



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:06 AM UTC

PDB ID : 4YDJ / pdb_00004ydj
Title : Crystal structure of broadly and potently neutralizing antibody 44-VRC13.01
in complex with HIV-1 clade AE strain 93TH057 gp120
Authors : Zhou, T.; Moquin, S.; Kwong, P.D.
Deposited on : 2015-02-22
Resolution : 2.31 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

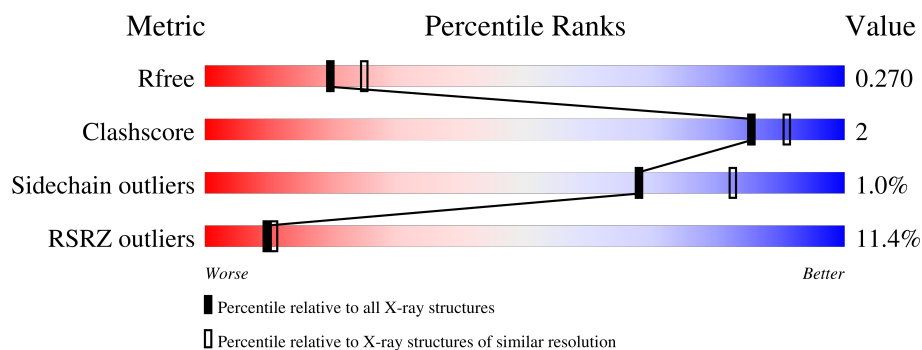
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	G	353	16% 79% 5% 16%
1	I	353	16% 77% 6% 17%
2	A	238	6% 95% 5%
2	H	238	7% 95% 5%
3	B	206	6% 94% 6%
3	L	206	7% 93% 6%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 23589 atoms, of which 11493 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 gp160,Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	G	298	Total	C	H	N	O	S	0	0	0
			4646	1476	2295	411	445	19			
1	I	292	Total	C	H	N	O	S	0	0	0
			4555	1451	2248	402	436	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	197	GLY	-	linker	UNP Q0ED31
G	198	GLY	-	linker	UNP Q0ED31
G	318	GLY	-	linker	UNP Q0ED31
G	319	GLY	-	linker	UNP Q0ED31
G	320	SER	-	linker	UNP Q0ED31
G	321	GLY	-	linker	UNP Q0ED31
G	322	SER	-	linker	UNP Q0ED31
G	323	GLY	-	linker	UNP Q0ED31
I	197	GLY	-	linker	UNP Q0ED31
I	198	GLY	-	linker	UNP Q0ED31
I	318	GLY	-	linker	UNP Q0ED31
I	319	GLY	-	linker	UNP Q0ED31
I	320	SER	-	linker	UNP Q0ED31
I	321	GLY	-	linker	UNP Q0ED31
I	322	SER	-	linker	UNP Q0ED31
I	323	GLY	-	linker	UNP Q0ED31

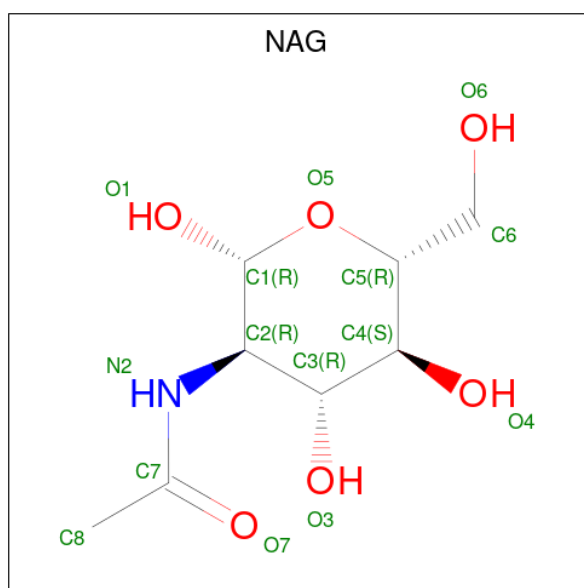
- Molecule 2 is a protein called HEAVY CHAIN OF ANTIBODY 44-VRC13.01.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	238	Total	C	H	N	O	S	0	0	0
			3583	1141	1787	308	339	8			
2	A	238	Total	C	H	N	O	S	0	0	0
			3582	1141	1786	308	339	8			

- Molecule 3 is a protein called LIGHT CHAIN OF ANTIBODY 44-VRC13.01.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	205	Total	C	H	N	O	S	0	0	0
			3052	967	1500	266	313	6			
3	B	205	Total	C	H	N	O	S	0	0	0
			3049	967	1497	266	313	6			

