



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 07:58 pm GMT

PDB ID : 2W67
Title : BtGH84 in complex with FMA34
Authors : He, Y.; Davies, G.J.
Deposited on : 2008-12-17
Resolution : 2.25 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 : 1.8.4, 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

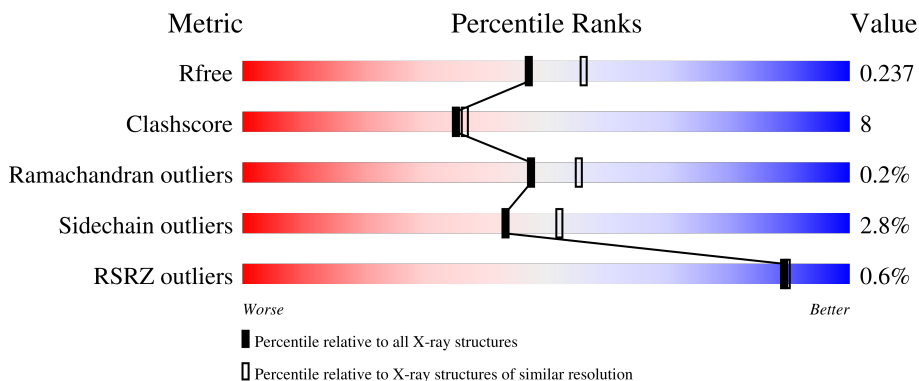
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	716	 % 73% 16% • 10%
1	B	716	 % 65% 15% • 20%

2 Entry composition [i](#)

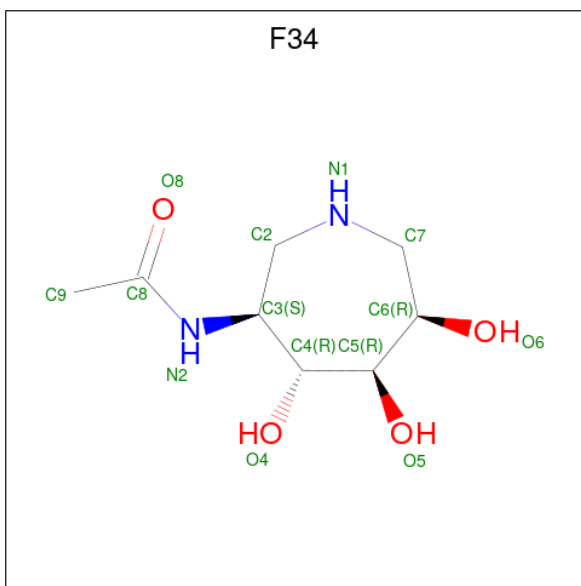
There are 5 unique types of molecules in this entry. The entry contains 10488 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 O-GLCNACASE BT_4395.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	642	Total 5230	C 3357	N 881	O 974	S 18	0	2	0
1	B	576	Total 4697	C 3009	N 791	O 881	S 16	0	2	0

- Molecule 2 is N-[(3S,4R,5R,6R)-4,5,6-trihydroxyazepan-3-yl]acetamide (three-letter code: F34) (formula: C₈H₁₆N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 14	C 8	N 2	O 4	0	0
2	B	1	Total 14	C 8	N 2	O 4	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

