Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:29 PM GMT

PDB ID	:	5CXF
Title	:	Crystal structure of the extracellular domain of glycoprotein B from Human Cytomegalovirus
Authors	:	Burke, H.G.; Heldwein, E.E.
Deposited on	:	2015-07-28
Resolution	:	3.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

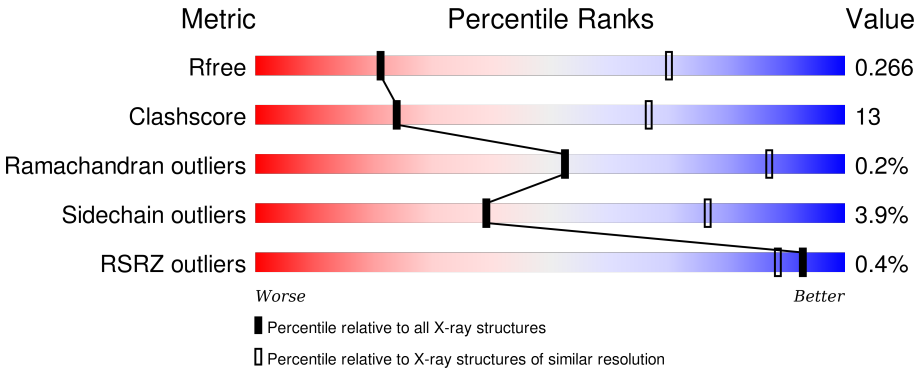
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 3.60 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}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	630	% 61% 26% • 11%
1	B	630	63% 26% • 10%
1	C	630	63% 27% • 9%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14373 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 Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	0	0
			4561	2894	781	862	24			
1	B	570	Total	C	N	O	S	0	0	0
			4626	2931	794	877	24			
1	C	576	Total	C	N	O	S	0	0	0
			4669	2958	801	886	24			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	GLY	TYR	engineered mutation	UNP P06473
A	156	HIS	ILE	engineered mutation	UNP P06473
A	157	ARG	TYR	engineered mutation	UNP P06473
A	206	HIS	TYR	engineered mutation	UNP P06473
A	240	ALA	TRP	engineered mutation	UNP P06473
A	241	THR	LEU	engineered mutation	UNP P06473
A	242	HIS	TYR	engineered mutation	UNP P06473
A	434V	ASP	-	engineered mutation	UNP P06473
A	434W	ASP	ARG	engineered mutation	UNP P06473
A	434X	ASP	THR	engineered mutation	UNP P06473
A	434Y	ASP	ARG	engineered mutation	UNP P06473
A	434Z	LYS	ARG	engineered mutation	UNP P06473
B	155	GLY	TYR	engineered mutation	UNP P06473
B	156	HIS	ILE	engineered mutation	UNP P06473
B	157	ARG	TYR	engineered mutation	UNP P06473
B	206	HIS	TYR	engineered mutation	UNP P06473
B	240	ALA	TRP	engineered mutation	UNP P06473
B	241	THR	LEU	engineered mutation	UNP P06473
B	242	HIS	TYR	engineered mutation	UNP P06473
B	438R	ASP	-	engineered mutation	UNP P06473
B	438S	ASP	ARG	engineered mutation	UNP P06473
B	438T	ASP	THR	engineered mutation	UNP P06473
B	438U	ASP	ARG	engineered mutation	UNP P06473

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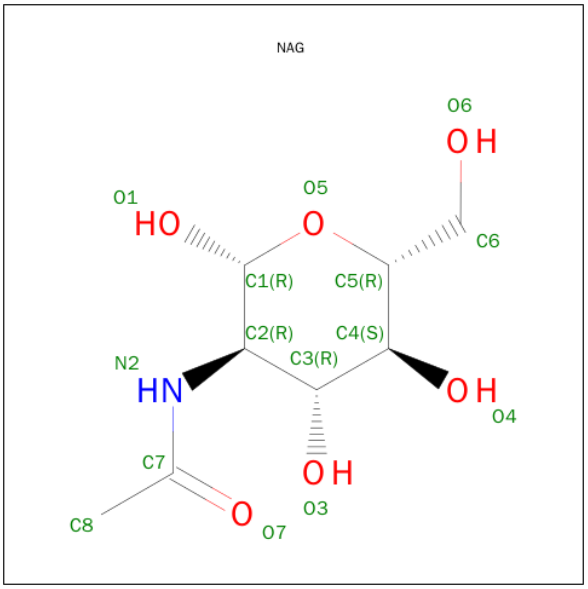
Chain	Residue	Modelled	Actual	Comment	Reference
B	438V	LYS	ARG	engineered mutation	UNP P06473
C	155	GLY	TYR	engineered mutation	UNP P06473
C	156	HIS	ILE	engineered mutation	UNP P06473
C	157	ARG	TYR	engineered mutation	UNP P06473
C	206	HIS	TYR	engineered mutation	UNP P06473
C	240	ALA	TRP	engineered mutation	UNP P06473
C	241	THR	LEU	engineered mutation	UNP P06473
C	242	HIS	TYR	engineered mutation	UNP P06473
C	440P	ASP	-	engineered mutation	UNP P06473
C	440Q	ASP	ARG	engineered mutation	UNP P06473
C	440R	ASP	THR	engineered mutation	UNP P06473
C	440S	ASP	ARG	engineered mutation	UNP P06473
C	440T	LYS	ARG	engineered mutation	UNP P06473

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: 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	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	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

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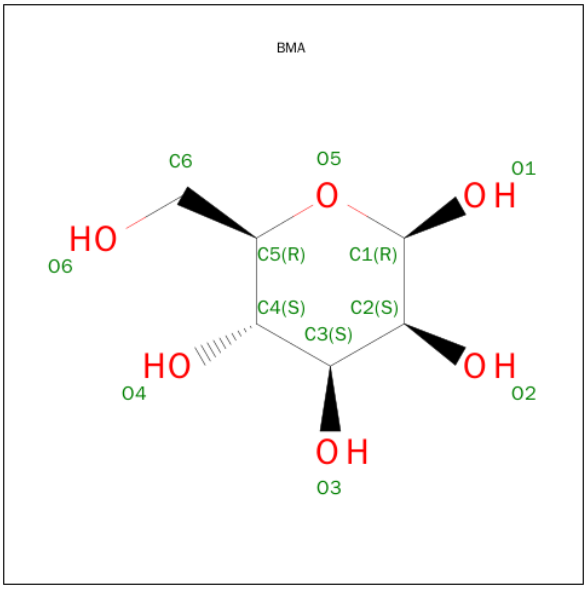
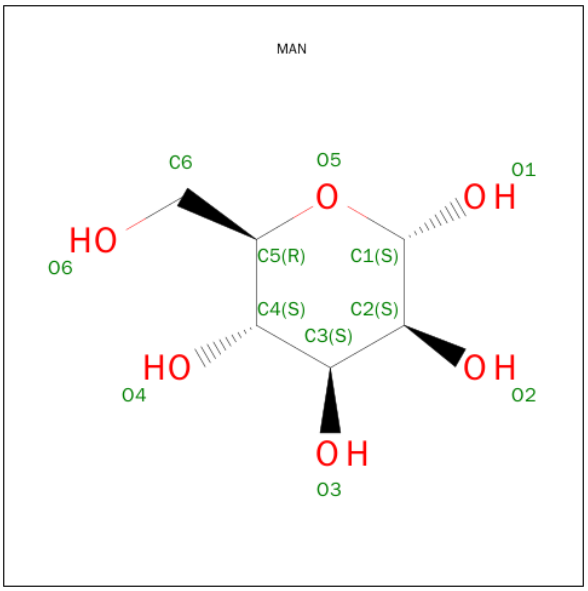
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0
3	C	1	Total C O 11 6 5	0	0

