



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:27 AM UTC

PDB ID : 7CEB / pdb_00007ceb
Title : Crystal structure of alpha6beta1 integrin headpiece
Authors : Arimori, T.; Takagi, J.
Deposited on : 2020-06-22
Resolution : 2.89 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

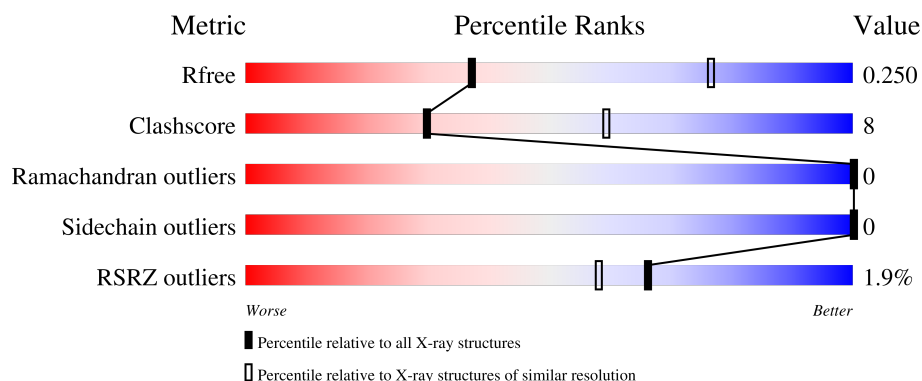
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	627	3% 67% 22% 12%
2	B	454	71% 12% 18%
3	C	172	% 67% 19% 15%
4	D	164	2% 73% 16% 11%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9632 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 Integrin alpha-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4308	2710	754	826	18			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	619	GLY	-	expression tag	UNP P23229
A	620	SER	-	expression tag	UNP P23229
A	621	LEU	-	expression tag	UNP P23229
A	622	GLU	-	expression tag	UNP P23229
A	623	ASN	-	expression tag	UNP P23229
A	624	LEU	-	expression tag	UNP P23229
A	625	TYR	-	expression tag	UNP P23229
A	626	PHE	-	expression tag	UNP P23229
A	627	GLN	-	expression tag	UNP P23229

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	374	Total	C	N	O	S	0	0	0
			2931	1846	492	577	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	446	GLY	-	expression tag	UNP P05556
B	447	GLY	-	expression tag	UNP P05556
B	448	LEU	-	expression tag	UNP P05556
B	449	GLU	-	expression tag	UNP P05556
B	450	ASN	-	expression tag	UNP P05556
B	451	LEU	-	expression tag	UNP P05556
B	452	TYR	-	expression tag	UNP P05556

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Chain	Residue	Modelled	Actual	Comment	Reference
B	453	PHE	-	expression tag	UNP P05556
B	454	GLN	-	expression tag	UNP P05556

- Molecule 3 is a protein called TS2/16 VH(S112C)-SARAH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	147	Total	C	N	O	S	0	0	0
			1155	725	191	230	9			

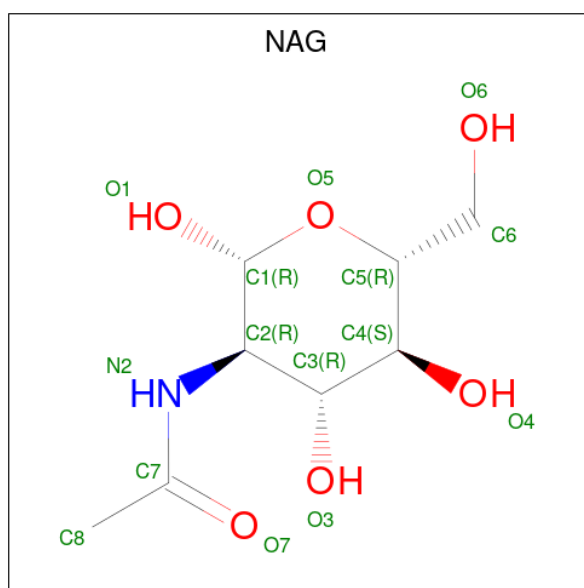
- Molecule 4 is a protein called TS2/16 VL-SARAH(S37C).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	146	Total	C	N	O	S	0	0	0
			1146	727	188	224	7			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Ca	0	0
			3	3		
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Mg 1 1	0	0

