



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:29 PM UTC

PDB ID : 8CJV / pdb_00008cjb
Title : Structure of bovine CD46 ectodomain (SCR 1-4)
Authors : Aitkenhead, H.; Stuart, D.I.; El Omari, K.
Deposited on : 2023-02-13
Resolution : 2.84 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

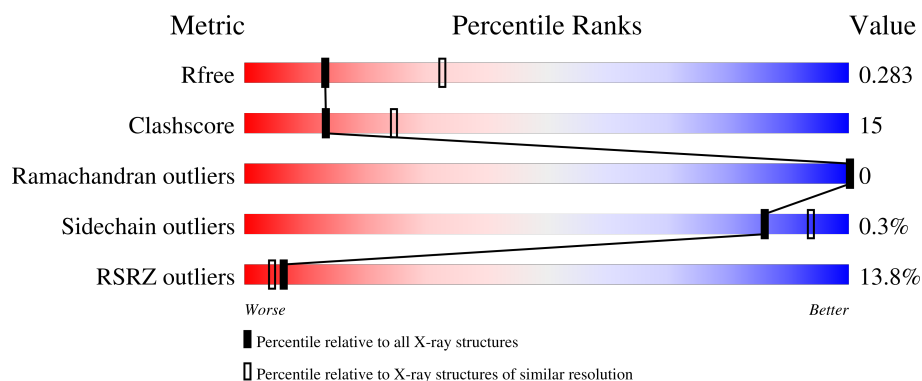
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	A	289	12% 64% 24% 12%
1	B	289	9% 47% 20% 33%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3504 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 Membrane cofactor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1950	1227	321	385	17			
1	B	194	Total	C	N	O	S	0	0	0
			1484	923	248	300	13			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	GLU	-	expression tag	UNP Q6VE48
A	41	THR	-	expression tag	UNP Q6VE48
A	42	GLY	-	expression tag	UNP Q6VE48
A	73	ARG	HIS	conflict	UNP Q6VE48
A	126	ALA	GLU	conflict	UNP Q6VE48
A	185	ASN	SER	conflict	UNP Q6VE48
A	296	GLY	-	expression tag	UNP Q6VE48
A	297	THR	-	expression tag	UNP Q6VE48
A	298	GLY	-	expression tag	UNP Q6VE48
A	299	GLY	-	expression tag	UNP Q6VE48
A	300	SER	-	expression tag	UNP Q6VE48
A	301	GLY	-	expression tag	UNP Q6VE48
A	302	GLY	-	expression tag	UNP Q6VE48
A	303	SER	-	expression tag	UNP Q6VE48
A	304	GLY	-	expression tag	UNP Q6VE48
A	305	LEU	-	expression tag	UNP Q6VE48
A	306	ASN	-	expression tag	UNP Q6VE48
A	307	ASP	-	expression tag	UNP Q6VE48
A	308	ILE	-	expression tag	UNP Q6VE48
A	309	PHE	-	expression tag	UNP Q6VE48
A	310	GLU	-	expression tag	UNP Q6VE48
A	311	ALA	-	expression tag	UNP Q6VE48
A	312	GLN	-	expression tag	UNP Q6VE48
A	313	LYS	-	expression tag	UNP Q6VE48
A	314	ILE	-	expression tag	UNP Q6VE48