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 6 5	0	0
4	C	1	Total C O 11 6 5	0	0
4	C	1	Total C O 11 6 5	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is water.

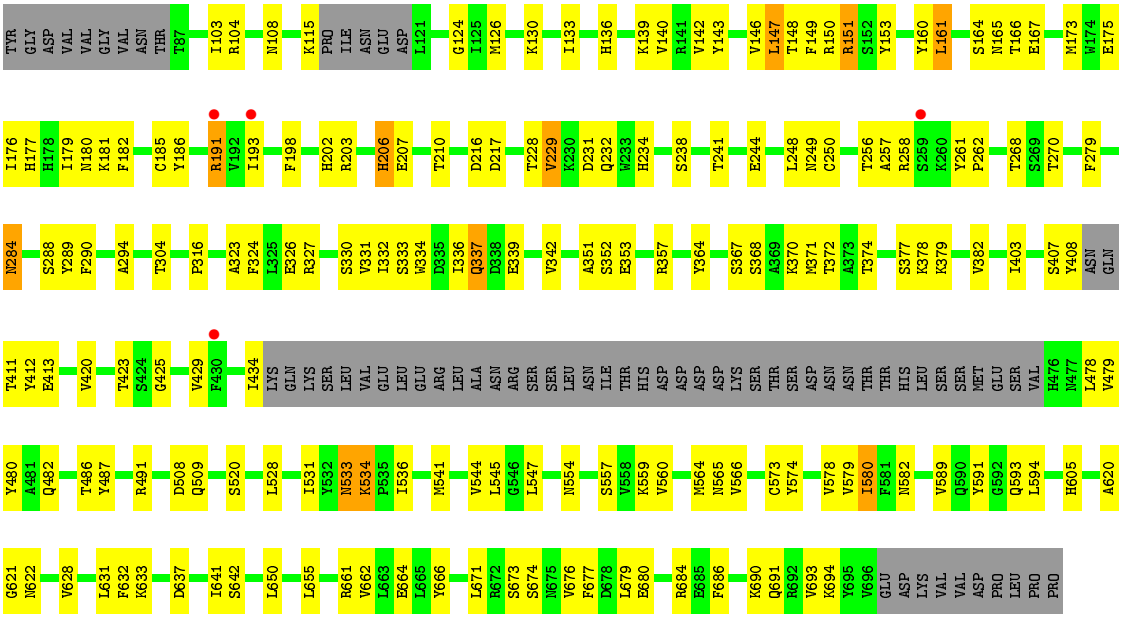
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0
6	C	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

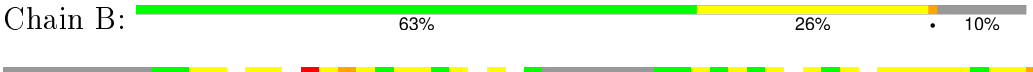
- Molecule 1: Envelope glycoprotein B

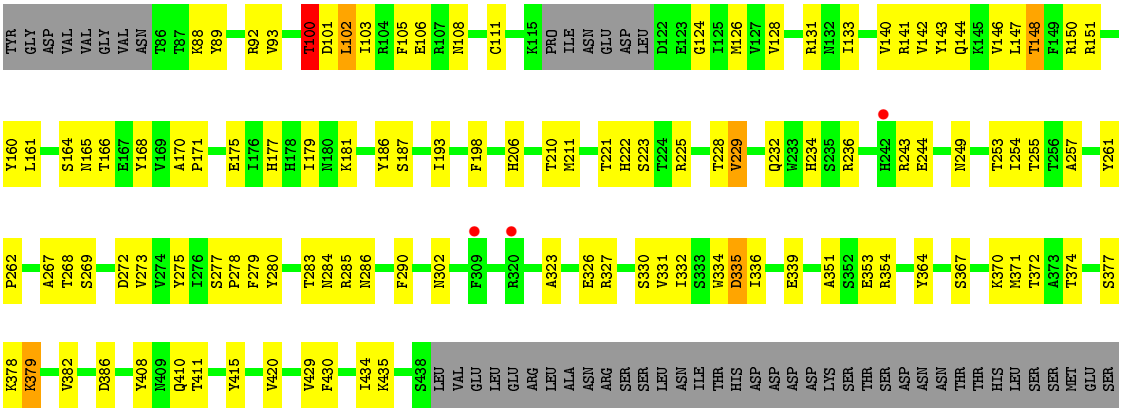
Chain A:

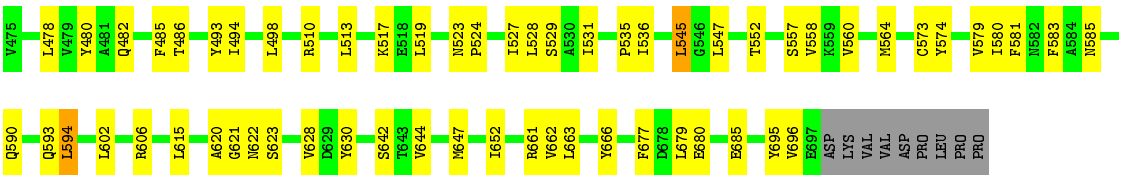


- Molecule 1: Envelope glycoprotein B

Chain B:

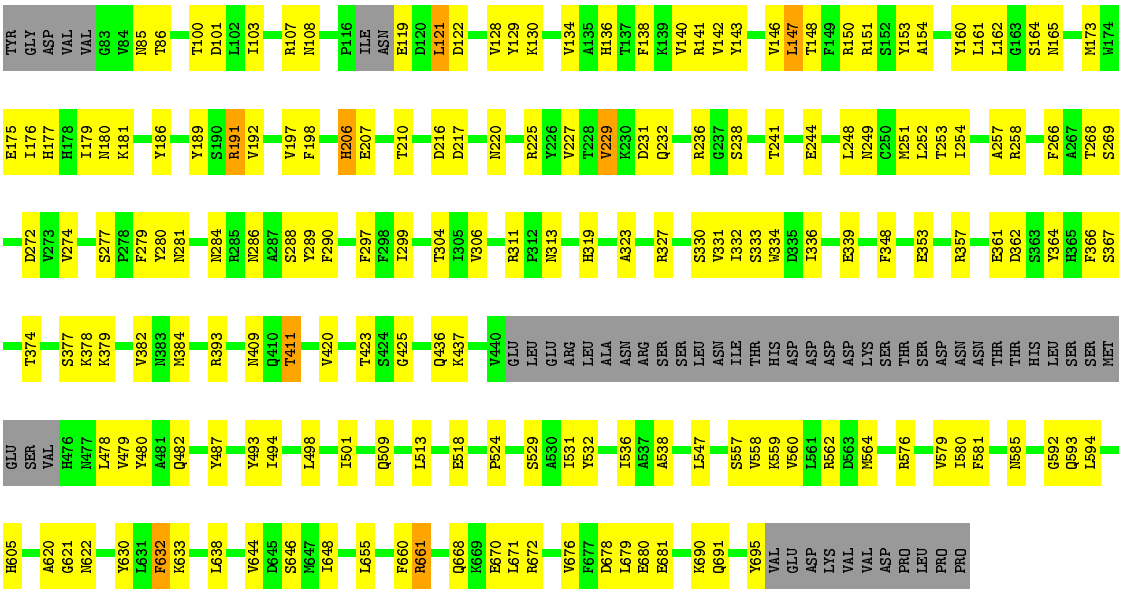






- Molecule 1: Envelope glycoprotein B

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.18Å 133.93Å 295.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.63 – 3.60 147.69 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (57.63-3.60) 86.7 (147.69-3.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 3.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.232 , 0.269 0.229 , 0.266	Depositor DCC
R_{free} test set	1666 reflections (4.45%)	DCC
Wilson B-factor (Å^2)	91.5	Xtriage
Anisotropy	0.844	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 42.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 42579 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	14373	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, BMA, NAG, MAN

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	0.42	0/4663	0.60	1/6314 (0.0%)
1	B	0.43	0/4729	0.61	0/6403
1	C	0.45	0/4773	0.62	0/6464
All	All	0.43	0/14165	0.61	1/19181 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	508	ASP	CB-CG-OD1	5.40	123.16	118.30

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	4561	0	4417	141	0
1	B	4626	0	4482	146	0
1	C	4669	0	4523	142	0
2	A	126	0	115	1	0
2	B	168	0	151	9	0
2	C	154	0	139	6	0
3	A	11	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	10	1	0
3	C	11	0	8	0	0
4	A	11	0	10	0	0
4	C	22	0	20	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
All	All	14373	0	13884	370	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 13.