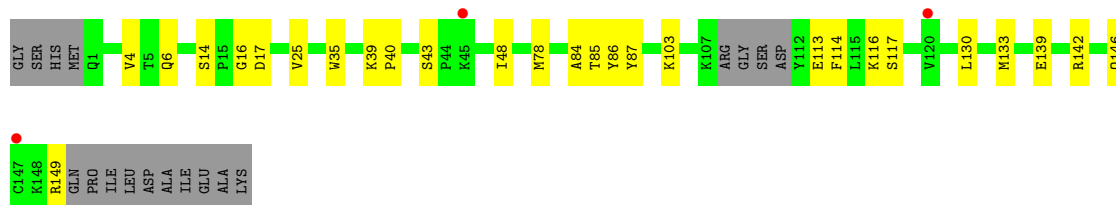
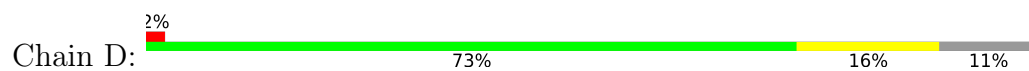
- Molecule 8 is water.

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

• Molecule 3: TS2/16 VH(S112C)-SARAH



• Molecule 4: TS2/16 VL-SARAH(S37C)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	116.52Å 251.31Å 63.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.57 – 2.89 44.57 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.57-2.89) 99.6 (44.57-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.207 , 0.249 0.207 , 0.250	Depositor DCC
R_{free} test set	2041 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	72.2	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9632	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: CA, NAG, MG

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	0.19	0/4400	0.46	0/5956
2	B	0.13	0/2982	0.37	0/4027
3	C	0.15	0/1178	0.39	0/1587
4	D	0.28	0/1169	0.53	2/1581 (0.1%)
All	All	0.18	0/9729	0.44	2/13151 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	16	GLY	CA-C-N	-5.52	113.98	122.87
4	D	16	GLY	C-N-CA	-5.52	113.98	122.87

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	4308	0	4186	96	0
2	B	2931	0	2902	32	0
3	C	1155	0	1119	21	0
4	D	1146	0	1142	16	0
5	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	28	0	26	1	0
6	B	56	0	52	0	0
7	B	1	0	0	0	0
8	A	2	0	0	0	0
8	B	1	0	0	0	0
All	All	9632	0	9427	162	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 8.

