Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 01:12 AM JST

PDB ID	:	7CEB
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:

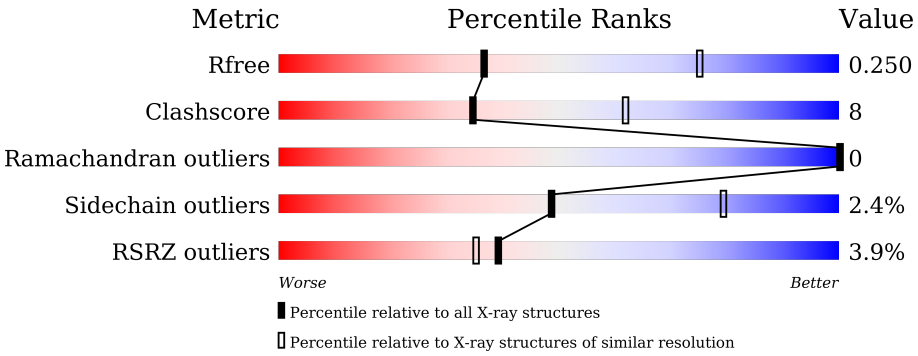
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 <=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	4% 67% 20% • 12%
2	B	454	3% 70% 11% • 18%
3	C	172	3% 68% 17% • 15%
4	D	164	2% 72% 16% • 11%

2 Entry composition (i)

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			

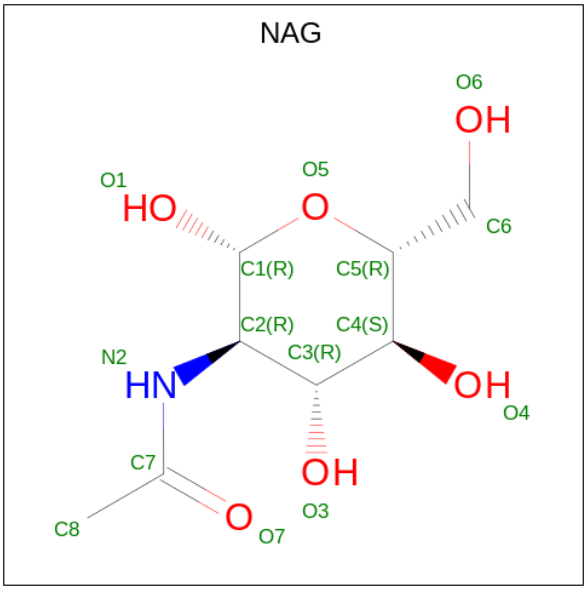
- Molecule 4 is a protein called TS2/16 VL-SARAH(S37C).

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 (three-letter code: 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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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 (three-letter code: MG) (formula: Mg).

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

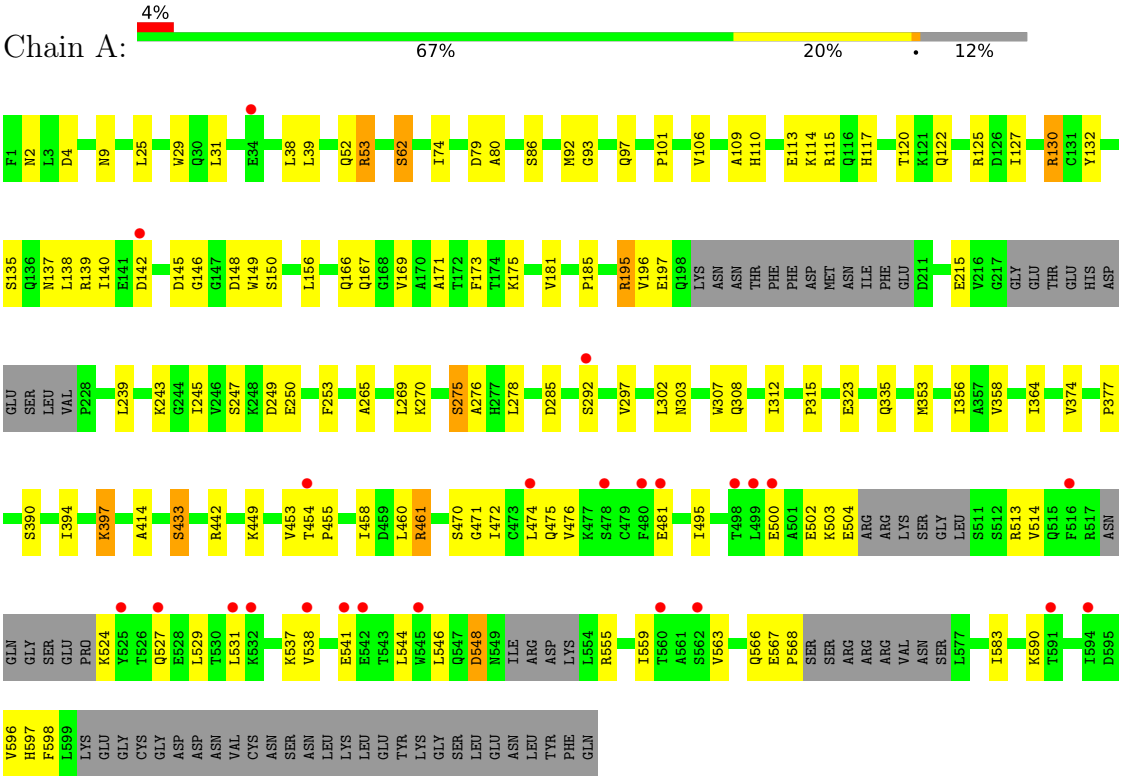
- Molecule 8 is water.