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



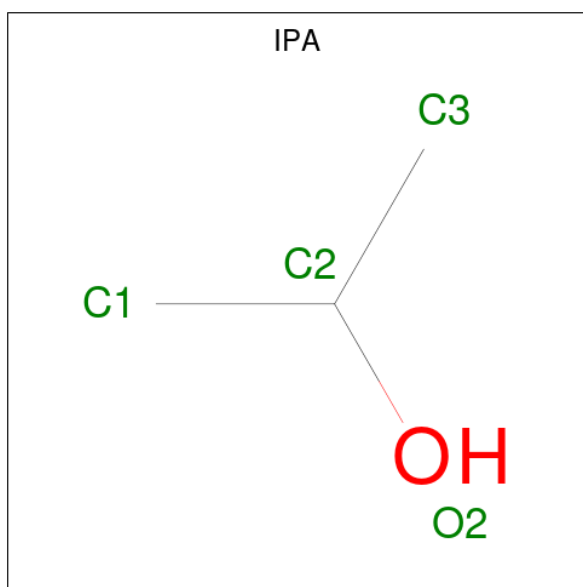
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	G	1	Total	C	H	N	O		0	0
			27	8	13	1	5			
4	G	1	Total	C	H	N	O		0	0
			27	8	13	1	5			
4	G	1	Total	C	H	N	O		0	0
			27	8	13	1	5			
4	G	1	Total	C	H	N	O		0	0
			27	8	13	1	5			
4	G	1	Total	C	H	N	O		0	0
			27	8	13	1	5			
4	G	1	Total	C	H	N	O		0	0
			27	8	13	1	5			
4	G	1	Total	C	H	N	O		0	0
			27	8	13	1	5			

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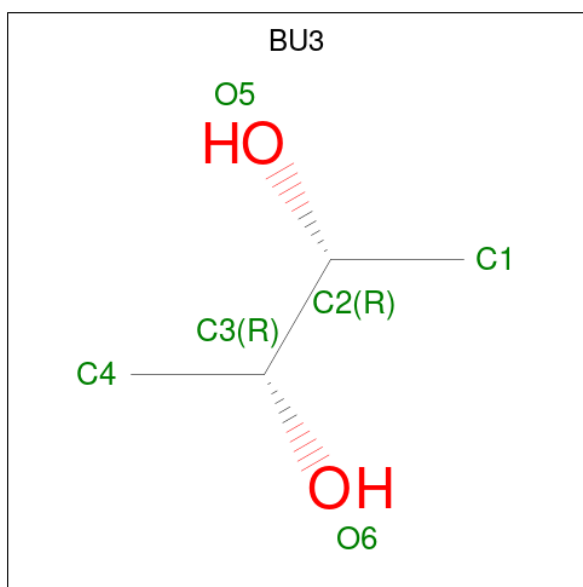
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	H	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	L	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	I	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	I	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	I	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	I	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	I	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	I	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	I	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 5 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	H	O	0	0
			12	3	8	1		
5	L	1	Total	C	H	O	0	0
			12	3	8	1		
5	A	1	Total	C	H	O	0	0
			12	3	8	1		

- Molecule 6 is (R,R)-2,3-BUTANEDIOL (CCD ID: BU3) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	H	O	0	0
			16	4	10	2		

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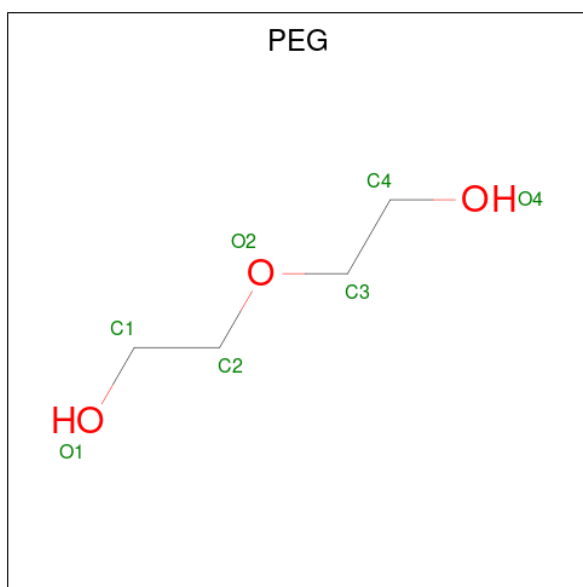
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			16	4	10	2		
6	B	1	Total	C	H	O	0	0
			16	4	10	2		
6	B	1	Total	C	H	O	0	0
			16	4	10	2		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	1	Total	Na	0	0
			1	1		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			17	4	10	3		
8	B	1	Total	C	H	O	0	0
			17	4	10	3		
8	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Cl 1 1	0	0