All (370) 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:C:327:ARG:HH21	1:C:332:ILE:HD11	1.29	0.96
1:B:225:ARG:HD3	1:B:253:THR:HG22	1.56	0.88
1:A:642:SER:HB2	1:B:103:ILE:HG22	1.60	0.83
1:B:103:ILE:HD11	1:B:528:LEU:HD21	1.60	0.83
1:A:559:LYS:HB2	1:A:580:ILE:HG13	1.61	0.83
1:B:524:PRO:HB3	1:B:545:LEU:HD13	1.63	0.80
1:B:198:PHE:HB3	1:C:161:LEU:HB2	1.63	0.79
1:B:124:GLY:HA2	1:B:434:ILE:HG12	1.63	0.79
1:B:206:HIS:HE2	1:C:160:TYR:HH	1.25	0.78
1:C:191:ARG:HH11	1:C:191:ARG:HB2	1.51	0.76
1:A:382:VAL:HB	1:A:420:VAL:HG23	1.67	0.75
1:A:533:ASN:O	1:A:533:ASN:ND2	2.17	0.74
1:A:124:GLY:HA2	1:A:434:ILE:HG12	1.69	0.74
1:B:382:VAL:HB	1:B:420:VAL:HG23	1.70	0.74
1:C:382:VAL:HB	1:C:420:VAL:HG23	1.69	0.74
1:B:323:ALA:HB2	1:B:336:ILE:HD11	1.70	0.73
1:A:161:LEU:HB3	1:C:198:PHE:HB3	1.72	0.72
1:A:238:SER:O	1:A:241:THR:OG1	2.06	0.72
1:A:594:LEU:HD11	1:A:620:ALA:HB2	1.72	0.71
1:C:384:MET:O	1:C:393:ARG:NH2	2.20	0.71
1:A:327:ARG:HH21	1:A:332:ILE:HD11	1.55	0.71
1:A:560:VAL:HA	1:A:579:VAL:HG22	1.74	0.70
1:C:411:THR:O	1:C:436:GLN:NE2	2.24	0.70
1:C:560:VAL:HA	1:C:579:VAL:HG22	1.74	0.70
1:B:151:ARG:HG2	1:B:244:GLU:HB3	1.74	0.69
1:C:227:VAL:HG12	1:C:251:MET:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:TYR:CE2	1:B:434:ILE:HD13	2.28	0.69
1:B:165:ASN:ND2	1:C:165:ASN:OD1	2.17	0.69
1:C:146:VAL:HG22	1:C:249:ASN:HB3	1.75	0.68
1:A:554:ASN:HB3	1:A:557:SER:HB3	1.75	0.68
1:A:160:TYR:OH	1:C:206:HIS:NE2	2.23	0.68
1:B:594:LEU:HD11	1:B:620:ALA:HB2	1.77	0.67
1:B:140:VAL:HG23	1:B:334:TRP:HB3	1.76	0.67
1:C:377:SER:OG	1:C:378:LYS:N	2.27	0.66
1:C:378:LYS:O	1:C:379:LYS:HG2	1.95	0.66
1:C:423:THR:HG22	1:C:425:GLY:H	1.60	0.66
1:A:146:VAL:HG22	1:A:249:ASN:HB3	1.77	0.66
1:C:594:LEU:HD11	1:C:620:ALA:HB2	1.79	0.65
1:C:189:TYR:OH	1:C:191:ARG:HD3	1.96	0.65
1:B:353:GLU:HG2	1:B:354:ARG:HG2	1.77	0.65
1:A:686:PHE:HE1	1:A:690:LYS:HE2	1.61	0.65
1:B:377:SER:OG	1:B:378:LYS:N	2.25	0.65
1:B:272:ASP:OD2	1:B:327:ARG:NH2	2.30	0.65
1:B:105:PHE:HD2	1:B:517:LYS:HA	1.62	0.65
1:C:478:LEU:HD23	1:C:480:TYR:HE1	1.62	0.64
1:A:191:ARG:HH12	1:A:193:ILE:HD11	1.62	0.64
1:A:593:GLN:HB2	1:A:605:HIS:CD2	2.33	0.64
1:C:564:MET:HB2	1:C:630:TYR:HB3	1.80	0.64
1:B:367:SER:HA	1:B:374:THR:HG22	1.81	0.63
1:A:378:LYS:O	1:A:379:LYS:HG2	1.99	0.63
1:A:593:GLN:HB2	1:A:605:HIS:HD2	1.63	0.63
1:B:144:GLN:NE2	1:B:330:SER:OG	2.31	0.63
1:A:231:ASP:HB3	1:B:696:VAL:HG21	1.81	0.63
1:A:326:GLU:HG2	1:A:331:VAL:HG12	1.80	0.63
1:B:279:PHE:O	1:B:284:ASN:ND2	2.29	0.62
1:B:128:VAL:HG12	1:B:429:VAL:HG22	1.81	0.62
1:A:650:LEU:HD11	1:C:501:ILE:HD12	1.82	0.62
1:C:672:ARG:NH2	1:C:678:ASP:OD2	2.33	0.61
1:C:323:ALA:HB2	1:C:336:ILE:HD11	1.82	0.61
1:A:202:HIS:CE1	1:A:203:ARG:HG3	2.36	0.61
1:A:216:ASP:OD1	1:A:217:ASP:N	2.33	0.61
1:B:89:TYR:OH	1:C:107:ARG:NH1	2.33	0.60
2:C:808:NAG:H3	2:C:808:NAG:H83	1.83	0.60
1:C:524:PRO:HB2	1:C:538:ALA:HB3	1.84	0.60
1:A:408:TYR:CE2	1:A:434:ILE:HD13	2.37	0.59
1:A:175:GLU:O	1:A:179:ILE:HG13	2.02	0.59
1:B:170:ALA:HB1	1:B:331:VAL:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:LEU:HD23	1:B:663:LEU:HD13	1.84	0.59
2:B:813:NAG:H3	2:B:813:NAG:H83	1.84	0.59
1:C:558:VAL:HG13	1:C:579:VAL:HG11	1.84	0.59
1:A:520:SER:HB2	1:A:545:LEU:HD21	1.83	0.59
1:B:88:LYS:NZ	1:B:535:PRO:HD3	2.18	0.59
1:C:173:MET:HA	1:C:176:ILE:HD12	1.83	0.59
1:B:206:HIS:CE1	1:C:160:TYR:HH	2.21	0.58
1:C:592:GLY:HA2	1:C:605:HIS:HE1	1.68	0.58
1:B:275:TYR:HE2	1:C:220:ASN:HB2	1.67	0.58
1:A:151:ARG:NH2	1:C:244:GLU:OE2	2.36	0.58
1:A:423:THR:HG22	1:A:425:GLY:H	1.68	0.58
1:B:232:GLN:HB3	1:C:695:TYR:CD2	2.39	0.58
1:C:103:ILE:HD11	1:C:547:LEU:HD11	1.86	0.58
1:B:326:GLU:HA	1:B:331:VAL:HG22	1.86	0.57
1:C:153:TYR:HB3	1:C:160:TYR:HB2	1.87	0.57
1:A:177:HIS:O	1:A:181:LYS:HG2	2.03	0.57
1:A:140:VAL:HG23	1:A:334:TRP:HB3	1.87	0.57
1:B:193:ILE:HB	1:B:198:PHE:HE1	1.68	0.57
1:B:302:ASN:OD1	2:B:805:NAG:N2	2.38	0.57
1:C:143:TYR:O	1:C:330:SER:HB3	2.05	0.57
1:C:353:GLU:OE1	1:C:353:GLU:N	2.37	0.57
1:A:126:MET:HG3	1:A:429:VAL:HG13	1.87	0.57
1:B:126:MET:HG3	1:B:429:VAL:HG13	1.87	0.56
1:B:615:LEU:HD13	1:B:628:VAL:HG22	1.87	0.56
1:C:140:VAL:HG23	1:C:334:TRP:HB3	1.85	0.56