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

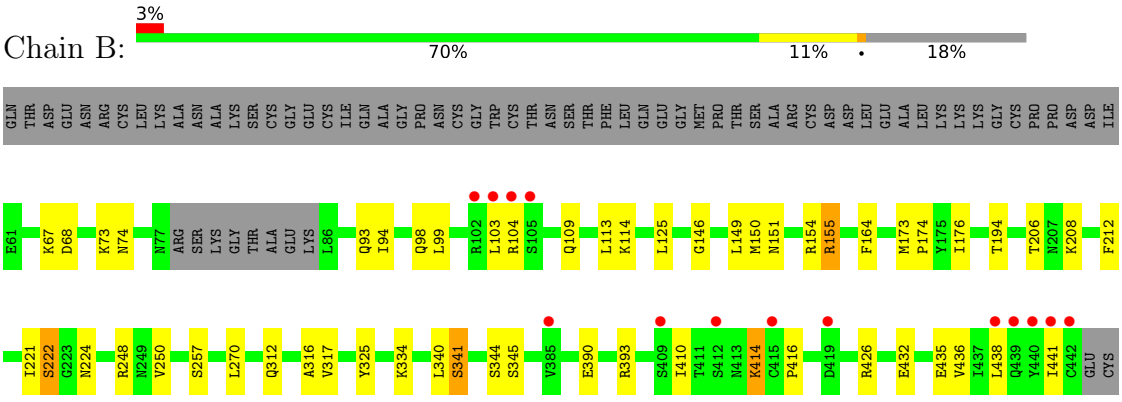
3 Residue-property plots (i)

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.