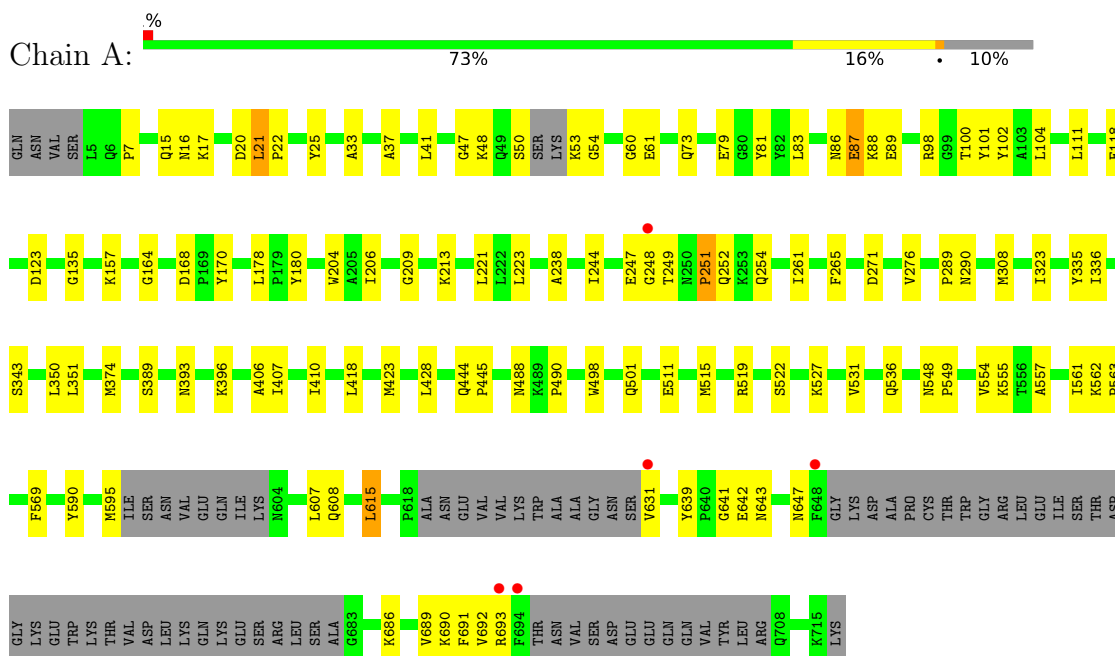
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	285	Total O 285 285	0	0
5	B	240	Total O 240 240	0	0

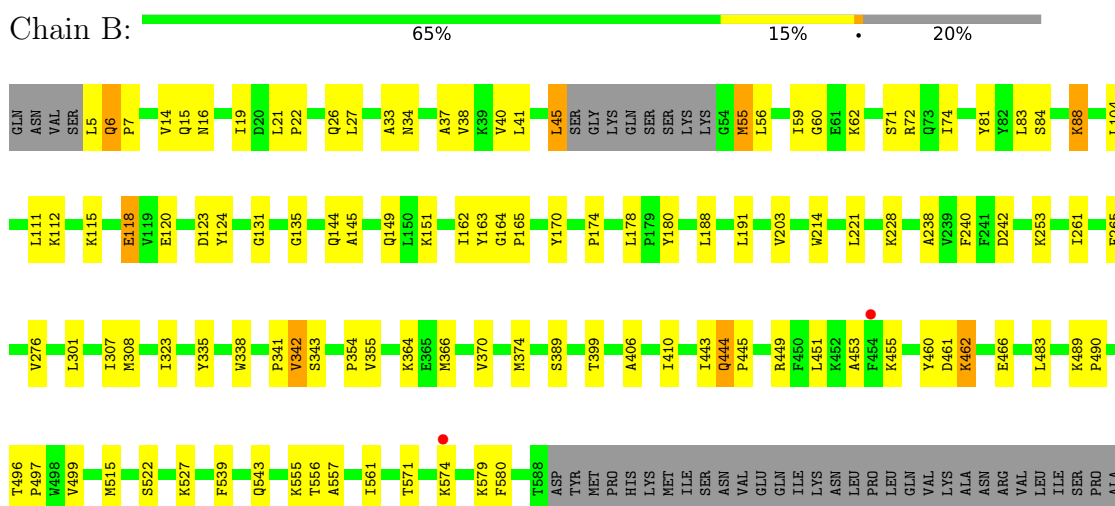
3 Residue-property plots [i](#)