2:B:812:NAG:H83	2:B:812:NAG:H3	1.87	0.56
1:B:378:LYS:O	1:B:379:LYS:HG3	2.04	0.56
1:A:143:TYR:OH	1:A:180:ASN:OD1	2.19	0.56
1:B:351:ALA:O	1:B:370:LYS:NZ	2.30	0.56
1:A:304:THR:HB	1:A:316:PRO:HB2	1.86	0.56
1:A:279:PHE:O	1:A:284:ASN:ND2	2.34	0.56
1:A:198:PHE:HB3	1:B:161:LEU:HB2	1.87	0.56
1:A:533:ASN:OD1	1:B:510:ARG:NH1	2.39	0.56
1:B:593:GLN:HE21	1:B:606:ARG:H	1.54	0.56
1:A:377:SER:OG	1:A:378:LYS:N	2.38	0.56
1:C:280:TYR:O	1:C:336:ILE:HD13	2.06	0.56
1:A:288:SER:OG	1:A:289:TYR:N	2.39	0.56
1:B:280:TYR:O	1:B:336:ILE:HD13	2.06	0.55
1:C:272:ASP:HB2	1:C:327:ARG:HH22	1.71	0.55
1:B:105:PHE:CD2	1:B:517:LYS:HA	2.41	0.55
1:B:88:LYS:HZ1	1:B:535:PRO:HD3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:GLU:OE1	1:A:370:LYS:NZ	2.38	0.55
1:A:337:GLN:HG3	1:A:342:VAL:HG21	1.88	0.55
1:A:139:LYS:HG2	1:A:256:THR:HG22	1.88	0.54
1:A:673:SER:HB2	1:C:134:VAL:HG12	1.88	0.54
1:B:529:SER:OG	1:B:536:ILE:N	2.39	0.54
1:B:524:PRO:HB3	1:B:545:LEU:CD1	2.37	0.54
1:C:478:LEU:HD23	1:C:480:TYR:CE1	2.42	0.54
1:C:277:SER:HG	1:C:288:SER:HG	1.55	0.54
1:C:288:SER:OG	1:C:289:TYR:N	2.40	0.54
1:B:353:GLU:OE1	1:B:353:GLU:N	2.32	0.54
1:B:267:ALA:HB2	1:B:273:VAL:HG13	1.88	0.54
1:B:335:ASP:N	1:B:335:ASP:OD1	2.41	0.54
1:C:225:ARG:HB3	1:C:253:THR:HG22	1.90	0.54
1:A:186:TYR:CE1	1:A:210:THR:HG22	2.43	0.53
1:A:677:PHE:HE2	1:B:680:GLU:HG3	1.72	0.53
1:C:297:PHE:CE1	1:C:323:ALA:HB1	2.43	0.53
1:B:144:GLN:HA	1:B:171:PRO:HD3	1.90	0.53
1:A:290:PHE:HZ	1:A:294:ALA:HA	1.74	0.53
1:A:186:TYR:HE1	1:A:210:THR:HG22	1.73	0.53
2:B:807:NAG:H83	2:B:807:NAG:H3	1.90	0.53
1:A:694:LYS:O	1:C:232:GLN:HB2	2.09	0.53
1:B:111:CYS:HB2	1:B:510:ARG:NH2	2.24	0.53
1:B:327:ARG:HH21	1:B:332:ILE:HD11	1.73	0.53
1:A:167:GLU:OE2	1:B:150:ARG:NH1	2.42	0.52
1:B:142:VAL:HG22	1:B:332:ILE:HG12	1.90	0.52
1:C:141:ARG:NH1	1:C:333:SER:OG	2.41	0.52
1:B:372:THR:HG21	1:C:660:PHE:HA	1.91	0.52
1:C:150:ARG:CZ	1:C:164:SER:HB3	2.39	0.52
1:A:479:VAL:HG11	1:C:479:VAL:HG12	1.92	0.52
1:B:106:GLU:O	1:B:513:LEU:HD21	2.09	0.52
1:A:191:ARG:NH1	1:A:193:ILE:HD11	2.22	0.52
1:A:679:LEU:HD12	1:C:679:LEU:HD12	1.91	0.52
1:B:101:ASP:HB3	1:B:547:LEU:HB2	1.92	0.52
1:B:243:ARG:HD2	1:B:244:GLU:H	1.75	0.51
1:A:557:SER:O	1:A:557:SER:OG	2.27	0.51
1:A:150:ARG:CZ	1:A:164:SER:HB3	2.40	0.51
1:C:192:VAL:HG22	1:C:197:VAL:HG22	1.92	0.51
1:C:189:TYR:HE2	1:C:191:ARG:NH1	2.08	0.51
1:A:368:SER:HB3	1:A:371:MET:HB3	1.92	0.51
1:A:411:THR:OG1	1:A:412:TYR:N	2.44	0.51
1:A:353:GLU:N	1:A:353:GLU:OE1	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:808:NAG:O3	2:B:809:NAG:O5	2.26	0.51
1:C:100:THR:OG1	1:C:101:ASP:N	2.44	0.51
1:B:677:PHE:CD2	1:C:680:GLU:HA	2.46	0.51
1:C:529:SER:OG	1:C:536:ILE:N	2.44	0.51
1:B:585:ASN:HA	2:B:811:NAG:H81	1.92	0.51
1:C:177:HIS:O	1:C:181:LYS:HG2	2.09	0.51
1:C:181:LYS:NZ	1:C:304:THR:OG1	2.37	0.51
1:A:628:VAL:HG21	1:A:633:LYS:HD2	1.93	0.51
1:A:270:THR:HA	1:B:685:GLU:HG2	1.93	0.51
1:A:367:SER:HA	1:A:374:THR:HG22	1.93	0.51
1:A:130:LYS:HD2	1:B:666:TYR:CE1	2.45	0.50
1:B:652:ILE:HG21	1:C:498:LEU:HD13	1.93	0.50
1:C:180:ASN:O	1:C:306:VAL:HG13	2.11	0.50
1:A:684:ARG:HD2	1:B:275:TYR:OH	2.12	0.50
1:B:679:LEU:HD12	1:C:679:LEU:HD12	1.93	0.50
1:A:491:ARG:HG3	1:C:655:LEU:HB3	1.94	0.50
1:C:576:ARG:O	1:C:593:GLN:NE2	2.43	0.50
1:B:478:LEU:HD23	1:B:480:TYR:HE1	1.77	0.50
1:C:119:GLU:OE2	1:C:121:LEU:HD23	2.11	0.50
1:A:686:PHE:CE1	1:A:690:LYS:HE2	2.43	0.50
1:C:409:ASN:CG	1:C:411:THR:HG1	2.14	0.50
1:B:386:ASP:HA	2:B:806:NAG:H82	1.92	0.50
1:B:557:SER:O	1:B:581:PHE:HA	2.11	0.50
1:C:138:PHE:CZ	1:C:266:PHE:CE1	3.00	0.49
1:A:153:TYR:HB3	1:A:160:TYR:HB2	1.94	0.49
1:B:93:VAL:HG11	1:B:602:LEU:HD12	1.94	0.49
1:B:148:THR:HG22	1:B:166:THR:HG23	1.93	0.49
1:C:146:VAL:CG2	1:C:249:ASN:HB3	2.41	0.49
1:A:148:THR:HG23	1:A:166:THR:HG22	1.94	0.49
1:A:193:ILE:HG21	1:B:234:HIS:HB3	1.94	0.49
1:B:564:MET:HB2	1:B:630:TYR:HB3	1.94	0.49
1:C:122:ASP:HB2	1:C:357:ARG:HB3	1.95	0.49
1:A:146:VAL:CG2	1:A:249:ASN:HB3	2.42	0.49
1:C:334:TRP:CZ3	1:C:336:ILE:HG12	2.47	0.49
1:B:482:GLN:NE2	1:C:661:ARG:O	2.38	0.49
1:B:581:PHE:HZ	1:B:602:LEU:HD11	1.77	0.49
1:A:147:LEU:HB3	1:A:248:LEU:HD12	1.94	0.49
1:B:371:MET:HA	1:C:661:ARG:HD3	1.94	0.48