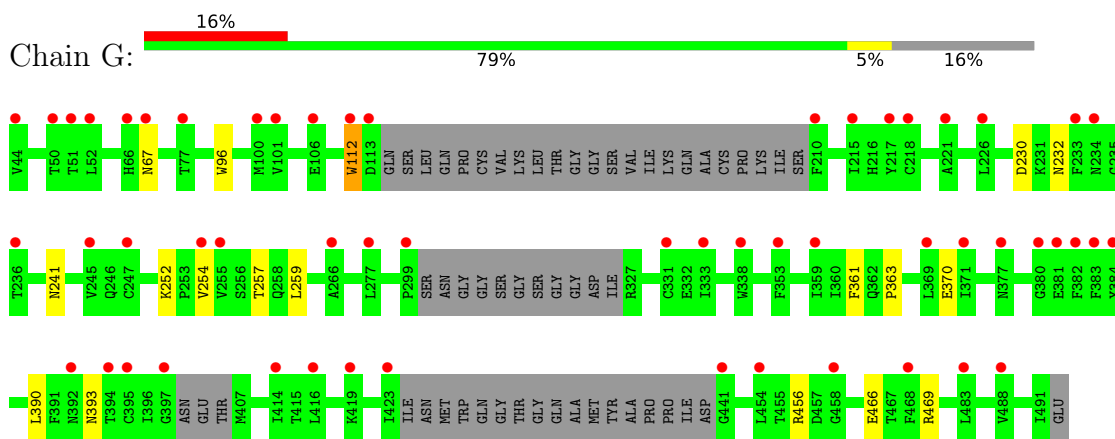
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	G	7	Total O 7 7	0	0
10	H	90	Total O 90 90	0	0
10	L	78	Total O 78 78	0	0
10	I	3	Total O 3 3	0	0
10	A	97	Total O 97 97	0	0
10	B	100	Total O 100 100	0	0

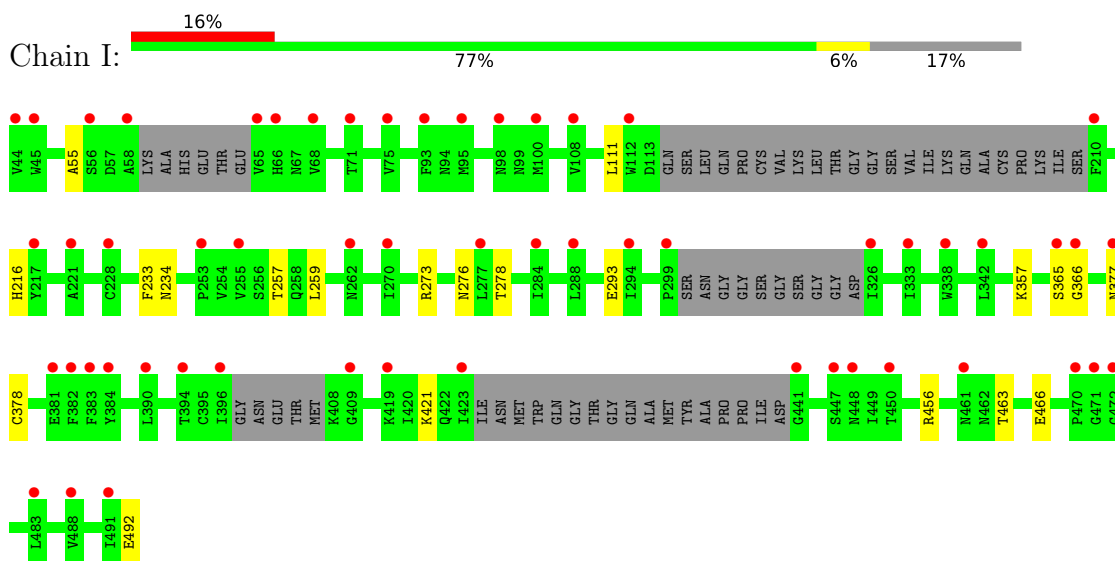
3 Residue-property plots [i](#)

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: Envelope glycoprotein gp160,Envelope glycoprotein gp160

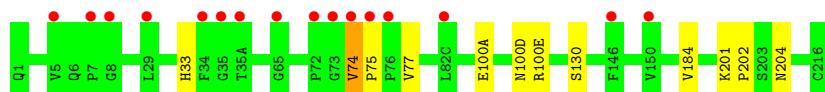


- Molecule 1: Envelope glycoprotein gp160,Envelope glycoprotein gp160

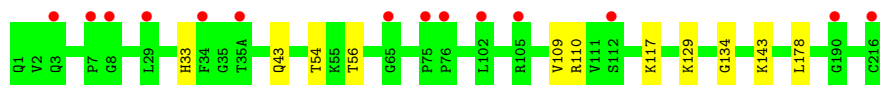


- Molecule 2: HEAVY CHAIN OF ANTIBODY 44-VRC13.01

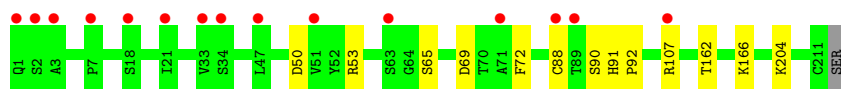
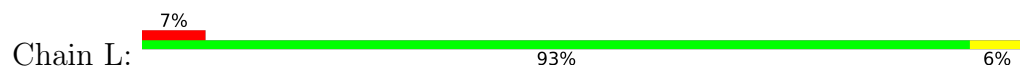