All (162) 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:A:566:GLN:O	1:A:567:GLU:HG3	1.72	0.88
1:A:567:GLU:HB3	1:A:568:PRO:HD2	1.58	0.85
1:A:140:ILE:HG23	1:A:146:GLY:HA3	1.61	0.83
3:C:87:THR:HG23	3:C:110:THR:HA	1.60	0.82
1:A:120:THR:HG22	1:A:122:GLN:H	1.45	0.82
1:A:461:ARG:O	1:A:461:ARG:NH2	2.17	0.78
1:A:461:ARG:HG2	1:A:461:ARG:HH21	1.49	0.77
1:A:502:GLU:OE2	1:A:513:ARG:N	2.16	0.77
1:A:86:SER:HB3	1:A:113:GLU:HG3	1.69	0.73
1:A:79:ASP:OD2	1:A:80:ALA:N	2.24	0.71
4:D:146:GLN:HA	4:D:149:ARG:HG3	1.73	0.71
3:C:163:ALA:HB3	4:D:116:LYS:HD3	1.72	0.70
1:A:495:ILE:HD13	1:A:531:LEU:HD11	1.74	0.69
2:B:155:ARG:HD2	2:B:155:ARG:H	1.59	0.66
1:A:150:SER:HA	1:A:167:GLN:HE22	1.61	0.66
1:A:135:SER:OG	1:A:137:ASN:O	2.13	0.66
1:A:245:ILE:HD13	1:A:308:GLN:HB2	1.76	0.65
1:A:454:THR:CG2	1:A:455:PRO:HD3	2.27	0.65
1:A:243:LYS:HD3	1:A:249:ASP:HA	1.79	0.65
1:A:358:VAL:HG12	1:A:374:VAL:HG22	1.79	0.65
1:A:475:GLN:HE21	1:A:541:GLU:HG2	1.62	0.64
3:C:83:LYS:HD2	3:C:84:SER:H	1.64	0.63
1:A:461:ARG:NH2	1:A:461:ARG:HG2	2.12	0.62
1:A:453:VAL:HG11	1:A:596:VAL:HG12	1.81	0.62
1:A:195:ARG:NH1	1:A:215:GLU:OE2	2.32	0.62
1:A:481:GLU:OE1	1:A:537:LYS:HG3	2.01	0.61
1:A:514:VAL:HB	1:A:544:LEU:HG	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:GLU:HG2	1:A:537:LYS:HG3	1.83	0.60
1:A:503:LYS:HG3	1:A:504:GLU:N	2.16	0.60
2:B:414:LYS:HB2	2:B:416:PRO:HG3	1.83	0.60
3:C:47:TRP:NE1	3:C:50:THR:OG1	2.29	0.59
2:B:94:ILE:HD11	2:B:113:LEU:HD13	1.84	0.59
2:B:410:ILE:HD11	2:B:438:LEU:HD21	1.84	0.59
2:B:104:ARG:HB2	2:B:441:ILE:HD11	1.86	0.58
4:D:6:GLN:NE2	4:D:86:TYR:O	2.37	0.58
1:A:302:LEU:HB2	1:A:332:MET:HE1	1.86	0.57
1:A:29:TRP:HB3	1:A:101:PRO:HA	1.85	0.57
1:A:454:THR:HG22	1:A:455:PRO:HD3	1.87	0.57
4:D:39:LYS:HD3	4:D:84:ALA:HB2	1.87	0.57
1:A:110:HIS:O	1:A:166:GLN:HG2	2.04	0.57
3:C:35:SER:HB3	3:C:50:THR:HG23	1.86	0.56
1:A:433:SER:O	1:A:433:SER:OG	2.23	0.56
4:D:139:GLU:HA	4:D:142:ARG:HG3	1.86	0.56
3:C:144:GLU:HG3	3:C:148:GLN:HE21	1.70	0.56
1:A:156:LEU:HD12	1:A:156:LEU:H	1.72	0.55
1:A:25:LEU:HD13	1:A:39:LEU:HD11	1.89	0.55
1:A:460:LEU:HD11	1:A:598:PHE:HD2	1.72	0.55
1:A:461:ARG:HH21	1:A:461:ARG:CG	2.16	0.54
1:A:307:TRP:CE2	1:A:335:GLN:HA	2.43	0.54
2:B:154:ARG:HB2	2:B:155:ARG:NH1	2.23	0.54
3:C:82:MET:HE1	3:C:109:VAL:HG21	1.90	0.53
4:D:14:SER:O	4:D:17:ASP:HB2	2.08	0.53
1:A:2:ASN:ND2	1:A:364:ILE:O	2.40	0.53
3:C:144:GLU:HG3	3:C:148:GLN:NE2	2.23	0.53
3:C:67:PHE:HB3	3:C:80:LEU:HD11	1.91	0.53
4:D:85:THR:HG22	4:D:103:LYS:HG3	1.91	0.53
1:A:315:PRO:HG3	1:A:356:ILE:HA	1.90	0.52
4:D:113:GLU:H	4:D:113:GLU:CD	2.18	0.52
1:A:247:SER:HB3	1:A:250:GLU:HB3	1.90	0.52
4:D:40:PRO:HB2	4:D:133:MET:HG2	1.90	0.52
1:A:460:LEU:HD11	1:A:598:PHE:CD2	2.45	0.52
1:A:4:ASP:OD2	1:A:9:ASN:ND2	2.43	0.51
2:B:390:GLU:OE2	2:B:393:ARG:NH1	2.43	0.51
1:A:130:ARG:HH21	1:A:148:ASP:CG	2.19	0.51
1:A:481:GLU:HG2	1:A:537:LYS:CG	2.41	0.51
2:B:93:GLN:HB2	2:B:432:GLU:OE2	2.10	0.51
1:A:92:MET:HE3	1:A:93:GLY:N	2.26	0.50
1:A:25:LEU:HD12	1:A:414:ALA:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:THR:HG23	1:A:455:PRO:HD3	1.94	0.50
1:A:460:LEU:HA	1:A:472:ILE:CD1	2.41	0.50
2:B:194:THR:O	2:B:222:SER:HB2	2.11	0.50
6:A:1005:NAG:H82	6:A:1005:NAG:O3	2.12	0.49
2:B:73:LYS:HD3	2:B:74:ASN:O	2.12	0.49
1:A:275:SER:OG	1:A:276:ALA:N	2.46	0.48
1:A:287:GLU:OE2	1:A:329:TYR:OH	2.23	0.48
2:B:312:GLN:HG2	2:B:334:LYS:HD2	1.95	0.48
1:A:38:LEU:HD22	1:A:62:SER:OG	2.13	0.48
1:A:166:GLN:NE2	2:B:270:LEU:O	2.46	0.48
1:A:292:SER:HB2	1:A:315:PRO:HD2	1.95	0.48
1:A:458:ILE:HD11	1:A:474:LEU:HD11	1.96	0.48