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: O-GLCNACASE BT_4395



• Molecule 1: O-GLCNACASE BT_4395



ASN
GLU
VAL
VAL
LYS
TRP
ALA
ALA
GLY
ASN
SER
VAL
GLU
ILE
GLU
LEU
LEU
ASN
ASP
ALA
ALA
ILE
TYR
PRO
GLY
GLU
ASN
ILE
GLN
ILE
PHE
GLY
LYS
ASP
ALA
PRO
CYS
THR
THR
GLY
ARG
LEU
GLU
ILE
SER
THR
ASP
GLY
LYS
GLU
TRP
LYS
THR
VAL
ASP
LEU
LYS
GLN
LYS
GLU
SER
ARG

LEU
SER
ALA
GLY
LEU
GLN
LYS
ALA
PRO
VAL
LYS
PHE
VAL
ARG
PHE
THR
ASN
VAL
SER
ASP
GLU
GLU
GLN
GLN
VAL
TYR
LEU
ARG
GLN
PHE
VAL
LEU
THR
ILE
GLU
LYS
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.25Å 92.10Å 98.29Å 103.42° 95.11° 100.60°	Depositor
Resolution (Å)	87.71 – 2.25 87.57 – 2.25	Depositor EDS
% Data completeness (in resolution range)	93.3 (87.71-2.25) 92.4 (87.57-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.25Å)	Xtrriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.181 , 0.229 0.192 , 0.237	Depositor DCC
R_{free} test set	3711 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtrriage
Anisotropy	0.144	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10488	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F34, GOL, 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	0.72	0/5367	0.71	0/7271
1	B	0.70	0/4826	0.71	0/6547
All	All	0.71	0/10193	0.71	0/13818