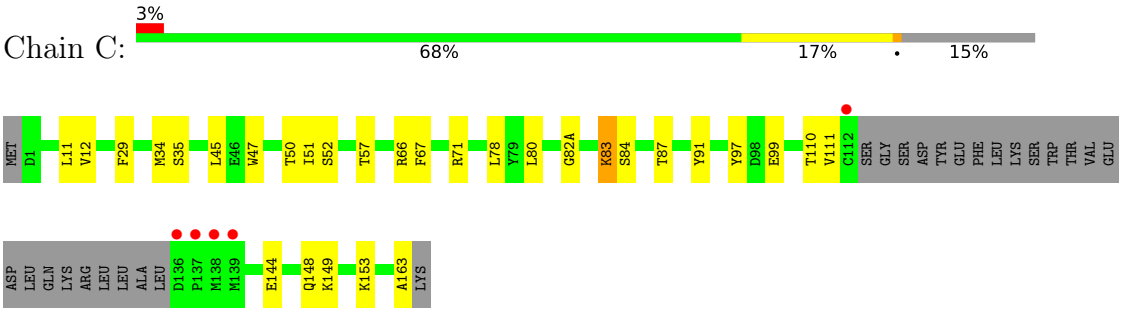
• Molecule 1: Integrin alpha-6



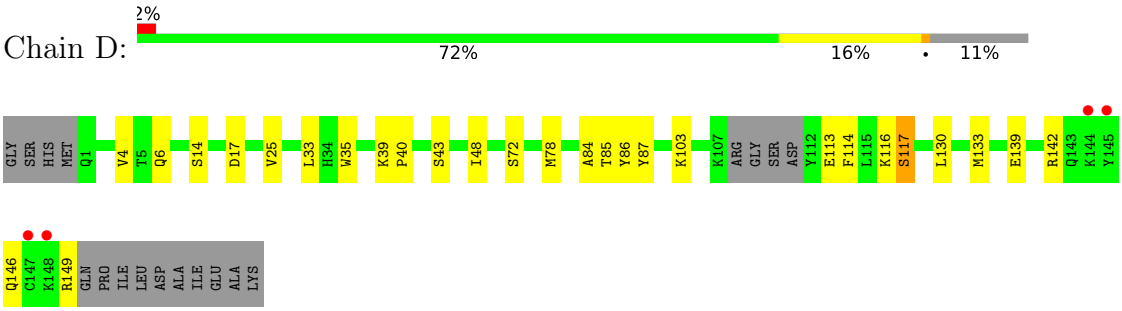
• Molecule 2: Integrin beta-1



• Molecule 3: TS2/16 VH(S112C)-SARAH



• Molecule 4: TS2/16 VL-SARAH(S37C)



4 Data and refinement statistics (i)

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 47.83 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.57-2.89) 99.6 (47.83-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.207 , 0.249 0.206 , 0.250	Depositor DCC
R_{free} test set	2041 reflections (4.83%)	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)	0.31 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NAG, CA

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	0.29	0/4400	0.53	0/5956
2	B	0.26	0/2982	0.46	0/4027
3	C	0.27	0/1178	0.48	0/1587
4	D	0.34	0/1169	0.53	0/1581
All	All	0.29	0/9729	0.50	0/13151

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	93	0
2	B	2931	0	2902	33	0
3	C	1155	0	1119	21	0
4	D	1146	0	1142	16	0
5	A	3	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	2	0	0	0	0
8	B	1	0	0	0	0
All	All	9632	0	9427	159	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 (159) 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
3:C:47:TRP:HE1	3:C:50:THR:HG1	1.34	0.76
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:29:TRP:HB3	1:A:101:PRO:HA	1.85	0.57
2:B:341:SER:HG	2:B:345:SER:HG	1.52	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:92:MET:HE3	1:A:93:GLY:N	2.22	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
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
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: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:25:LEU:HD12	1:A:414:ALA:HB3	1.93	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:113:GLU:H	4:D:113:GLU:CD	2.18	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:130:ARG:HH21	1:A:148:ASP:CG	2.19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:113:GLU:OE1	2:B:173:MET:HE1	2.17	0.44
1:A:323:GLU:O	1:A:323:GLU:HG3	2.17	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	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 (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	467/535 (87%)	452 (97%)	15 (3%)	39	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	336/402 (84%)	330 (98%)	6 (2%)	59 85
3	C	126/149 (85%)	125 (99%)	1 (1%)	81 94
4	D	130/144 (90%)	127 (98%)	3 (2%)	50 80
All	All	1059/1230 (86%)	1034 (98%)	25 (2%)	49 79

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	62	SER
1	A	114	LYS
1	A	130	ARG
1	A	195	ARG
1	A	270	LYS
1	A	275	SER
1	A	397	LYS
1	A	433	SER
1	A	449	LYS
1	A	461	ARG
1	A	548	ASP
1	A	555	ARG
1	A	590	LYS
1	A	597	HIS
2	B	155	ARG
2	B	222	SER
2	B	224	ASN
2	B	341	SER
2	B	414	LYS
2	B	426	ARG
3	C	83	LYS
4	D	33	LEU
4	D	72	SER
4	D	117	SER