4:D:130:LEU:O	4:D:133:MET:HB2	2.14	0.48
1:A:470:SER:OG	1:A:471:GLY:N	2.47	0.48
3:C:51:ILE:HG13	3:C:57:THR:HG22	1.94	0.48
1:A:97:GLN:HG3	1:A:171:ALA:O	2.14	0.48
1:A:265:ALA:HA	1:A:285:ASP:HA	1.96	0.48
2:B:103:LEU:O	2:B:441:ILE:HG12	2.13	0.48
4:D:114:PHE:O	4:D:117:SER:HB3	2.14	0.48
2:B:125:LEU:HD13	2:B:149:LEU:HD21	1.95	0.47
2:B:151:ASN:O	2:B:155:ARG:NH1	2.48	0.47
1:A:53:ARG:HE	1:A:53:ARG:HB2	1.49	0.47
1:A:92:MET:HG2	1:A:109:ALA:HB2	1.96	0.47
1:A:139:ARG:CZ	1:A:139:ARG:HB3	2.43	0.47
2:B:154:ARG:HB2	2:B:155:ARG:HH11	1.77	0.47
1:A:453:VAL:HG11	1:A:596:VAL:CG1	2.45	0.46
2:B:164:PHE:HB2	2:B:212:PHE:CE2	2.50	0.46
1:A:253:PHE:HB2	1:A:269:LEU:HB2	1.97	0.46
1:A:442:ARG:HH11	1:A:583:ILE:HD12	1.81	0.46
1:A:502:GLU:OE1	1:A:513:ARG:NE	2.41	0.46
1:A:476:VAL:HG21	1:A:559:ILE:HG21	1.97	0.46
1:A:353:MET:HB2	1:A:377:PRO:HD2	1.98	0.46
4:D:35:TRP:HB2	4:D:48:ILE:HB	1.97	0.46
2:B:206:THR:OG1	2:B:208:LYS:HE3	2.16	0.46
1:A:297:VAL:HG12	1:A:312:ILE:HG12	1.98	0.46
2:B:99:LEU:HD11	2:B:436:VAL:HG22	1.98	0.46
1:A:500:GLU:HG2	1:A:524:LYS:HA	1.98	0.45
1:A:52:GLN:HA	1:A:80:ALA:HB2	1.99	0.45
2:B:340:LEU:HD22	2:B:344:SER:HA	1.99	0.45
1:A:142:ASP:HB2	1:A:145:ASP:CB	2.47	0.45
1:A:150:SER:HA	1:A:167:GLN:NE2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:MET:HB3	3:C:78:LEU:HD22	1.98	0.45
2:B:98:GLN:HA	2:B:435:GLU:O	2.17	0.45
3:C:11:LEU:HD13	3:C:110:THR:HB	1.98	0.45
1:A:514:VAL:HG12	1:A:546:LEU:HD12	1.99	0.45
2:B:248:ARG:HB2	2:B:250:VAL:HG22	1.99	0.45
1:A:106:VAL:HG12	1:A:173:PHE:CE2	2.52	0.44
1:A:115:ARG:HE	1:A:125:ARG:HG2	1.81	0.44
1:A:195:ARG:NE	1:A:197:GLU:OE1	2.44	0.44
1:A:302:LEU:HD13	1:A:394:ILE:HB	1.99	0.44
2:B:303:VAL:O	2:B:307:SER:OG	2.36	0.44
3:C:12:VAL:HG13	3:C:111:VAL:HG13	2.00	0.44
3:C:144:GLU:O	3:C:148:GLN:HG3	2.17	0.44
1:A:31:LEU:HA	1:A:31:LEU:HD23	1.57	0.44
2:B:94:ILE:HA	2:B:114:LYS:O	2.18	0.44
1:A:323:GLU:O	1:A:323:GLU:HG3	2.17	0.44
2:B:173:MET:HG2	2:B:176:ILE:O	2.18	0.43
1:A:142:ASP:HB2	1:A:145:ASP:HB3	1.99	0.43
1:A:117:HIS:O	1:A:120:THR:HB	2.18	0.43
1:A:196:VAL:HG23	1:A:278:LEU:HD11	1.99	0.43
3:C:29:PHE:O	3:C:71:ARG:NH2	2.52	0.43
3:C:52:SER:O	3:C:71:ARG:NH1	2.48	0.43
1:A:379:ASP:CG	1:A:383:LYS:HD2	2.44	0.43
1:A:27:MET:HE3	1:A:415:GLY:HA2	2.01	0.43
1:A:74:ILE:HG12	1:A:138:LEU:HD23	2.01	0.43
1:A:303:ASN:HA	1:A:390:SER:O	2.18	0.43
1:A:481:GLU:CG	1:A:537:LYS:HG3	2.47	0.43
1:A:529:LEU:HD23	1:A:538:VAL:HG12	2.00	0.43
3:C:45:LEU:HD23	3:C:45:LEU:HA	1.84	0.43
2:B:103:LEU:HD23	2:B:109:GLN:HG2	2.01	0.42
3:C:91:TYR:CE1	4:D:43:SER:HB3	2.54	0.42
3:C:149:LYS:O	3:C:153:LYS:HG3	2.18	0.42
2:B:146:GLY:O	2:B:150:MET:HG3	2.20	0.42
1:A:548:ASP:N	1:A:548:ASP:OD1	2.52	0.42
3:C:66:ARG:HB3	3:C:82(A):GLY:O	2.20	0.42
3:C:97:TYR:HB3	3:C:99:GLU:HG2	2.01	0.42
1:A:149:TRP:CD1	1:A:149:TRP:N	2.88	0.42
1:A:130:ARG:NE	1:A:148:ASP:OD2	2.53	0.42
1:A:169:VAL:HG11	1:A:185:PRO:HG2	2.02	0.41
1:A:181:VAL:HG12	1:A:239:LEU:HD13	2.01	0.41
4:D:4:VAL:HG22	4:D:25:VAL:HG12	2.02	0.41
2:B:67:LYS:HG2	2:B:68:ASP:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:GLN:HB3	1:A:529:LEU:CD1	2.51	0.41
1:A:166:GLN:OE1	2:B:174:PRO:HG3	2.21	0.41
2:B:194:THR:HG22	2:B:221:ILE:O	2.21	0.41
1:A:175:LYS:HD3	1:A:175:LYS:HA	1.87	0.41
4:D:6:GLN:HE22	4:D:87:TYR:HA	1.86	0.41
4:D:17:ASP:O	4:D:78:MET:HB2	2.21	0.41
1:A:397:LYS:HD3	1:A:397:LYS:HA	1.75	0.41
2:B:257:SER:HA	2:B:316:ALA:O	2.21	0.40
1:A:127:ILE:HG12	1:A:166:GLN:HG3	2.03	0.40
1:A:495:ILE:HB	1:A:563:VAL:HG23	2.02	0.40
2:B:317:VAL:HG11	2:B:325:TYR:CD2	2.56	0.40
1:A:106:VAL:HA	1:A:132:TYR:O	2.21	0.40