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	5230	0	5149	81	0
1	B	4697	0	4594	80	0
2	A	14	0	16	0	0
2	B	14	0	16	0	0
3	A	6	0	8	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	285	0	0	0	0
5	B	240	0	0	5	0
All	All	10488	0	9783	161	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 (161) 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:53:LYS:HG3	1:A:54:GLY:N	1.54	1.12
1:A:53:LYS:HG3	1:A:54:GLY:H	0.95	1.08
1:A:53:LYS:CG	1:A:54:GLY:H	1.64	1.08
1:A:21:LEU:HD23	1:A:22:PRO:HD2	1.35	1.06
1:A:47:GLY:O	1:A:48:LYS:HG2	1.64	0.97
1:A:88:LYS:HG3	1:A:89:GLU:HG2	1.67	0.76
1:A:536:GLN:HG2	1:A:590:TYR:CD1	2.21	0.75
1:A:393:ASN:ND2	1:A:396:LYS:HD3	2.02	0.74
1:A:47:GLY:C	1:A:48:LYS:HG2	2.03	0.74
1:B:301:LEU:HD12	1:B:307:ILE:HD11	1.67	0.74
1:B:444:GLN:N	1:B:445:PRO:HD2	2.00	0.74
1:B:6:GLN:NE2	1:B:389:SER:OG	2.24	0.70
1:B:406:ALA:O	1:B:410[A]:ILE:HG12	1.90	0.70
1:B:461:ASP:OD1	1:B:462:LYS:N	2.29	0.66
1:B:41:LEU:O	1:B:45:LEU:HD22	1.97	0.65
1:B:527:LYS:HA	1:B:527:LYS:HE2	1.78	0.65
1:A:393:ASN:HD21	1:A:396:LYS:HD3	1.61	0.65
1:A:562:LYS:HB3	1:A:563:PRO:HD3	1.78	0.65
1:A:690:LYS:HG2	1:A:691:PHE:CD2	2.32	0.65
1:A:690:LYS:HG2	1:A:691:PHE:CE2	2.32	0.64
1:A:25:TYR:O	1:A:50:SER:HA	1.97	0.64
1:B:19:ILE:HG13	1:B:19:ILE:O	1.97	0.64
1:A:557:ALA:HB1	1:A:561:ILE:HB	1.79	0.63
1:A:21:LEU:HD12	1:A:111:LEU:HD11	1.81	0.63
1:A:244:ILE:HD11	1:A:248:GLY:O	1.98	0.62
1:B:489:LYS:HB2	1:B:490:PRO:HD3	1.80	0.62
1:A:53:LYS:CD	1:A:54:GLY:H	2.13	0.62
1:B:135:GLY:HA2	1:B:164:GLY:O	2.00	0.61
1:A:631:VAL:O	1:A:693:ARG:HA	2.01	0.61
1:A:17:LYS:HD2	1:A:87:GLU:OE2	2.01	0.60
1:A:515:MET:HG2	1:A:527:LYS:HB2	1.83	0.60
1:A:86:ASN:HA	1:A:118:GLU:HG3	1.83	0.59
1:B:170:TYR:HB2	1:B:180:TYR:CE1	2.38	0.58
1:B:15:GLN:HB3	1:B:118:GLU:HB3	1.84	0.57
1:B:451:LEU:O	1:B:455:LYS:HB2	2.04	0.57
1:A:289:PRO:O	1:A:290:ASN:HB2	2.06	0.56
1:B:72:ARG:NH2	5:B:2020:HOH:O	2.38	0.56
1:A:444:GLN:HB3	1:A:445:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ASN:HD21	1:A:396:LYS:CD	2.18	0.55
1:A:53:LYS:CG	1:A:54:GLY:N	2.31	0.55
1:A:81:TYR:CE2	1:A:123:ASP:HB3	2.41	0.55
1:A:608:GLN:HB2	1:A:615:LEU:CD2	2.37	0.55
1:B:22:PRO:HB3	1:B:55:MET:CE	2.37	0.54
1:A:615:LEU:HD22	1:A:615:LEU:O	2.07	0.54
1:A:536:GLN:HG2	1:A:590:TYR:CG	2.43	0.54
1:A:88:LYS:HE2	1:A:89:GLU:OE2	2.08	0.53
1:A:308:MET:HA	1:A:335:TYR:O	2.09	0.53
1:B:308:MET:HA	1:B:335:TYR:O	2.08	0.53
1:B:34:ASN:O	1:B:38:VAL:HG23	2.08	0.53
1:A:238:ALA:HA	1:A:276:VAL:O	2.09	0.53