1:A:165:ASN:ND2	1:B:164:SER:O	2.46	0.48
1:B:494:ILE:HG13	1:C:494:ILE:HD11	1.95	0.48
1:B:374:THR:HG23	1:B:485:PHE:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:GLU:HG2	1:C:362:ASP:OD1	2.14	0.48
1:B:229:VAL:HG22	1:B:249:ASN:HB3	1.95	0.48
1:B:581:PHE:HE2	1:B:583:PHE:CE1	2.31	0.48
1:C:257:ALA:HB2	1:C:268:THR:HG22	1.95	0.48
1:B:221:THR:OG1	1:B:222:HIS:N	2.47	0.48
1:C:173:MET:HG3	1:C:177:HIS:CD2	2.49	0.47
1:A:234:HIS:HD2	1:C:198:PHE:CZ	2.31	0.47
1:A:679:LEU:HD12	1:B:679:LEU:HD12	1.95	0.47
1:C:367:SER:HA	1:C:374:THR:HG22	1.96	0.47
1:B:177:HIS:O	1:B:181:LYS:HG2	2.14	0.47
1:A:147:LEU:HD13	1:A:149:PHE:CE1	2.49	0.47
1:B:141:ARG:NH1	1:B:143:TYR:OH	2.47	0.47
1:C:148:THR:HG21	1:C:232:GLN:NE2	2.30	0.47
1:A:661:ARG:O	1:C:482:GLN:NE2	2.34	0.47
1:A:151:ARG:HB3	1:A:244:GLU:CG	2.44	0.47
1:B:244:GLU:OE1	1:C:162:LEU:HD13	2.13	0.47
1:C:286:ASN:OD1	2:C:808:NAG:N2	2.47	0.47
1:B:228:THR:HG22	1:B:229:VAL:HG12	1.97	0.47
1:C:136:HIS:O	1:C:258:ARG:HA	2.14	0.47
1:A:691:GLN:NE2	1:B:327:ARG:HH11	2.12	0.47
1:B:193:ILE:HB	1:B:198:PHE:CE1	2.48	0.47
1:A:193:ILE:HB	1:A:198:PHE:CE1	2.50	0.47
1:B:279:PHE:CD2	1:B:339:GLU:HB3	2.50	0.47
1:C:290:PHE:HE2	1:C:297:PHE:CD2	2.33	0.47
1:A:231:ASP:CB	1:B:696:VAL:HG21	2.45	0.47
1:A:676:VAL:HG13	1:C:258:ARG:HB2	1.97	0.47
1:B:286:ASN:OD1	2:B:804:NAG:N2	2.48	0.47
1:A:664:GLU:HG3	1:A:664:GLU:O	2.14	0.47
1:B:564:MET:O	1:B:574:TYR:HB2	2.16	0.46
1:B:560:VAL:HA	1:B:579:VAL:HG22	1.96	0.46
1:C:436:GLN:HE21	1:C:437:LYS:H	1.63	0.46
1:A:147:LEU:HD12	1:A:167:GLU:HB2	1.97	0.46
1:B:621:GLY:HA2	1:B:622:ASN:HA	1.51	0.46
1:B:410:GLN:N	1:B:410:GLN:OE1	2.47	0.46
1:A:206:HIS:CE1	1:B:160:TYR:HH	2.30	0.46
1:A:244:GLU:OE2	1:B:151:ARG:NE	2.49	0.46
1:C:147:LEU:HD23	1:C:248:LEU:HD11	1.97	0.46
1:B:527:ILE:O	1:B:531:ILE:HG23	2.16	0.46
1:B:257:ALA:HB2	1:B:268:THR:HG22	1.98	0.46
1:B:165:ASN:ND2	1:C:164:SER:O	2.49	0.46
1:C:141:ARG:O	1:C:333:SER:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:GLN:H	1:B:696:VAL:HG23	1.81	0.46
1:C:141:ARG:HG2	1:C:254:ILE:HG12	1.98	0.45
1:C:238:SER:O	1:C:241:THR:OG1	2.34	0.45
1:A:582:ASN:HD21	1:A:589:VAL:HG22	1.81	0.45
1:C:186:TYR:HE1	1:C:210:THR:HG22	1.79	0.45
1:A:257:ALA:HB2	1:A:268:THR:HG22	1.99	0.45
1:A:261:TYR:CG	1:A:262:PRO:HA	2.51	0.45
1:C:411:THR:HG22	1:C:436:GLN:NE2	2.31	0.45
1:A:181:LYS:HB2	1:A:182:PHE:CD2	2.52	0.45
1:A:165:ASN:HD22	1:B:164:SER:N	2.13	0.45
1:B:229:VAL:HG13	1:B:249:ASN:HB3	1.98	0.45
1:B:269:SER:OG	1:C:681:GLU:HB3	2.17	0.45
1:C:272:ASP:HB2	1:C:327:ARG:NH2	2.31	0.45
1:A:279:PHE:CD2	1:A:339:GLU:HB3	2.52	0.45
1:C:366:PHE:O	1:C:374:THR:HA	2.16	0.45
1:B:285:ARG:NE	1:B:290:PHE:HB3	2.32	0.45
1:A:680:GLU:O	1:A:684:ARG:HG2	2.17	0.45
1:B:677:PHE:HE2	1:C:680:GLU:HG3	1.82	0.45
1:B:558:VAL:HG13	1:B:579:VAL:HG11	1.98	0.45
1:A:541:MET:HB2	1:A:544:VAL:O	2.17	0.45
1:A:372:THR:O	1:A:482:GLN:HG2	2.17	0.45
1:B:103:ILE:HD11	1:B:528:LEU:CD2	2.41	0.45
1:A:425:GLY:HA3	1:A:480:TYR:OH	2.17	0.45
1:A:554:ASN:HD22	2:A:810:NAG:H83	1.82	0.45
1:B:364:TYR:CD1	1:B:379:LYS:HA	2.51	0.45
1:A:679:LEU:HD23	1:A:679:LEU:O	2.17	0.45
1:B:223:SER:HB3	1:B:255:THR:HG22	1.99	0.44
1:B:523:ASN:ND2	1:C:518:GLU:OE2	2.50	0.44
1:A:185:CYS:HB3	1:A:228:THR:HG21	1.98	0.44
1:B:223:SER:CB	1:B:255:THR:HG22	2.47	0.44
1:B:280:TYR:HE1	1:B:285:ARG:HD3	1.82	0.44
1:A:334:TRP:HZ3	1:A:336:ILE:HG12	1.82	0.44
1:C:279:PHE:CD2	1:C:339:GLU:HB3	2.52	0.44
1:B:644:VAL:O	1:C:108:ASN:ND2	2.50	0.44
1:C:143:TYR:HB2	1:C:331:VAL:CG1	2.46	0.44
1:B:573:CYS:HB3	1:B:630:TYR:CE2	2.53	0.44
1:C:621:GLY:HA2	1:C:622:ASN:HA	1.49	0.44
1:A:547:LEU:H	1:A:547:LEU:HD23	1.81	0.44
1:B:186:TYR:CE1	1:B:210:THR:HG22	2.52	0.44
1:A:351:ALA:O	1:A:370:LYS:NZ	2.36	0.44
1:A:334:TRP:CZ3	1:A:336:ILE:HG12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:GLN:OE1	1:C:648:ILE:HG22	2.18	0.44
1:B:415:TYR:CD2	1:B:435:LYS:HE2	2.52	0.44
1:A:147:LEU:HB3	1:A:248:LEU:CD1	2.48	0.44
1:B:244:GLU:OE2	1:C:151:ARG:NH2	2.49	0.43
1:A:323:ALA:HB2	1:A:336:ILE:HD11	1.99	0.43
1:C:277:SER:OG	1:C:288:SER:OG	2.27	0.43
1:B:272:ASP:OD2	1:B:332:ILE:HD11	2.17	0.43
1:C:632:PHE:HD1	1:C:633:LYS:N	2.16	0.43
1:C:142:VAL:HG22	1:C:332:ILE:HG23	2.00	0.43