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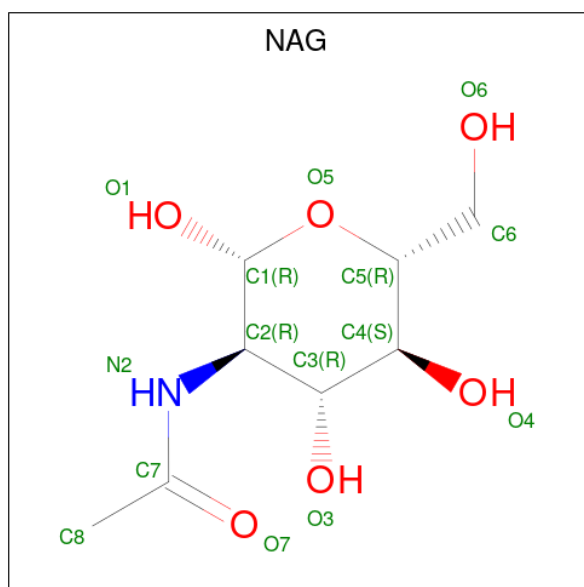
Chain	Residue	Modelled	Actual	Comment	Reference
A	315	GLU	-	expression tag	UNP Q6VE48
A	316	TRP	-	expression tag	UNP Q6VE48
A	317	HIS	-	expression tag	UNP Q6VE48
A	318	GLU	-	expression tag	UNP Q6VE48
A	319	GLY	-	expression tag	UNP Q6VE48
A	320	ARG	-	expression tag	UNP Q6VE48
A	321	THR	-	expression tag	UNP Q6VE48
A	322	LYS	-	expression tag	UNP Q6VE48
A	323	HIS	-	expression tag	UNP Q6VE48
A	324	HIS	-	expression tag	UNP Q6VE48
A	325	HIS	-	expression tag	UNP Q6VE48
A	326	HIS	-	expression tag	UNP Q6VE48
A	327	HIS	-	expression tag	UNP Q6VE48
A	328	HIS	-	expression tag	UNP Q6VE48
B	40	GLU	-	expression tag	UNP Q6VE48
B	41	THR	-	expression tag	UNP Q6VE48
B	42	GLY	-	expression tag	UNP Q6VE48
B	73	ARG	HIS	conflict	UNP Q6VE48
B	126	ALA	GLU	conflict	UNP Q6VE48
B	185	ASN	SER	conflict	UNP Q6VE48
B	296	GLY	-	expression tag	UNP Q6VE48
B	297	THR	-	expression tag	UNP Q6VE48
B	298	GLY	-	expression tag	UNP Q6VE48
B	299	GLY	-	expression tag	UNP Q6VE48
B	300	SER	-	expression tag	UNP Q6VE48
B	301	GLY	-	expression tag	UNP Q6VE48
B	302	GLY	-	expression tag	UNP Q6VE48
B	303	SER	-	expression tag	UNP Q6VE48
B	304	GLY	-	expression tag	UNP Q6VE48
B	305	LEU	-	expression tag	UNP Q6VE48
B	306	ASN	-	expression tag	UNP Q6VE48
B	307	ASP	-	expression tag	UNP Q6VE48
B	308	ILE	-	expression tag	UNP Q6VE48
B	309	PHE	-	expression tag	UNP Q6VE48
B	310	GLU	-	expression tag	UNP Q6VE48
B	311	ALA	-	expression tag	UNP Q6VE48
B	312	GLN	-	expression tag	UNP Q6VE48
B	313	LYS	-	expression tag	UNP Q6VE48
B	314	ILE	-	expression tag	UNP Q6VE48
B	315	GLU	-	expression tag	UNP Q6VE48
B	316	TRP	-	expression tag	UNP Q6VE48
B	317	HIS	-	expression tag	UNP Q6VE48

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Chain	Residue	Modelled	Actual	Comment	Reference
B	318	GLU	-	expression tag	UNP Q6VE48
B	319	GLY	-	expression tag	UNP Q6VE48
B	320	ARG	-	expression tag	UNP Q6VE48
B	321	THR	-	expression tag	UNP Q6VE48
B	322	LYS	-	expression tag	UNP Q6VE48
B	323	HIS	-	expression tag	UNP Q6VE48
B	324	HIS	-	expression tag	UNP Q6VE48
B	325	HIS	-	expression tag	UNP Q6VE48
B	326	HIS	-	expression tag	UNP Q6VE48
B	327	HIS	-	expression tag	UNP Q6VE48
B	328	HIS	-	expression tag	UNP Q6VE48

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



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

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.73Å 129.73Å 120.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.17 – 2.84 88.17 – 2.84	Depositor EDS
% Data completeness (in resolution range)	43.9 (88.17-2.84) 44.0 (88.17-2.84)	Depositor EDS
R_{merge}	0.49	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.253 , 0.285 0.249 , 0.283	Depositor DCC
R_{free} test set	529 reflections (2.14%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	3504	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.36% 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: NAG

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	0.71	0/2003	1.09	2/2735 (0.1%)
1	B	0.70	0/1523	1.09	1/2081 (0.0%)
All	All	0.71	0/3526	1.09	3/4816 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	LYS	CB-CG-CD	7.51	128.57	111.30
1	A	142	LEU	CA-CB-CG	-5.35	97.57	116.30
1	B	89	CYS	N-CA-C	-5.16	102.01	109.59