1:A:244:ILE:CD1	1:A:248:GLY:O	2.57	0.53
1:A:81:TYR:CZ	1:A:123:ASP:HB3	2.44	0.52
1:B:15:GLN:CB	1:B:118:GLU:HB3	2.39	0.52
1:A:209:GLY:O	1:A:248:GLY:HA3	2.10	0.52
1:B:445:PRO:O	1:B:449:ARG:HG3	2.10	0.52
1:A:511:GLU:O	1:A:515:MET:HG3	2.10	0.52
1:B:15:GLN:O	1:B:16:ASN:HB2	2.09	0.52
1:A:423:MET:O	1:A:423:MET:HG3	2.11	0.51
1:B:6:GLN:HA	1:B:7:PRO:C	2.29	0.51
1:B:37:ALA:HB1	1:B:104:LEU:HD23	1.92	0.51
1:B:81:TYR:CZ	1:B:123:ASP:HB3	2.45	0.51
1:B:228:LYS:CD	5:B:2093:HOH:O	2.57	0.51
1:A:135:GLY:HA2	1:A:164:GLY:O	2.11	0.51
1:A:406:ALA:O	1:A:410[B]:ILE:HG13	2.10	0.50
1:B:81:TYR:CE2	1:B:123:ASP:HB3	2.46	0.50
1:A:531:VAL:HG11	1:A:569:PHE:CE1	2.46	0.50
1:A:641:GLY:O	1:A:686:LYS:HA	2.11	0.50
1:B:571:THR:O	1:B:574:LYS:HB3	2.12	0.49
1:A:608:GLN:HB2	1:A:615:LEU:HD22	1.94	0.49
1:B:443:ILE:C	1:B:445:PRO:HD2	2.33	0.49
1:A:7:PRO:HB3	1:A:389:SER:HA	1.93	0.49
1:B:14:VAL:HG12	1:B:15:GLN:N	2.28	0.49
1:A:170:TYR:HB2	1:A:180:TYR:CE1	2.48	0.49
1:B:444:GLN:N	1:B:445:PRO:CD	2.73	0.49
1:A:15:GLN:O	1:A:16:ASN:HB2	2.13	0.49
1:B:343[B]:SER:HB2	1:B:374:MET:HG2	1.94	0.49
1:B:111:LEU:HD12	1:B:115:LYS:O	2.12	0.48
1:A:204:TRP:CZ3	1:A:206:ILE:HB	2.49	0.48
1:B:145:ALA:O	1:B:149:GLN:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:THR:O	1:B:557:ALA:C	2.51	0.48
1:A:393:ASN:ND2	1:A:396:LYS:CD	2.75	0.48
1:A:102:TYR:CE1	1:A:157:LYS:HA	2.48	0.48
1:B:55:MET:HG3	1:B:56:LEU:N	2.28	0.48
1:B:261:ILE:O	1:B:265:PHE:HB3	2.14	0.47
1:B:14:VAL:HG12	1:B:15:GLN:H	1.79	0.47
1:B:22:PRO:HB3	1:B:55:MET:HE2	1.95	0.47
1:B:338:TRP:CH2	1:B:355:VAL:HG13	2.48	0.47
1:B:214:TRP:HB3	1:B:253:LYS:HD2	1.95	0.47
1:A:527:LYS:HE2	1:A:527:LYS:HA	1.97	0.47
1:B:341:PRO:O	1:B:342:VAL:C	2.53	0.47
1:A:15:GLN:HB3	1:A:118:GLU:HB3	1.96	0.47
1:A:531:VAL:HG11	1:A:569:PHE:CD1	2.50	0.47
1:B:163:TYR:CD2	1:B:163:TYR:C	2.88	0.47
1:B:164:GLY:N	1:B:165:PRO:HD3	2.30	0.47
1:A:350:LEU:O	1:A:351:LEU:HD23	2.15	0.46
1:B:489:LYS:N	1:B:490:PRO:CD	2.78	0.46
1:B:539:PHE:O	1:B:543:GLN:HG2	2.15	0.46
1:B:579:LYS:HG2	1:B:580:PHE:CD2	2.50	0.46
1:A:61:GLU:OE2	1:A:100:THR:OG1	2.21	0.46
1:B:483:LEU:HG	1:B:499:VAL:HG11	1.96	0.46
1:A:79:GLU:OE2	1:A:98:ARG:HD2	2.14	0.46
1:B:515:MET:HG3	1:B:527:LYS:HB2	1.97	0.46
1:B:71:SER:HA	1:B:74:ILE:HD12	1.97	0.46
1:A:41:LEU:HB2	1:A:104:LEU:HD11	1.97	0.45
1:B:7:PRO:HB3	1:B:389:SER:HA	1.97	0.45
1:A:692:VAL:O	1:A:692:VAL:HG12	2.17	0.45
1:B:238:ALA:HA	1:B:276:VAL:O	2.15	0.45
1:B:26:GLN:N	1:B:55:MET:O	2.41	0.45
1:A:73:GLN:H	1:A:73:GLN:HG2	1.56	0.45