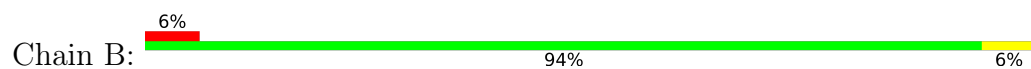
• Molecule 2: HEAVY CHAIN OF ANTIBODY 44-VRC13.01



• Molecule 3: LIGHT CHAIN OF ANTIBODY 44-VRC13.01



• Molecule 3: LIGHT CHAIN OF ANTIBODY 44-VRC13.01



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	293.80Å 67.05Å 93.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.30 – 2.31 38.30 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.9 (38.30-2.31) 92.7 (38.30-2.31)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.31Å)	Xtriage
Refinement program	PHENIX dev_1702	Depositor
R, R_{free}	0.223 , 0.249 (Not available) , 0.270	Depositor DCC
R_{free} test set	4079 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23589	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8071e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PEG, NAG, IPA, BU3, CL, NA

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	0.27	0/2398	0.58	0/3249
1	I	0.26	0/2352	0.57	0/3187
2	A	0.30	0/1844	0.58	0/2510
2	H	0.30	0/1844	0.60	2/2510 (0.1%)
3	B	0.32	0/1591	0.60	0/2170
3	L	0.30	0/1591	0.59	0/2170
All	All	0.29	0/11620	0.59	2/15796 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	74	VAL	CA-C-N	-6.01	114.19	120.38
2	H	74	VAL	C-N-CA	-6.01	114.19	120.38

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	2351	2295	2285	11	0
1	I	2307	2248	2245	11	0
2	A	1796	1786	1781	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1796	1787	1782	7	0
3	B	1552	1497	1493	9	0
3	L	1552	1500	1494	8	0
4	A	14	13	13	0	0
4	B	14	13	13	0	0
4	G	126	117	117	1	0
4	H	14	13	13	0	0
4	I	126	117	117	0	0
4	L	14	13	13	0	0
5	A	4	8	8	1	0
5	H	4	8	8	0	0
5	L	4	8	8	1	0
6	A	6	10	10	0	0
6	B	12	20	20	4	0
6	H	6	10	10	0	0
7	L	1	0	0	0	0
8	A	7	10	10	0	0
8	B	14	20	20	0	0
9	B	1	0	0	0	0
10	A	97	0	0	4	0
10	B	100	0	0	1	0
10	G	7	0	0	0	0
10	H	90	0	0	1	1
10	I	3	0	0	0	0
10	L	78	0	0	1	1
All	All	12096	11493	11460	51	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 2.