1:A:641:ILE:HG12	1:B:102:LEU:HD13	1.99	0.43
2:C:813:NAG:H83	2:C:813:NAG:H3	2.00	0.43
1:B:236:ARG:HA	1:B:236:ARG:HD2	1.73	0.43
1:B:146:VAL:HG22	1:B:168:TYR:CD1	2.53	0.43
1:A:143:TYR:O	1:A:330:SER:HB2	2.19	0.43
1:C:531:ILE:HG13	1:C:532:TYR:CD1	2.54	0.43
1:C:216:ASP:OD1	1:C:217:ASP:N	2.48	0.43
1:A:136:HIS:O	1:A:258:ARG:HA	2.19	0.43
2:C:806:NAG:O3	2:C:806:NAG:O7	2.31	0.43
1:B:334:TRP:CZ3	1:B:336:ILE:HG12	2.53	0.43
1:A:564:MET:O	1:A:574:TYR:HB2	2.18	0.43
1:B:519:LEU:HD23	1:B:519:LEU:HA	1.81	0.43
1:B:420:VAL:HG12	1:B:430:PHE:CD1	2.54	0.43
1:B:100:THR:HB	1:B:101:ASP:H	1.68	0.43
1:C:632:PHE:CD1	1:C:632:PHE:C	2.92	0.43
1:C:229:VAL:O	1:C:249:ASN:ND2	2.51	0.43
1:C:281:ASN:OD1	1:C:284:ASN:ND2	2.52	0.42
1:B:133:ILE:HD11	1:C:670:GLU:HB3	2.01	0.42
1:A:691:GLN:NE2	1:B:327:ARG:NH1	2.68	0.42
1:B:695:TYR:CE1	1:C:191:ARG:NE	2.87	0.42
1:A:270:THR:HG22	1:B:685:GLU:HG2	2.00	0.42
1:B:141:ARG:HG2	1:B:254:ILE:HG12	2.00	0.42
1:B:283:THR:C	1:B:285:ARG:H	2.23	0.42
1:C:409:ASN:OD1	1:C:411:THR:OG1	2.34	0.42
1:A:151:ARG:HB3	1:A:244:GLU:HG2	2.02	0.42
1:C:284:ASN:OD1	2:C:806:NAG:H83	2.20	0.42
1:C:668:GLN:HA	1:C:671:LEU:HG	2.01	0.42
1:A:486:THR:HG23	1:C:487:TYR:HD2	1.84	0.42
1:A:207:GLU:OE1	1:A:207:GLU:N	2.53	0.42
1:A:621:GLY:HA2	1:A:622:ASN:HA	1.43	0.42
1:A:142:VAL:HG22	1:A:332:ILE:HG23	2.02	0.42
1:C:191:ARG:HH11	1:C:191:ARG:CB	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:LYS:HD3	1:B:378:LYS:O	2.20	0.42
1:B:647:MET:SD	1:C:509:GLN:HG2	2.59	0.42
1:A:104:ARG:O	1:C:644:VAL:HG23	2.19	0.42
1:C:311:ARG:HB3	1:C:313:ASN:OD1	2.18	0.42
1:C:690:LYS:HB2	1:C:691:GLN:HE22	1.85	0.42
1:B:142:VAL:HB	1:B:253:THR:OG1	2.19	0.42
1:A:352:SER:HB2	1:A:371:MET:HE3	2.02	0.42
1:A:228:THR:HG21	1:A:250:CYS:HB3	2.01	0.42
1:B:261:TYR:CG	1:B:262:PRO:HA	2.53	0.42
1:B:277:SER:HA	1:B:278:PRO:HD3	1.91	0.42
1:A:103:ILE:HG13	1:A:547:LEU:HD22	2.02	0.42
1:B:175:GLU:O	1:B:179:ILE:HG13	2.20	0.42
1:C:268:THR:OG1	1:C:272:ASP:OD1	2.35	0.42
1:A:487:TYR:HD2	1:B:486:THR:HG23	1.84	0.42
1:A:528:LEU:HA	1:A:528:LEU:HD23	1.86	0.42
1:A:478:LEU:HD12	1:A:480:TYR:HE1	1.84	0.41
1:C:585:ASN:N	2:C:813:NAG:O7	2.53	0.41
1:B:372:THR:O	1:B:482:GLN:HG2	2.19	0.41
1:C:638:LEU:HD23	1:C:638:LEU:HA	1.77	0.41
1:C:189:TYR:CE2	1:C:191:ARG:NH1	2.88	0.41
1:C:357:ARG:NH2	1:C:364:TYR:HE2	2.18	0.41
1:B:580:ILE:HA	1:B:590:GLN:O	2.20	0.41
1:A:160:TYR:HH	1:C:206:HIS:CD2	2.29	0.41
1:A:554:ASN:HB3	1:A:557:SER:CB	2.48	0.41
1:A:173:MET:O	1:A:176:ILE:HG12	2.21	0.41
1:A:176:ILE:HA	1:A:179:ILE:HD12	2.03	0.41
1:C:559:LYS:HE2	1:C:580:ILE:HG13	2.03	0.41
1:A:229:VAL:HG22	1:A:231:ASP:H	1.86	0.41
1:A:655:LEU:HD13	1:C:493:TYR:CG	2.55	0.41
1:C:272:ASP:CB	1:C:327:ARG:HH22	2.34	0.41
1:C:129:TYR:CZ	1:C:348:PHE:HB2	2.56	0.41
1:B:187:SER:OG	1:B:211:MET:SD	2.79	0.41
1:A:324:PHE:CD1	1:A:333:SER:HB2	2.56	0.41
1:C:297:PHE:HE1	1:C:323:ALA:HB1	1.85	0.41
1:A:279:PHE:CG	1:A:339:GLU:HB3	2.56	0.41
2:B:802:NAG:H4	3:B:803:BMA:H2	1.78	0.41
1:C:85:ASN:O	1:C:86:THR:OG1	2.31	0.41
1:B:225:ARG:CD	1:B:253:THR:HG22	2.40	0.40
1:C:153:TYR:HD1	1:C:154:ALA:N	2.19	0.40
1:C:266:PHE:HB3	1:C:274:VAL:HB	2.02	0.40
1:A:403:ILE:O	1:A:407:SER:OG	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:TYR:HE2	1:B:434:ILE:HD13	1.81	0.40
1:A:352:SER:HA	1:A:370:LYS:NZ	2.36	0.40
1:A:206:HIS:NE2	1:B:160:TYR:OH	2.39	0.40
1:A:357:ARG:NH2	1:A:364:TYR:HE1	2.18	0.40
1:A:173:MET:HG3	1:A:177:HIS:CE1	2.56	0.40
1:C:576:ARG:H	1:C:593:GLN:HE22	1.69	0.40
1:C:557:SER:O	1:C:581:PHE:HA	2.22	0.40
1:A:143:TYR:HB2	1:A:331:VAL:CG2	2.52	0.40
1:C:107:ARG:HA	1:C:513:LEU:HD21	2.03	0.40
1:B:493:TYR:CG	1:C:655:LEU:HD13	2.56	0.40
1:C:175:GLU:O	1:C:179:ILE:HG13	2.21	0.40
1:A:666:TYR:CE1	1:C:130:LYS:HD2	2.56	0.40
1:A:534:LYS:O	1:A:536:ILE:HG13	2.20	0.40
1:A:655:LEU:HA	1:A:655:LEU:HD12	1.93	0.40
1:A:565:ASN:HA	1:A:573:CYS:HA	2.02	0.40
1:A:671:LEU:O	1:A:674:SER:OG	2.40	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	554/630 (88%)	541 (98%)	11 (2%)	2 (0%)	39 80
1	B	564/630 (90%)	541 (96%)	22 (4%)	1 (0%)	52 87
1	C	570/630 (90%)	544 (95%)	26 (5%)	0	100 100
All	All	1688/1890 (89%)	1626 (96%)	59 (4%)	3 (0%)	52 87