1:A:536:GLN:HG2	1:A:590:TYR:CE1	2.51	0.45
1:B:131:GLY:O	1:B:370:VAL:HA	2.16	0.45
1:B:174:PRO:HD2	5:B:2064:HOH:O	2.16	0.45
1:B:83:LEU:HD23	1:B:83:LEU:C	2.38	0.45
1:A:343[B]:SER:OG	1:A:374:MET:HG2	2.17	0.44
1:B:188:LEU:HD23	1:B:191:LEU:HD12	1.99	0.44
1:B:444:GLN:NE2	5:B:2192:HOH:O	2.50	0.44
1:B:59:ILE:HG23	1:B:59:ILE:O	2.18	0.44
1:B:557:ALA:HB1	1:B:561:ILE:HB	1.99	0.44
1:A:251:PRO:O	1:A:254:GLN:N	2.50	0.44
1:B:240:PHE:HB3	1:B:242:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:HD23	1:A:22:PRO:CD	2.26	0.44
1:A:247:GLU:C	1:A:249:THR:H	2.21	0.44
1:A:323:ILE:CD1	1:A:336:ILE:HD11	2.48	0.43
1:A:37:ALA:HB2	1:A:101:TYR:HA	1.99	0.43
1:B:355:VAL:O	1:B:399:THR:HG23	2.18	0.43
1:A:428:LEU:HD12	1:A:428:LEU:N	2.34	0.43
1:A:595:MET:HB2	1:A:607:LEU:HD11	1.99	0.43
1:A:498:TRP:CD1	1:A:554:VAL:HG13	2.54	0.43
1:B:83:LEU:HD23	1:B:84:SER:N	2.34	0.43
1:A:168:ASP:OD1	1:A:168:ASP:C	2.56	0.43
1:B:41:LEU:O	1:B:45:LEU:CD2	2.65	0.43
1:B:40:VAL:HG12	1:B:104:LEU:HD12	2.00	0.43
1:B:515:MET:HG3	1:B:527:LYS:CB	2.49	0.43
1:A:271:ASP:OD1	1:A:271:ASP:N	2.52	0.42
1:B:6:GLN:HE21	1:B:7:PRO:HA	1.85	0.42
1:B:21:LEU:HG	1:B:22:PRO:HD2	2.01	0.42
1:B:123:ASP:O	1:B:124:TYR:HB3	2.19	0.42
1:A:407:ILE:HG23	1:A:418:LEU:HD23	2.01	0.42
1:A:33:ALA:HB2	1:A:60:GLY:HA2	2.02	0.42
1:B:144:GLN:HG2	5:B:2046:HOH:O	2.20	0.42
1:A:83:LEU:C	1:A:83:LEU:HD23	2.40	0.42
1:A:261:ILE:O	1:A:265:PHE:HB3	2.19	0.42
1:A:444:GLN:N	1:A:445:PRO:CD	2.82	0.42
1:B:162:ILE:HA	1:B:203:VAL:HB	2.02	0.41
1:A:501:GLN:HA	1:A:501:GLN:OE1	2.20	0.41
1:B:453:ALA:CB	1:B:460:TYR:HA	2.50	0.41
1:A:608:GLN:HB2	1:A:615:LEU:HD21	2.00	0.41
1:A:251:PRO:HG2	1:A:252:GLN:H	1.85	0.41
1:B:496:THR:O	1:B:497:PRO:C	2.59	0.41
1:A:548:ASN:HB2	1:A:549:PRO:HD2	2.02	0.41
1:B:354:PRO:HB2	1:B:399:THR:CG2	2.51	0.41
1:B:323:ILE:HD11	1:B:366:MET:HB3	2.02	0.41
1:B:364:LYS:HE3	1:B:364:LYS:HB3	1.70	0.41
1:B:443:ILE:C	1:B:443:ILE:HD12	2.41	0.41
1:B:33:ALA:HB2	1:B:60:GLY:HA2	2.02	0.41
1:B:188:LEU:HD23	1:B:188:LEU:HA	1.83	0.40
1:B:112:LYS:HD3	1:B:112:LYS:HA	1.89	0.40
1:A:488:ASN:OD1	1:A:490:PRO:HD2	2.21	0.40
1:A:639:TYR:O	1:A:689:VAL:HG12	2.21	0.40
1:B:5:LEU:O	1:B:6:GLN:HG2	2.22	0.40
1:B:88:LYS:H	1:B:88:LYS:HG2	1.50	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	632/716 (88%)	605 (96%)	26 (4%)	1 (0%)	47 55
1	B	574/716 (80%)	547 (95%)	26 (4%)	1 (0%)	47 55
All	All	1206/1432 (84%)	1152 (96%)	52 (4%)	2 (0%)	47 55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	342	VAL
1	A	251	PRO