All (51) 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:I:233:PHE:O	1:I:273:ARG:NH2	2.25	0.69
2:H:204:ASN:ND2	10:H:401:HOH:O	2.29	0.66
2:A:117:LYS:NZ	10:A:401:HOH:O	2.30	0.65
2:A:134:GLY:H	5:A:302:IPA:H12	1.67	0.60
1:G:361:PHE:O	1:G:393:ASN:ND2	2.35	0.60
1:I:357:LYS:NZ	1:I:463:THR:O	2.36	0.59
3:B:50:ASP:OD2	3:B:53:ARG:NH1	2.36	0.58
3:B:31:ASP:OD1	3:B:32:ARG:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:107:ARG:HD3	5:L:302:IPA:H31	1.86	0.57
2:A:129:LYS:NZ	10:A:403:HOH:O	2.38	0.57
3:B:138:ASP:OD1	3:B:167:GLN:NE2	2.39	0.56
3:B:149:LYS:CE	6:B:302:BU3:H11	2.37	0.55
1:I:492:GLU:OE1	1:I:492:GLU:N	2.41	0.54
1:I:377:ASN:OD1	1:I:378:CYS:N	2.41	0.54
1:I:276:ASN:OD1	1:I:278:THR:OG1	2.20	0.54
2:A:110:ARG:NH1	10:A:484:HOH:O	2.41	0.53
1:G:96:TRP:O	2:H:100(E):ARG:NH1	2.39	0.52
2:A:143:LYS:NZ	10:A:495:HOH:O	2.43	0.52
1:G:241:ASN:ND2	4:G:502:NAG:O7	2.45	0.50
1:G:370:GLU:N	1:G:370:GLU:OE2	2.43	0.50
1:G:230:ASP:O	1:G:232:ASN:N	2.45	0.50
3:B:201:THR:HB	6:B:303:BU3:H13	1.94	0.49
2:A:54:THR:O	2:A:56:THR:N	2.44	0.47
3:L:50:ASP:OD2	3:L:53:ARG:NH1	2.45	0.47
1:G:257:THR:O	1:G:259:LEU:N	2.46	0.46
3:L:90:SER:OG	3:L:91:HIS:N	2.47	0.46
3:B:203:GLU:OE1	6:B:302:BU3:O5	2.33	0.46
3:L:65:SER:O	3:L:72:PHE:N	2.48	0.46
1:I:293:GLU:OE1	1:I:293:GLU:N	2.47	0.46
1:G:456:ARG:NH1	1:G:466:GLU:OE2	2.49	0.45
3:B:126:GLN:NE2	10:B:403:HOH:O	2.49	0.45
2:H:74:VAL:HB	2:H:75:PRO:CD	2.47	0.45
1:I:55:ALA:N	1:I:216:HIS:O	2.51	0.44
1:I:456:ARG:NH1	1:I:466:GLU:OE2	2.49	0.44
3:B:194:GLN:NE2	3:B:203:GLU:OE2	2.49	0.44
2:H:74:VAL:HB	2:H:75:PRO:HD3	2.00	0.43
1:I:257:THR:O	1:I:259:LEU:N	2.46	0.43
3:B:149:LYS:HE3	6:B:302:BU3:H11	1.99	0.43
2:H:100(A):GLU:OE2	2:H:100(D):ASN:N	2.49	0.42
1:I:234:ASN:O	1:I:273:ARG:NE	2.52	0.42
1:I:365:SER:OG	1:I:366:GLY:N	2.51	0.42
1:G:252:LYS:O	1:G:254:VAL:N	2.50	0.42
3:L:91:HIS:HA	3:L:92:PRO:C	2.45	0.41
1:G:67:ASN:OD1	1:G:67:ASN:N	2.52	0.41
2:H:201:LYS:N	2:H:202:PRO:HD2	2.35	0.41
3:L:69:ASP:OD1	3:L:69:ASP:N	2.53	0.41
3:L:162:THR:OG1	10:L:464:HOH:O	2.22	0.40
2:A:178:LEU:C	2:A:178:LEU:HD12	2.46	0.40
2:H:130:SER:OG	3:L:204:LYS:NZ	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:TRP:HA	1:G:112:TRP:CE3	2.56	0.40
1:G:363:PRO:O	1:G:469:ARG:NH1	2.54	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)
10:H:425:HOH:O	10:L:412:HOH:O[3_453]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	268/311 (86%)	266 (99%)	2 (1%)	76	87
1	I	264/311 (85%)	262 (99%)	2 (1%)	73	86
2	A	202/202 (100%)	199 (98%)	3 (2%)	57	75
2	H	202/202 (100%)	199 (98%)	3 (2%)	57	75
3	B	175/176 (99%)	174 (99%)	1 (1%)	78	89
3	L	175/176 (99%)	173 (99%)	2 (1%)	65	81
All	All	1286/1378 (93%)	1273 (99%)	13 (1%)	68	82