There are no symmetry-related clashes.

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	539/627 (86%)	515 (96%)	24 (4%)	0	100	100
2	B	370/454 (82%)	353 (95%)	17 (5%)	0	100	100
3	C	143/172 (83%)	140 (98%)	3 (2%)	0	100	100
4	D	142/164 (87%)	137 (96%)	5 (4%)	0	100	100
All	All	1194/1417 (84%)	1145 (96%)	49 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	467/535 (87%)	467 (100%)	0	100	100
2	B	336/402 (84%)	336 (100%)	0	100	100
3	C	126/149 (85%)	126 (100%)	0	100	100
4	D	130/144 (90%)	130 (100%)	0	100	100
All	All	1059/1230 (86%)	1059 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	78	ASN
1	A	122	GLN
1	A	167	GLN
1	A	366	GLN
1	A	448	GLN
3	C	151	GLN
4	D	124	GLN
4	D	136	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	$\# Z > 2$
6	NAG	B	1003	2	14,14,15	0.83	1 (7%)	17,19,21	0.70	0
6	NAG	A	1004	1	14,14,15	0.84	1 (7%)	17,19,21	0.67	0
6	NAG	B	1005	2	14,14,15	0.64	1 (7%)	17,19,21	0.98	1 (5%)
6	NAG	B	1006	2	14,14,15	0.26	0	17,19,21	0.50	0
6	NAG	A	1005	1	14,14,15	1.22	2 (14%)	17,19,21	1.04	1 (5%)
6	NAG	B	1004	2	14,14,15	0.39	0	17,19,21	0.59	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
6	NAG	B	1003	2	-	1/6/23/26	0/1/1/1
6	NAG	A	1004	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1005	2	-	3/6/23/26	0/1/1/1
6	NAG	B	1006	2	-	2/6/23/26	0/1/1/1
6	NAG	A	1005	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1004	2	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1005	NAG	C1-C2	3.13	1.56	1.52
6	A	1004	NAG	O5-C1	-3.05	1.38	1.43
6	A	1005	NAG	O5-C1	-2.80	1.39	1.43
6	B	1003	NAG	C1-C2	2.66	1.56	1.52
6	B	1005	NAG	O5-C1	2.11	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1005	NAG	C1-O5-C5	3.31	116.62	112.19
6	A	1005	NAG	C2-N2-C7	2.30	125.98	122.90