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	1950	0	1846	56	0
1	B	1484	0	1387	51	0
2	A	28	0	26	3	0
2	B	42	0	39	2	0
All	All	3504	0	3298	100	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (100) 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:B:169:ILE:HG23	1:B:222:ASN:HA	1.56	0.88
1:B:94:THR:HG21	2:B:402:NAG:H82	1.60	0.82
1:B:106:ARG:HG2	1:B:126:ALA:HA	1.63	0.79
1:B:42:GLY:HA2	1:B:64:PRO:HD3	1.69	0.74
1:A:50:VAL:HA	1:B:117:GLN:HE22	1.52	0.73
1:A:197:THR:HG22	1:A:216:LYS:HG2	1.71	0.72
1:A:242:ILE:HG13	1:A:263:LEU:HD23	1.71	0.72
1:A:106:ARG:HG2	1:A:126:ALA:HA	1.75	0.69
1:B:222:ASN:OD1	1:B:223:GLY:N	2.27	0.68
1:A:175:PRO:HG2	1:A:229:PRO:HG3	1.76	0.68
1:A:222:ASN:OD1	1:A:223:GLY:N	2.28	0.66
1:A:179:ASN:HB3	1:A:201:ASP:HB2	1.77	0.65
1:A:182:TYR:CE1	1:A:185:ASN:HA	2.32	0.65
1:B:112:ASP:OD1	1:B:118:VAL:HG12	1.98	0.64
1:B:203:SER:HB2	1:B:208:GLU:OE1	1.97	0.64
1:B:177:ILE:HD11	1:B:232:CYS:HB3	1.79	0.63
1:B:145:ASN:ND2	2:B:403:NAG:O7	2.33	0.61
1:A:112:ASP:OD1	1:A:118:VAL:HG12	2.00	0.61
1:B:177:ILE:HD13	1:B:232:CYS:H	1.65	0.60
1:B:190:PHE:HB3	1:B:194:GLU:HB2	1.83	0.60
1:A:169:ILE:HG23	1:A:222:ASN:HA	1.84	0.59
1:B:182:TYR:HB2	1:B:196:VAL:CG1	2.33	0.59
1:A:176:GLU:HG3	1:A:182:TYR:CD2	2.38	0.58
1:A:176:GLU:HG3	1:A:182:TYR:CE2	2.37	0.58
1:B:170:LEU:HB3	1:B:189:VAL:HG11	1.86	0.58
1:A:168:LYS:NZ	1:A:191:GLU:HG2	2.20	0.57
1:A:150:GLU:OE2	1:B:106:ARG:HD3	2.05	0.57
1:B:55:GLN:HA	1:B:71:GLU:HG2	1.88	0.56
1:A:251:PHE:N	1:A:255:TYR:OH	2.36	0.55
1:B:221:GLY:HA3	1:B:224:GLU:HB2	1.89	0.55
1:B:176:GLU:HG3	1:B:182:TYR:CD2	2.42	0.54
1:B:195:VAL:HG22	1:B:218:THR:HG22	1.89	0.54
1:A:144:THR:HG21	1:B:103:LYS:NZ	2.22	0.54
1:B:200:CYS:SG	1:B:211:LEU:HD12	2.48	0.53
1:A:207:ASP:HB3	1:A:254:LYS:NZ	2.24	0.53
1:A:146:ILE:HD11	2:A:402:NAG:H82	1.91	0.52
1:A:51:SER:HB2	1:A:102:CYS:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:SER:N	1:B:100:GLU:OE2	2.39	0.52
1:A:190:PHE:HB3	1:A:194:GLU:HB2	1.92	0.52
1:A:261:VAL:HG12	1:A:263:LEU:CD1	2.39	0.52
1:B:177:ILE:CD1	1:B:232:CYS:H	2.23	0.52
1:B:183:THR:HG1	1:B:197:THR:HG1	1.54	0.52
1:A:182:TYR:HB2	1:A:196:VAL:HG11	1.93	0.51
1:A:49:PHE:CG	1:A:52:MET:HE3	2.45	0.51
1:B:182:TYR:HB2	1:B:196:VAL:HG11	1.93	0.51
1:A:168:LYS:HE2	1:A:191:GLU:HG2	1.93	0.50
1:A:50:VAL:CA	1:B:117:GLN:HE22	2.23	0.50
1:A:45:ASP:HA	1:A:46:PRO:HD3	1.68	0.49
1:A:182:TYR:HB2	1:A:196:VAL:CG1	2.43	0.48
1:A:249:SER:O	1:A:261:VAL:HG13	2.13	0.48
1:A:177:ILE:HD11	1:A:232:CYS:HB3	1.96	0.48
1:B:190:PHE:HB3	1:B:194:GLU:CB	2.44	0.47