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	112	TRP

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Mol	Chain	Res	Type
1	G	390	LEU
2	H	33	HIS
2	H	77	VAL
2	H	184	VAL
3	L	88	CYS
3	L	166	LYS
1	I	111	LEU
1	I	421	LYS
2	A	33	HIS
2	A	43	GLN
2	A	109	VAL
3	B	209	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	258	GLN
2	H	1	GLN
3	L	66	HIS
1	I	94	ASN
1	I	362	GLN
2	A	43	GLN
3	B	37	GLN
3	B	91	HIS
3	B	105	ASN
3	B	108	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	I	501	1	14,14,15	0.20	0	17,19,21	0.51	0
4	NAG	H	301	2	14,14,15	0.25	0	17,19,21	0.52	0
4	NAG	G	504	1	14,14,15	0.24	0	17,19,21	0.44	0
6	BU3	B	302	-	4,5,5	1.41	0	6,6,6	0.31	0
4	NAG	G	503	1	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	I	505	1	14,14,15	0.23	0	17,19,21	0.48	0
5	IPA	H	302	-	3,3,3	0.57	0	3,3,3	0.18	0
4	NAG	G	506	1	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	L	301	3	14,14,15	0.22	0	17,19,21	0.50	0
4	NAG	I	504	1	14,14,15	0.29	0	17,19,21	0.42	0
5	IPA	L	302	-	3,3,3	0.53	0	3,3,3	0.13	0
4	NAG	G	508	1	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	I	503	1	14,14,15	0.23	0	17,19,21	0.43	0
6	BU3	H	303	-	4,5,5	1.41	0	6,6,6	0.36	0
4	NAG	G	502	1	14,14,15	0.55	0	17,19,21	0.72	1 (5%)
8	PEG	A	304	-	6,6,6	0.55	0	5,5,5	0.28	0
4	NAG	I	502	1	14,14,15	0.25	0	17,19,21	0.43	0
4	NAG	I	506	1	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	B	301	3	14,14,15	0.28	0	17,19,21	0.42	0
4	NAG	G	507	1	14,14,15	0.20	0	17,19,21	0.55	0
6	BU3	A	303	-	4,5,5	1.44	0	6,6,6	0.37	0
4	NAG	I	509	1	14,14,15	0.25	0	17,19,21	0.48	0
4	NAG	A	301	2	14,14,15	0.20	0	17,19,21	0.53	0
4	NAG	I	508	1	14,14,15	0.28	0	17,19,21	0.48	0
5	IPA	A	302	-	3,3,3	0.55	0	3,3,3	0.18	0
8	PEG	B	304	-	6,6,6	0.55	0	5,5,5	0.39	0
4	NAG	G	509	1	14,14,15	0.26	0	17,19,21	0.53	0
6	BU3	B	303	-	4,5,5	1.47	0	6,6,6	0.40	0
4	NAG	I	507	1	14,14,15	0.21	0	17,19,21	0.55	0
4	NAG	G	505	1	14,14,15	0.30	0	17,19,21	0.51	0
4	NAG	G	501	1	14,14,15	0.19	0	17,19,21	0.47	0
8	PEG	B	305	-	6,6,6	0.54	0	5,5,5	0.48	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
4	NAG	I	501	1	-	3/6/23/26	0/1/1/1
4	NAG	H	301	2	-	2/6/23/26	0/1/1/1
4	NAG	G	504	1	-	1/6/23/26	0/1/1/1
6	BU3	B	302	-	-	0/4/4/4	-
4	NAG	G	503	1	-	2/6/23/26	0/1/1/1
4	NAG	I	505	1	-	0/6/23/26	0/1/1/1
4	NAG	G	506	1	-	0/6/23/26	0/1/1/1
4	NAG	L	301	3	-	4/6/23/26	0/1/1/1
4	NAG	I	504	1	-	0/6/23/26	0/1/1/1
4	NAG	G	508	1	-	0/6/23/26	0/1/1/1
4	NAG	I	503	1	-	2/6/23/26	0/1/1/1
6	BU3	H	303	-	-	0/4/4/4	-
4	NAG	G	502	1	-	3/6/23/26	0/1/1/1
8	PEG	A	304	-	-	2/4/4/4	-
4	NAG	I	502	1	-	2/6/23/26	0/1/1/1
4	NAG	I	506	1	-	2/6/23/26	0/1/1/1
4	NAG	B	301	3	-	1/6/23/26	0/1/1/1
4	NAG	G	507	1	-	2/6/23/26	0/1/1/1
6	BU3	A	303	-	-	0/4/4/4	-
4	NAG	I	509	1	-	2/6/23/26	0/1/1/1
4	NAG	A	301	2	-	4/6/23/26	0/1/1/1
4	NAG	I	508	1	-	2/6/23/26	0/1/1/1
8	PEG	B	304	-	-	1/4/4/4	-
4	NAG	G	509	1	-	2/6/23/26	0/1/1/1
6	BU3	B	303	-	-	0/4/4/4	-
4	NAG	I	507	1	-	3/6/23/26	0/1/1/1
4	NAG	G	505	1	-	0/6/23/26	0/1/1/1
4	NAG	G	501	1	-	2/6/23/26	0/1/1/1
8	PEG	B	305	-	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	502	NAG	C1-O5-C5	2.30	115.27	112.19

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	503	NAG	O5-C5-C6-O6
4	G	502	NAG	O5-C5-C6-O6
4	I	508	NAG	O5-C5-C6-O6
4	G	509	NAG	O5-C5-C6-O6
4	I	503	NAG	C4-C5-C6-O6
4	I	508	NAG	C4-C5-C6-O6
4	A	301	NAG	O5-C5-C6-O6
4	G	509	NAG	C4-C5-C6-O6
4	G	502	NAG	C4-C5-C6-O6
4	A	301	NAG	C4-C5-C6-O6
4	L	301	NAG	O5-C5-C6-O6
4	G	501	NAG	C8-C7-N2-C2
4	G	501	NAG	O7-C7-N2-C2
4	G	507	NAG	C8-C7-N2-C2
4	G	507	NAG	O7-C7-N2-C2
4	H	301	NAG	C8-C7-N2-C2
4	H	301	NAG	O7-C7-N2-C2
4	L	301	NAG	C8-C7-N2-C2
4	L	301	NAG	O7-C7-N2-C2
4	I	501	NAG	C8-C7-N2-C2
4	I	501	NAG	O7-C7-N2-C2
4	I	507	NAG	C8-C7-N2-C2
4	I	507	NAG	O7-C7-N2-C2
4	A	301	NAG	C8-C7-N2-C2
4	A	301	NAG	O7-C7-N2-C2
4	L	301	NAG	C4-C5-C6-O6
4	I	509	NAG	O5-C5-C6-O6
8	B	305	PEG	O1-C1-C2-O2
8	A	304	PEG	O2-C3-C4-O4
4	G	504	NAG	O5-C5-C6-O6
4	G	503	NAG	C4-C5-C6-O6
4	I	502	NAG	C4-C5-C6-O6
4	I	506	NAG	C4-C5-C6-O6
4	I	506	NAG	O5-C5-C6-O6
4	I	507	NAG	O5-C5-C6-O6
4	G	503	NAG	O5-C5-C6-O6
4	I	509	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	I	502	NAG	O5-C5-C6-O6
8	B	305	PEG	C4-C3-O2-C2
8	A	304	PEG	C4-C3-O2-C2
8	B	304	PEG	C1-C2-O2-C3
8	B	305	PEG	C1-C2-O2-C3
4	I	501	NAG	O5-C5-C6-O6
4	G	502	NAG	C1-C2-N2-C7
4	B	301	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	302	BU3	3	0
5	L	302	IPA	1	0
4	G	502	NAG	1	0
5	A	302	IPA	1	0
6	B	303	BU3	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