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	567/630 (90%)	553 (98%)	14 (2%)	47 56
1	B	507/630 (80%)	491 (97%)	16 (3%)	39 47
All	All	1074/1260 (85%)	1044 (97%)	30 (3%)	43 52

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASP

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Mol	Chain	Res	Type
1	A	21	LEU
1	A	87	GLU
1	A	178	LEU
1	A	213	LYS
1	A	221	LEU
1	A	223	LEU
1	A	519	ARG
1	A	522	SER
1	A	555	LYS
1	A	615	LEU
1	A	642	GLU
1	A	643	ASN
1	A	647	ASN
1	B	6	GLN
1	B	27	LEU
1	B	45	LEU
1	B	55	MET
1	B	62	LYS
1	B	88	LYS
1	B	118	GLU
1	B	120	GLU
1	B	151	LYS
1	B	178	LEU
1	B	221	LEU
1	B	444	GLN
1	B	462	LYS
1	B	466	GLU
1	B	522	SER
1	B	555	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	10	GLN
1	A	49	GLN
1	A	156	ASN
1	A	252	GLN
1	A	274	GLN
1	A	349	HIS
1	A	529	ASN
1	A	578	GLN

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Mol	Chain	Res	Type
1	A	643	ASN
1	A	647	ASN
1	A	708	GLN
1	B	6	GLN
1	B	10	GLN
1	B	28	ASN
1	B	149	GLN
1	B	156	ASN
1	B	274	GLN
1	B	444	GLN
1	B	459	ASN
1	B	529	ASN
1	B	536	GLN
1	B	547	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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
2	F34	B	1589	-	11,14,14	0.55	0	10,19,19	2.46	3 (30%)
2	F34	A	1716	-	11,14,14	0.94	0	10,19,19	2.25	3 (30%)
3	GOL	A	1717	-	5,5,5	0.30	0	5,5,5	0.49	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	F34	B	1589	-	-	1/4/22/22	0/1/1/1
2	F34	A	1716	-	-	1/4/22/22	0/1/1/1
3	GOL	A	1717	-	-	0/4/4/4	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1716	F34	C2-C3-N2	5.98	120.87	109.61
2	B	1589	F34	C2-C3-N2	5.70	120.34	109.61
2	B	1589	F34	C3-N2-C8	3.21	127.47	122.90
2	B	1589	F34	C6-C5-C4	2.63	119.43	115.20
2	A	1716	F34	O5-C5-C4	-2.35	103.70	108.93
2	A	1716	F34	C3-N2-C8	2.33	126.22	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1716	F34	C4-C3-N2-C8
2	B	1589	F34	C4-C3-N2-C8

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [\(i\)](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	642/716 (89%)	-0.25	5 (0%) 86 87	4, 16, 41, 55	0
1	B	576/716 (80%)	-0.23	2 (0%) 94 94	6, 17, 42, 51	0
All	All	1218/1432 (85%)	-0.24	7 (0%) 89 89	4, 17, 41, 55	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	454	PHE	3.8
1	A	694	PHE	3.2
1	A	648	PHE	2.4
1	A	631	VAL	2.3
1	A	693	ARG	2.3
1	B	574	LYS	2.1
1	A	248	GLY	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, 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(\AA^2)	Q<0.9
4	CA	B	1590	1/1	0.93	0.11	32,32,32,32	0
4	CA	A	1718	1/1	0.96	0.15	25,25,25,25	0
2	F34	A	1716	14/14	0.96	0.12	7,13,17,20	0
2	F34	B	1589	14/14	0.97	0.12	12,15,17,20	0
3	GOL	A	1717	6/6	0.97	0.10	20,23,25,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.