1:A:127:PHE:CE1	1:A:151:VAL:HG23	2.49	0.47
1:A:168:LYS:HG2	1:A:170:LEU:CD1	2.44	0.47
1:B:131:VAL:HG22	1:B:147:SER:O	2.13	0.47
1:A:272:TYR:CG	1:A:293:ILE:HD12	2.49	0.47
1:A:242:ILE:CG1	1:A:263:LEU:HD23	2.43	0.47
1:A:50:VAL:HG13	1:B:117:GLN:NE2	2.29	0.47
1:B:191:GLU:H	1:B:194:GLU:HG3	1.80	0.47
1:B:80:THR:HB	1:B:83:GLN:HB2	1.97	0.46
1:A:168:LYS:CE	1:A:191:GLU:HG2	2.46	0.46
1:B:141:LEU:CD2	1:B:145:ASN:HB3	2.45	0.46
1:B:177:ILE:HD12	1:B:178:GLN:O	2.14	0.46
1:A:228:GLN:HG3	1:A:229:PRO:HD2	1.97	0.46
1:A:236:LYS:HE2	1:A:254:LYS:HD3	1.97	0.46
1:A:182:TYR:HB3	1:A:198:TYR:CZ	2.51	0.46
1:B:74:LEU:HA	1:B:74:LEU:HD23	1.55	0.46
1:A:207:ASP:HB3	1:A:254:LYS:HZ3	1.80	0.45
1:A:79:VAL:HG12	1:A:80:THR:HG23	1.98	0.45
1:A:242:ILE:HG22	1:A:243:GLU:O	2.17	0.45
1:B:182:TYR:CE1	1:B:185:ASN:HA	2.51	0.45
1:A:262:VAL:C	1:A:263:LEU:HD12	2.43	0.44
1:B:151:VAL:O	1:B:151:VAL:HG12	2.17	0.44
2:A:401:NAG:H83	1:B:110:LEU:O	2.17	0.44
1:A:261:VAL:HG12	1:A:263:LEU:HD11	1.98	0.44
1:A:195:VAL:HG22	1:A:218:THR:CG2	2.48	0.43
1:A:74:LEU:HA	1:A:74:LEU:HD23	1.59	0.43
1:A:200:CYS:SG	1:A:211:LEU:HD12	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:VAL:HG22	1:A:157:VAL:HG12	2.00	0.42
1:B:107:CYS:SG	1:B:157:VAL:HB	2.58	0.42
1:A:49:PHE:CD1	1:A:52:MET:HE3	2.55	0.42
1:B:110:LEU:HD23	1:B:110:LEU:HA	1.30	0.42
1:B:176:GLU:HG3	1:B:182:TYR:HD2	1.84	0.42
1:A:144:THR:CG2	1:B:103:LYS:NZ	2.82	0.42
1:A:44:ASP:HA	1:A:61:SER:HA	2.01	0.42
1:A:87:LEU:HA	1:A:87:LEU:HD23	1.75	0.42
1:A:274:ASN:OD1	1:A:287:PRO:HG2	2.20	0.42
1:B:177:ILE:HG12	1:B:230:PRO:O	2.20	0.42
1:B:168:LYS:HE2	1:B:191:GLU:HG2	2.02	0.42
1:B:51:SER:HB2	1:B:102:CYS:HB2	2.02	0.41
1:B:168:LYS:HE2	1:B:191:GLU:CG	2.50	0.41
1:B:107:CYS:HB3	1:B:159:TRP:CE2	2.56	0.41
1:A:127:PHE:HA	1:A:149:CYS:SG	2.60	0.41
1:A:195:VAL:HG22	1:A:218:THR:HG22	2.01	0.41
1:A:144:THR:HG21	1:B:103:LYS:HZ2	1.86	0.41
2:A:401:NAG:H3	1:B:109:THR:OG1	2.20	0.41
1:B:183:THR:OG1	1:B:197:THR:OG1	2.27	0.40
1:A:76:PHE:CD1	1:A:76:PHE:N	2.88	0.40
1:B:198:TYR:CE1	1:B:217:LEU:HD21	2.56	0.40
1:B:90:GLN:NE2	1:B:96:SER:HA	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	252/289 (87%)	242 (96%)	10 (4%)	0	100	100
1	B	192/289 (66%)	182 (95%)	10 (5%)	0	100	100
All	All	444/578 (77%)	424 (96%)	20 (4%)	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	225/251 (90%)	224 (100%)	1 (0%)	84	92
1	B	173/251 (69%)	173 (100%)	0	100	100
All	All	398/502 (79%)	397 (100%)	1 (0%)	86	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	HIS
1	B	90	GLN
1	B	117	GLN
1	B	132	HIS