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	G	298/353 (84%)	1.25	55 (18%) 3 4	75, 131, 199, 255	0
1	I	292/353 (82%)	1.36	56 (19%) 3 3	74, 141, 210, 295	0
2	A	238/238 (100%)	0.53	14 (5%) 28 30	37, 63, 116, 165	0
2	H	238/238 (100%)	0.72	16 (6%) 24 26	41, 69, 120, 156	0
3	B	205/206 (99%)	0.47	12 (5%) 28 30	36, 62, 108, 175	0
3	L	205/206 (99%)	0.67	15 (7%) 21 23	44, 71, 146, 222	0
All	All	1476/1594 (92%)	0.88	168 (11%) 10 11	36, 85, 184, 295	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	58	ALA	6.2
1	I	217	TYR	5.5
1	G	382	PHE	5.1
1	G	112	TRP	4.9
1	I	299	PRO	4.7
1	G	380	GLY	4.5
1	I	112	TRP	4.3
1	G	397	GLY	4.3
1	I	326	ILE	4.2
1	I	423	ILE	4.2
1	I	383	PHE	4.2
1	I	288	LEU	4.1
1	I	221	ALA	4.0
3	L	33	VAL	3.8
1	I	255	VAL	3.7
1	G	255	VAL	3.7
1	G	51	THR	3.6
1	I	377	ASN	3.6
1	I	333	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	488	VAL	3.5
1	I	488	VAL	3.5
2	H	73	GLY	3.4
1	G	414	ILE	3.4
1	G	113	ASP	3.4
2	H	74	VAL	3.4
1	I	394	THR	3.4
3	L	1	GLN	3.4
2	A	102	LEU	3.4
1	G	217	TYR	3.3
1	I	441	GLY	3.3
2	A	65	GLY	3.3
1	I	483	LEU	3.3
1	G	333	ILE	3.2
1	I	396	ILE	3.2
2	H	8	GLY	3.2
1	G	233	PHE	3.2
1	I	93	PHE	3.2
1	G	277	LEU	3.2
3	L	7	PRO	3.2
2	A	105	ARG	3.1
1	G	416	LEU	3.1
1	G	384	TYR	3.0
1	I	277	LEU	3.0
1	G	454	LEU	3.0
2	H	150	VAL	3.0
1	I	100	MET	3.0
2	H	7	PRO	3.0
1	I	448	ASN	2.9
2	H	5	VAL	2.9
3	B	211	CYS	2.9
1	I	384	TYR	2.9
1	I	382	PHE	2.9
2	H	146	PHE	2.9
1	I	419	LYS	2.8
3	B	27	SER	2.8
1	G	395	CYS	2.8
1	G	483	LEU	2.8
1	G	101	VAL	2.8
1	I	71	THR	2.8
3	B	107	ARG	2.8
3	L	34	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	A	34	PHE	2.8
3	L	51	VAL	2.8
1	I	472	GLY	2.8
1	G	423	ILE	2.7
1	I	491	ILE	2.7
1	G	218	CYS	2.7
1	G	100	MET	2.7
1	G	266	ALA	2.7
1	I	471	GLY	2.7
2	A	216	CYS	2.7
1	I	342	LEU	2.7
3	L	18	SER	2.7
1	I	66	HIS	2.7
1	G	353	PHE	2.6
1	G	67	ASN	2.6
1	G	377	ASN	2.6
1	G	338	TRP	2.6
3	B	20	ASN	2.6
1	G	44	VAL	2.6
1	G	299	PRO	2.6
3	B	1	GLN	2.6
1	I	365	SER	2.6
1	I	98	ASN	2.6
1	I	44	VAL	2.6
1	G	221	ALA	2.5
1	I	409	GLY	2.5
2	H	75	PRO	2.5
2	A	35(A)	THR	2.5
2	A	112	SER	2.5
1	G	441	GLY	2.5
2	A	7	PRO	2.5
2	H	76	PRO	2.5
3	L	88	CYS	2.5
1	G	381	GLU	2.5
3	L	63	SER	2.5
3	B	19	ILE	2.5
1	G	236	THR	2.4
2	H	35(A)	THR	2.4
3	L	47	LEU	2.4
2	A	8	GLY	2.4
1	G	247	CYS	2.4
1	G	468	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
3	B	21	ILE	2.4
2	A	3	GLN	2.4
1	I	95	MET	2.4
1	I	253	PRO	2.4
1	G	215	ILE	2.4
3	B	62	PHE	2.4
1	I	56	SER	2.3
3	L	21	ILE	2.3
1	G	77	THR	2.3
2	H	82(C)	LEU	2.3
2	H	65	GLY	2.3
1	I	75	VAL	2.3
1	G	369	LEU	2.3
2	H	29	LEU	2.3
3	B	173	ALA	2.3
