:ASP:OD1	2.54	0.41
1:A:269:GLU:OE2	1:A:348:LYS:NZ	2.53	0.41

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	Distance(Å)	Clash(Å)
10:A:4133:HOH:O	10:A:4133:HOH:O[4_556]	1.55	0.65

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	303/317 (96%)	284 (94%)	16 (5%)	3 (1%)	22	9
2	B	180/184 (98%)	173 (96%)	7 (4%)	0	100	100
3	C	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
4	D	219/229 (96%)	214 (98%)	5 (2%)	0	100	100
All	All	914/944 (97%)	874 (96%)	37 (4%)	3 (0%)	50	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	464	GLU
1	A	462	ASN

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Mol	Chain	Res	Type
1	A	398	SER

5.3.2 Protein sidechains ⓘ

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	271/280 (97%)	265 (98%)	6 (2%)	64	60
2	B	165/166 (99%)	155 (94%)	10 (6%)	26	16
3	C	184/184 (100%)	176 (96%)	8 (4%)	40	31
4	D	188/193 (97%)	180 (96%)	8 (4%)	40	31
All	All	808/823 (98%)	776 (96%)	32 (4%)	42	33

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	371	ILE
1	A	416	LEU
1	A	462	ASN
1	A	490	LYS
1	A	491	ILE
2	B	1002	LYS
2	B	1037	LEU
2	B	1064	GLN
2	B	1069	LEU
2	B	1074	LEU
2	B	1077	GLU
2	B	1096	LEU
2	B	1104	SER
2	B	1109	LEU
2	B	1149	LEU
3	C	2073	LEU
3	C	2090	GLN
3	C	2107	GLU
3	C	2119	ILE
3	C	2127	LEU

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Mol	Chain	Res	Type
3	C	2171	LYS
3	C	2183	LEU
3	C	2204	SER
4	D	3054	ILE
4	D	3055	LEU
4	D	3064	LEU
4	D	3081	LEU
4	D	3083	LEU
4	D	3165	VAL
4	D	3203	SER
4	D	3220	THR