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

Mol	Chain	Res	Type
1	A	32	GLN
1	A	167	GLN
1	A	448	GLN

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Mol	Chain	Res	Type
4	D	124	GLN
4	D	136	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	1006	2	14,14,15	0.25	0	17,19,21	0.48	0
6	NAG	A	1005	1	14,14,15	1.20	2 (14%)	17,19,21	1.01	1 (5%)
6	NAG	A	1004	1	14,14,15	0.88	1 (7%)	17,19,21	0.66	0
6	NAG	B	1005	2	14,14,15	0.66	1 (7%)	17,19,21	0.96	1 (5%)
6	NAG	B	1003	2	14,14,15	0.79	1 (7%)	17,19,21	0.70	0
6	NAG	B	1004	2	14,14,15	0.37	0	17,19,21	0.57	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	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	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	1003	2	-	1/6/23/26	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	1004	NAG	O5-C1	-3.22	1.38	1.43
6	A	1005	NAG	O5-C1	-2.96	1.39	1.43
6	A	1005	NAG	C1-C2	2.86	1.56	1.52
6	B	1003	NAG	C1-C2	2.43	1.56	1.52
6	B	1005	NAG	O5-C1	2.21	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1005	NAG	C1-O5-C5	3.27	116.62	112.19
6	A	1005	NAG	C2-N2-C7	2.17	125.99	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	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	1006	NAG	O5-C5-C6-O6
6	B	1006	NAG	C4-C5-C6-O6
6	B	1003	NAG	O5-C5-C6-O6
6	B	1005	NAG	O5-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

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, 95^{th} 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%)	0.26	24 (4%)	35	31	39, 75, 124, 158	0
2	B	374/454 (82%)	0.20	14 (3%)	41	37	39, 70, 119, 169	0
3	C	147/172 (85%)	-0.08	5 (3%)	45	40	48, 78, 128, 157	0
4	D	146/164 (89%)	0.05	4 (2%)	54	50	38, 69, 132, 163	0
All	All	1220/1417 (86%)	0.17	47 (3%)	39	35	38, 73, 126, 169	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	442	CYS	11.6
2	B	441	ILE	5.5
4	D	147	CYS	5.0
4	D	148	LYS	4.9
2	B	105	SER	4.7
2	B	104	ARG	4.0
1	A	525	TYR	3.6
2	B	419	ASP	3.6
1	A	499	LEU	3.3
3	C	138	MET	3.3
1	A	142	ASP	3.2
1	A	481	GLU	3.2
1	A	474	LEU	3.2
1	A	454	THR	3.2
4	D	145	TYR	3.1
2	B	440	TYR	3.1
1	A	516	PHE	3.1
1	A	478	SER	3.0
3	C	139	MET	3.0
3	C	137	PRO	2.9
1	A	532	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	412	SER	2.8
1	A	531	LEU	2.8
2	B	103	LEU	2.8
2	B	439	GLN	2.7
1	A	560	THR	2.7
1	A	292	SER	2.7
1	A	541	GLU	2.7
1	A	538	VAL	2.6
1	A	34	GLU	2.6
2	B	438	LEU	2.6
2	B	102	ARG	2.6
3	C	136	ASP	2.4
2	B	415	CYS	2.4
1	A	594	ILE	2.4
1	A	527	GLN	2.4
2	B	385	VAL	2.3
1	A	542	GLU	2.3
4	D	144	LYS	2.2
1	A	545	TRP	2.2
2	B	409	SER	2.2
1	A	480	PHE	2.2
1	A	498	THR	2.2
1	A	500	GLU	2.1
3	C	112	CYS	2.1
1	A	591	THR	2.0
1	A	562	SER	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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	B	1005	14/15	0.70	0.30	116,124,129,135	0
6	NAG	B	1003	14/15	0.77	0.16	87,103,113,113	0
6	NAG	B	1006	14/15	0.82	0.28	90,105,113,114	0
6	NAG	A	1004	14/15	0.83	0.25	88,102,116,117	0
7	MG	B	1002	1/1	0.86	0.16	83,83,83,83	1
6	NAG	A	1005	14/15	0.91	0.18	50,76,92,97	0
5	CA	B	1001	1/1	0.94	0.20	104,104,104,104	1
6	NAG	B	1004	14/15	0.95	0.17	58,72,83,87	0
5	CA	A	1002	1/1	0.96	0.17	78,78,78,78	0
5	CA	A	1001	1/1	0.98	0.27	78,78,78,78	0
5	CA	A	1003	1/1	0.99	0.11	71,71,71,71	0

6.5 Other polymers (i)

There are no such residues in this entry.