3	L	89	THR	2.3
3	B	2	SER	2.3
1	I	381	GLU	2.3
1	G	458	GLY	2.2
2	A	190	GLY	2.2
1	G	52	LEU	2.2
2	A	29	LEU	2.2
1	I	228	CYS	2.2
1	G	106	GLU	2.2
1	I	270	ILE	2.2
1	I	390	LEU	2.2
1	G	254	VAL	2.2
1	I	65	VAL	2.2
2	H	34	PHE	2.2
1	I	262	ASN	2.2
2	H	72	PRO	2.2
2	H	35	GLY	2.2
3	B	153	SER	2.2
1	I	45	TRP	2.2
1	G	226	LEU	2.2
1	G	234	ASN	2.2
1	G	392	ASN	2.2
1	I	68	VAL	2.2
1	I	461	ASN	2.2
1	I	366	GLY	2.2
3	L	2	SER	2.2
1	G	383	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	470	PRO	2.1
1	G	331	CYS	2.1
1	G	394	THR	2.1
3	L	71	ALA	2.1
1	I	284	ILE	2.1
1	I	338	TRP	2.1
1	G	50	THR	2.1
1	I	450	THR	2.1
3	L	3	ALA	2.1
1	I	294	ILE	2.1
1	G	66	HIS	2.1
1	G	245	VAL	2.1
1	I	210	PHE	2.1
3	L	107	ARG	2.1
1	I	447	SER	2.0
1	G	359	ILE	2.0
1	I	108	VAL	2.0
3	B	51	VAL	2.0
1	G	210	PHE	2.0
1	G	419	LYS	2.0
1	G	371	ILE	2.0
2	A	75	PRO	2.0
2	A	76	PRO	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 oligosaccharides 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	L	301	14/15	0.23	0.15	94,103,124,125	0
4	NAG	I	507	14/15	0.36	0.14	96,107,128,129	0
4	NAG	G	502	14/15	0.37	0.15	86,97,115,115	0
4	NAG	G	509	14/15	0.47	0.13	81,91,109,109	0
4	NAG	I	509	14/15	0.50	0.13	81,88,105,107	0
4	NAG	B	301	14/15	0.54	0.16	79,92,109,112	0
4	NAG	I	506	14/15	0.55	0.15	104,110,132,133	0
4	NAG	G	507	14/15	0.61	0.12	79,90,107,107	0
4	NAG	I	502	14/15	0.61	0.13	93,100,120,120	0
4	NAG	A	301	14/15	0.62	0.11	71,82,99,99	0
4	NAG	G	506	14/15	0.62	0.13	81,86,103,106	0
4	NAG	G	504	14/15	0.64	0.12	88,97,116,119	0
4	NAG	I	501	14/15	0.64	0.13	84,92,110,111	0
8	PEG	A	304	7/7	0.67	0.24	89,107,109,109	0
4	NAG	H	301	14/15	0.69	0.10	80,91,109,110	0
4	NAG	I	504	14/15	0.69	0.12	83,93,113,113	0
5	IPA	H	302	4/4	0.72	0.31	80,96,96,96	0
4	NAG	G	501	14/15	0.72	0.12	77,83,99,101	0
6	BU3	H	303	6/6	0.75	0.18	96,116,117,117	0
5	IPA	L	302	4/4	0.76	0.21	78,96,97,97	0
6	BU3	B	302	6/6	0.77	0.16	80,97,98,98	0
8	PEG	B	304	7/7	0.77	0.36	111,133,134,134	0
4	NAG	I	508	14/15	0.80	0.11	72,79,94,96	0
4	NAG	I	503	14/15	0.80	0.11	80,93,112,112	0
4	NAG	G	505	14/15	0.81	0.09	63,69,82,84	0
4	NAG	G	503	14/15	0.81	0.11	75,82,99,100	0
8	PEG	B	305	7/7	0.82	0.26	93,112,117,117	0
5	IPA	A	302	4/4	0.83	0.22	64,77,79,81	0
6	BU3	B	303	6/6	0.84	0.22	104,125,126,126	0
4	NAG	I	505	14/15	0.86	0.08	75,79,94,96	0
4	NAG	G	508	14/15	0.86	0.10	70,78,93,95	0
9	CL	B	306	1/1	0.86	0.16	106,106,106,106	0
6	BU3	A	303	6/6	0.90	0.21	105,126,127,127	0
7	NA	L	303	1/1	0.93	0.10	59,59,59,59	0

6.5 Other polymers

There are no such residues in this entry.