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

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

19 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	EDO	A	4001	-	3,3,3	0.51	0	2,2,2	0.37	0
7	EDO	A	4003	-	3,3,3	0.54	0	2,2,2	0.38	0
8	HEZ	A	4005	-	7,7,7	0.27	0	6,6,6	0.56	0
5	NAG	A	588	1	12,14,15	0.66	0	15,19,21	0.89	1 (6%)
5	NAG	A	697	1	12,14,15	0.58	0	15,19,21	0.74	1 (6%)
5	NAG	A	730	1	12,14,15	0.68	1 (8%)	15,19,21	1.30	2 (13%)
5	NAG	A	734	1	12,14,15	0.68	0	15,19,21	0.82	1 (6%)
5	NAG	A	741	1	12,14,15	0.73	1 (8%)	15,19,21	1.09	2 (13%)
5	NAG	A	762	1	12,14,15	0.65	0	15,19,21	1.04	1 (6%)
5	NAG	A	776	1	12,14,15	0.71	1 (8%)	15,19,21	1.19	2 (13%)
5	NAG	A	789	1	12,14,15	0.69	1 (8%)	15,19,21	0.99	1 (6%)
5	NAG	A	795	1	12,14,15	0.71	1 (8%)	15,19,21	1.31	2 (13%)
5	NAG	A	839	1	12,14,15	0.71	1 (8%)	15,19,21	1.14	2 (13%)
5	NAG	A	886	1	12,14,15	0.65	0	15,19,21	1.12	2 (13%)
5	NAG	A	892	1	12,14,15	0.69	1 (8%)	15,19,21	0.94	1 (6%)
5	NAG	A	948	1	12,14,15	0.67	1 (8%)	15,19,21	1.07	2 (13%)
9	IPA	B	4004	-	3,3,3	1.36	0	3,3,3	1.15	0
7	EDO	C	4002	-	3,3,3	0.54	0	2,2,2	0.36	0
6	SUC	D	4000	-	24,24,24	0.41	0	36,36,36	0.70	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
7	EDO	A	4001	-	-	0/1/1/1	0/0/0/0
7	EDO	A	4003	-	-	0/1/1/1	0/0/0/0
8	HEZ	A	4005	-	-	0/5/5/5	0/0/0/0
5	NAG	A	588	1	-	0/6/23/26	0/1/1/1
5	NAG	A	697	1	-	0/6/23/26	0/1/1/1
5	NAG	A	730	1	-	0/6/23/26	0/1/1/1
5	NAG	A	734	1	-	0/6/23/26	0/1/1/1
5	NAG	A	741	1	-	0/6/23/26	0/1/1/1
5	NAG	A	762	1	-	0/6/23/26	0/1/1/1
5	NAG	A	776	1	-	0/6/23/26	0/1/1/1
5	NAG	A	789	1	-	0/6/23/26	0/1/1/1
5	NAG	A	795	1	-	0/6/23/26	0/1/1/1
5	NAG	A	839	1	-	0/6/23/26	0/1/1/1
5	NAG	A	886	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	892	1	-	0/6/23/26	0/1/1/1
5	NAG	A	948	1	-	0/6/23/26	0/1/1/1
9	IPA	B	4004	-	-	0/0/0/0	0/0/0/0
7	EDO	C	4002	-	-	0/1/1/1	0/0/0/0
6	SUC	D	4000	-	-	0/12/51/51	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	741	NAG	O5-C5	-2.24	1.41	1.45
5	A	839	NAG	O5-C5	-2.24	1.41	1.45
5	A	776	NAG	O5-C5	-2.19	1.41	1.45
5	A	892	NAG	O5-C5	-2.09	1.41	1.45
5	A	789	NAG	O5-C5	-2.07	1.41	1.45
5	A	730	NAG	O5-C5	-2.06	1.41	1.45
5	A	795	NAG	O5-C5	-2.05	1.41	1.45
5	A	948	NAG	O5-C5	-2.04	1.41	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	730	NAG	O5-C5-C6	3.71	110.87	106.98
5	A	795	NAG	C3-C2-N2	-3.26	106.80	111.76
5	A	776	NAG	O5-C5-C6	3.17	110.31	106.98
5	A	839	NAG	O5-C5-C4	-2.67	107.27	110.65
5	A	789	NAG	O5-C5-C6	2.64	109.75	106.98
5	A	795	NAG	O5-C5-C6	2.62	109.73	106.98
5	A	948	NAG	O5-C5-C6	2.59	109.70	106.98
5	A	741	NAG	O5-C5-C6	2.57	109.68	106.98
5	A	730	NAG	O5-C5-C4	-2.57	107.40	110.65
5	A	588	NAG	O5-C5-C6	2.56	109.67	106.98
5	A	892	NAG	O5-C5-C6	2.48	109.58	106.98
5	A	762	NAG	O5-C5-C6	2.37	109.47	106.98
5	A	886	NAG	C3-C2-N2	-2.36	108.16	111.76
5	A	886	NAG	O5-C5-C6	2.35	109.44	106.98
5	A	839	NAG	O5-C5-C6	2.17	109.25	106.98
5	A	734	NAG	O5-C5-C6	2.16	109.25	106.98
5	A	741	NAG	O5-C5-C4	-2.16	107.92	110.65
5	A	697	NAG	O5-C5-C6	2.13	109.21	106.98
5	A	776	NAG	O5-C5-C4	-2.07	108.02	110.65
5	A	948	NAG	C3-C2-N2	-2.05	108.63	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	306/317 (96%)	0.38	25 (8%)	12 11	7, 24, 56, 87	0
2	B	181/184 (98%)	0.21	10 (5%)	24 23	11, 29, 51, 61	0
3	C	214/214 (100%)	-0.11	1 (0%)	88 91	6, 22, 50, 60	0
4	D	222/229 (96%)	-0.08	3 (1%)	72 74	7, 18, 47, 69	0
All	All	923/944 (97%)	0.12	39 (4%)	33 33	6, 23, 53, 87	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	399	THR	6.8
1	A	129	ALA	4.9
1	A	89	VAL	4.9
1	A	462	ASN	4.6
2	B	1001	LYS	4.5
1	A	88	ASN	4.3
1	A	398	SER	4.0
1	A	84	VAL	3.8
1	A	127	VAL	3.8
1	A	410	GLY	3.7
1	A	195	SER	3.6
2	B	1105	ASP	3.5
1	A	196	CYS	3.2
1	A	83	GLU	3.2
1	A	463	ASN	3.1
1	A	461	SER	3.1
4	D	3229	LYS	3.0
1	A	194	GLY	3.0
1	A	197	ASN	2.8
1	A	128	GLY	2.8
1	A	397	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	1181	LYS	2.7
1	A	87	VAL	2.6
1	A	242	VAL	2.6
1	A	85	VAL	2.4
1	A	228	CYS	2.4
2	B	1089	GLN	2.4
2	B	1106	THR	2.4
2	B	1165	GLN	2.4
1	A	356	ASN	2.2
2	B	1104	SER	2.2
2	B	1125	SER	2.2
1	A	445	CYS	2.2
4	D	3205	GLY	2.2
1	A	411	SER	2.2
2	B	1027[A]	HIS	2.1
2	B	1103	ASN	2.1
4	D	3001	GLU	2.1
3	C	2001	ASP	2.1

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	A	892	14/15	0.41	29.30	38,42,43,44	0
5	NAG	A	730	14/15	0.51	10.47	58,63,65,65	0
8	HEZ	A	4005	8/8	0.33	9.21	41,43,44,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	A	734	14/15	0.24	6.65	41,45,47,47	0
7	EDO	C	4002	4/4	0.19	6.28	32,33,33,33	0
7	EDO	A	4003	4/4	0.18	5.42	31,31,32,32	0
5	NAG	A	741	14/15	0.39	4.47	43,47,48,48	0
5	NAG	A	839	14/15	0.42	3.11	42,47,48,48	0
5	NAG	A	789	14/15	0.20	2.36	29,31,33,33	0
5	NAG	A	588	14/15	0.47	1.96	36,49,52,52	0
9	IPA	B	4004	4/4	0.19	1.95	31,31,31,31	0
6	SUC	D	4000	23/23	0.23	1.91	39,41,41,42	0
5	NAG	A	886	14/15	0.14	0.92	30,33,34,35	0
5	NAG	A	948	14/15	0.21	0.85	37,39,41,42	0
5	NAG	A	795	14/15	0.17	0.44	23,26,28,28	0
5	NAG	A	776	14/15	0.15	0.20	31,34,36,37	0
7	EDO	A	4001	4/4	0.11	-0.05	16,17,18,18	0
5	NAG	A	762	14/15	0.14	-0.41	21,25,27,28	0
5	NAG	A	697	14/15	0.44	-	44,48,49,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.