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

5 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$
2	NAG	A	402	1	14,14,15	0.24	0	17,19,21	0.55	0
2	NAG	B	401	1	14,14,15	0.46	0	17,19,21	0.68	1 (5%)
2	NAG	B	402	1	14,14,15	0.53	0	17,19,21	0.39	0
2	NAG	A	401	1	14,14,15	0.40	0	17,19,21	0.97	1 (5%)
2	NAG	B	403	1	14,14,15	0.41	0	17,19,21	0.62	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
2	NAG	A	402	1	-	0/6/23/26	0/1/1/1
2	NAG	B	401	1	-	2/6/23/26	0/1/1/1
2	NAG	B	402	1	-	2/6/23/26	0/1/1/1
2	NAG	A	401	1	-	0/6/23/26	0/1/1/1
2	NAG	B	403	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	401	NAG	O4-C4-C5	-3.00	101.94	109.32
2	B	401	NAG	C1-O5-C5	2.26	115.21	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	403	NAG	C3-C2-N2-C7
2	B	402	NAG	C4-C5-C6-O6
2	B	402	NAG	O5-C5-C6-O6
2	B	401	NAG	O5-C5-C6-O6
2	B	401	NAG	C4-C5-C6-O6
2	B	403	NAG	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	NAG	1	0
2	B	402	NAG	1	0
2	A	401	NAG	2	0
2	B	403	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

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	254/289 (87%)	0.83	35 (13%) 6 4	15, 86, 144, 186	0
1	B	194/289 (67%)	0.70	27 (13%) 6 4	17, 87, 196, 243	0
All	All	448/578 (77%)	0.78	62 (13%) 6 4	15, 87, 171, 243	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	ARG	4.6
1	A	152	SER	4.0
1	A	294	LYS	4.0
1	B	206	PRO	3.9
1	A	170	LEU	3.6
1	A	291	LYS	3.6
1	B	202	PRO	3.5
1	A	228	GLN	3.5
1	B	156	GLY	3.5
1	A	60	PRO	3.5
1	B	153	SER	3.5
1	A	264	LYS	3.4
1	A	46	PRO	3.4
1	A	65	GLY	3.3
1	B	48	ARG	3.1
1	B	154	GLY	3.1
1	A	156	GLY	3.1
1	A	243	GLU	3.1
1	B	87	LEU	3.1
1	B	41	THR	3.1
1	A	154	GLY	3.1
1	A	222	ASN	3.0
1	A	247	ILE	2.9
1	B	46	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	175	PRO	2.7
1	B	234	VAL	2.7
1	B	201	ASP	2.7
1	B	205	GLY	2.6
1	A	158	ASN	2.6
1	B	203	SER	2.6
1	A	172	GLN	2.6
1	A	91	ASP	2.5
1	B	195	VAL	2.5
1	A	70	TYR	2.5
1	A	236	LYS	2.5
1	A	274	ASN	2.5
1	A	238	VAL	2.5
1	A	214	GLU	2.4
1	A	212	VAL	2.4
1	A	239	TYR	2.4
1	B	204	ASN	2.4
1	A	227	SER	2.4
1	B	210	SER	2.4
1	A	186	HIS	2.3
1	A	202	PRO	2.3
1	B	233	LYS	2.3
1	B	212	VAL	2.3
1	A	41	THR	2.3
1	B	174	PRO	2.2
1	B	141	LEU	2.2
1	B	188	ASP	2.2
1	B	158	ASN	2.1
1	B	170	LEU	2.1
1	A	281	GLU	2.1
1	A	67	GLN	2.1
1	B	229	PRO	2.1
1	A	211	LEU	2.1
1	A	267	GLU	2.1
1	B	187	LYS	2.0
1	A	263	LEU	2.0
1	B	60	PRO	2.0
1	A	293	ILE	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 [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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	402	14/15	0.71	0.12	96,109,113,113	0
2	NAG	A	402	14/15	0.89	0.09	40,44,56,56	0
2	NAG	B	403	14/15	0.91	0.09	49,52,56,58	0
2	NAG	B	401	14/15	0.94	0.09	18,19,22,23	0
2	NAG	A	401	14/15	0.96	0.08	19,21,24,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.