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1004	NAG	O5-C5-C6-O6
6	A	1004	NAG	C4-C5-C6-O6
6	B	1006	NAG	O5-C5-C6-O6
6	A	1005	NAG	C8-C7-N2-C2
6	A	1005	NAG	O7-C7-N2-C2
6	B	1005	NAG	C8-C7-N2-C2
6	B	1005	NAG	O7-C7-N2-C2
6	B	1003	NAG	O5-C5-C6-O6
6	B	1005	NAG	O5-C5-C6-O6
6	B	1006	NAG	C4-C5-C6-O6
6	B	1004	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1005	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	553/627 (88%)	0.12	16 (2%) 53 45	39, 75, 124, 158	0
2	B	374/454 (82%)	-0.08	2 (0%) 87 83	39, 70, 119, 169	0
3	C	147/172 (85%)	0.00	2 (1%) 73 65	48, 78, 128, 157	0
4	D	146/164 (89%)	0.05	3 (2%) 63 54	38, 69, 132, 163	0
All	All	1220/1417 (86%)	0.04	23 (1%) 66 58	38, 73, 126, 169	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	597	HIS	4.2
2	B	86	LEU	3.9
2	B	442	CYS	3.7
1	A	568	PRO	3.6
1	A	321	ASP	3.3
1	A	599	LEU	3.1
1	A	549	ASN	2.7
4	D	120	VAL	2.7
1	A	147	GLY	2.5
1	A	144	MET	2.4
1	A	292	SER	2.4
1	A	481	GLU	2.4
3	C	105	GLN	2.4
1	A	454	THR	2.4
1	A	228	PRO	2.3
1	A	148	ASP	2.3
4	D	45	LYS	2.3
1	A	63	CYS	2.2
1	A	473	CYS	2.1
4	D	147	CYS	2.1
1	A	53	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	61	ASP	2.0
1	A	581	LEU	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	B	1005	14/15	0.46	0.15	116,124,129,135	0
6	NAG	A	1004	14/15	0.61	0.15	88,102,116,117	0
6	NAG	B	1006	14/15	0.72	0.12	90,105,113,114	0
6	NAG	B	1003	14/15	0.73	0.15	87,103,113,113	0
6	NAG	A	1005	14/15	0.83	0.11	50,76,92,97	0
6	NAG	B	1004	14/15	0.85	0.10	58,72,83,87	0
7	MG	B	1002	1/1	0.86	0.09	83,83,83,83	1
5	CA	B	1001	1/1	0.95	0.09	104,104,104,104	1
5	CA	A	1002	1/1	0.98	0.05	78,78,78,78	0
5	CA	A	1001	1/1	0.99	0.08	78,78,78,78	0
5	CA	A	1003	1/1	0.99	0.02	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.