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	GLU

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Mol	Chain	Res	Type
1	A	284	ASN
1	B	100	THR

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	504/569 (89%)	482 (96%)	22 (4%)	35	74
1	B	512/569 (90%)	493 (96%)	19 (4%)	41	77
1	C	517/569 (91%)	498 (96%)	19 (4%)	41	77
All	All	1533/1707 (90%)	1473 (96%)	60 (4%)	39	77

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	115	LYS
1	A	133	ILE
1	A	147	LEU
1	A	151	ARG
1	A	161	LEU
1	A	191	ARG
1	A	206	HIS
1	A	229	VAL
1	A	337	GLN
1	A	531	ILE
1	A	533	ASN
1	A	534	LYS
1	A	566	VAL
1	A	578	VAL
1	A	580	ILE
1	A	591	TYR
1	A	631	LEU
1	A	632	PHE
1	A	637	ASP

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Mol	Chain	Res	Type
1	A	662	VAL
1	A	693	VAL
1	B	92	ARG
1	B	100	THR
1	B	102	LEU
1	B	108	ASN
1	B	131	ARG
1	B	147	LEU
1	B	148	THR
1	B	229	VAL
1	B	335	ASP
1	B	379	LYS
1	B	411	THR
1	B	498	LEU
1	B	545	LEU
1	B	552	THR
1	B	594	LEU
1	B	623	SER
1	B	642	SER
1	B	661	ARG
1	B	662	VAL
1	C	121	LEU
1	C	128	VAL
1	C	147	LEU
1	C	191	ARG
1	C	206	HIS
1	C	207	GLU
1	C	229	VAL
1	C	231	ASP
1	C	236	ARG
1	C	252	LEU
1	C	269	SER
1	C	299	ILE
1	C	319	HIS
1	C	411	THR
1	C	562	ARG
1	C	632	PHE
1	C	646	SER
1	C	661	ARG
1	C	676	VAL

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

Mol	Chain	Res	Type
1	A	165	ASN
1	A	582	ASN
1	A	691	GLN
1	B	144	GLN
1	C	605	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 1 is monoatomic - leaving 38 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	NAG	A	801	1,2	14,14,15	0.29	0	15,19,21	0.60	0
2	NAG	A	802	3,2	14,14,15	0.30	0	15,19,21	0.60	0
3	BMA	A	803	2,4	11,11,12	0.92	1 (9%)	15,15,17	1.64	4 (26%)
4	MAN	A	804	3	11,11,12	1.27	2 (18%)	15,15,17	1.35	2 (13%)
2	NAG	A	805	1	14,14,15	0.24	0	15,19,21	0.44	0
2	NAG	A	806	1	14,14,15	0.41	0	15,19,21	0.33	0
2	NAG	A	807	1	14,14,15	0.66	1 (7%)	15,19,21	0.73	0
2	NAG	A	808	1	14,14,15	0.27	0	15,19,21	0.57	0
2	NAG	A	809	1	14,14,15	0.53	0	15,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	810	1	14,14,15	0.35	0	15,19,21	0.21	0
2	NAG	A	811	1	14,14,15	0.77	1 (7%)	15,19,21	0.57	0
2	NAG	B	801	1,2	14,14,15	0.66	1 (7%)	15,19,21	0.75	0
2	NAG	B	802	3,2	14,14,15	0.19	0	15,19,21	0.76	1 (6%)
3	BMA	B	803	2	11,11,12	1.36	1 (9%)	15,15,17	1.17	1 (6%)
2	NAG	B	804	1	14,14,15	0.34	0	15,19,21	0.59	0
2	NAG	B	805	1	14,14,15	0.29	0	15,19,21	0.40	0
2	NAG	B	806	1,2	14,14,15	0.85	1 (7%)	15,19,21	0.98	1 (6%)
2	NAG	B	807	2	14,14,15	0.59	0	15,19,21	1.30	1 (6%)
2	NAG	B	808	1,2	14,14,15	0.46	0	15,19,21	0.68	0
2	NAG	B	809	2	14,14,15	0.60	1 (7%)	15,19,21	0.72	0
2	NAG	B	810	1	14,14,15	0.36	0	15,19,21	0.86	0
2	NAG	B	811	1	14,14,15	0.27	0	15,19,21	0.42	0
2	NAG	B	812	1,2	14,14,15	0.46	0	15,19,21	1.41	2 (13%)
2	NAG	B	813	2	14,14,15	1.32	2 (14%)	15,19,21	1.28	1 (6%)
2	NAG	C	801	1,2	14,14,15	0.36	0	15,19,21	0.85	1 (6%)
2	NAG	C	802	3,2	14,14,15	0.55	0	15,19,21	0.60	0
3	BMA	C	803	2,4	11,11,12	1.14	0	15,15,17	1.22	2 (13%)
4	MAN	C	804	3	11,11,12	1.31	1 (9%)	15,15,17	0.93	1 (6%)
4	MAN	C	805	3	11,11,12	1.51	2 (18%)	15,15,17	1.10	1 (6%)
2	NAG	C	806	1,2	14,14,15	0.67	0	15,19,21	0.95	1 (6%)
2	NAG	C	807	2	14,14,15	0.58	0	15,19,21	1.28	2 (13%)
2	NAG	C	808	1	14,14,15	1.02	1 (7%)	15,19,21	1.29	1 (6%)
2	NAG	C	809	1	14,14,15	0.45	0	15,19,21	0.60	0
2	NAG	C	810	1	14,14,15	0.59	0	15,19,21	0.55	0
2	NAG	C	811	1	14,14,15	0.39	0	15,19,21	0.52	0
2	NAG	C	812	1	14,14,15	0.60	1 (7%)	15,19,21	0.68	1 (6%)
2	NAG	C	813	1,2	14,14,15	0.90	1 (7%)	15,19,21	1.80	2 (13%)
2	NAG	C	814	2	14,14,15	0.37	0	15,19,21	0.25	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	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	802	3,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	A	803	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	804	3	-	0/2/19/22	0/1/1/1
2	NAG	A	805	1	-	0/6/23/26	0/1/1/1
2	NAG	A	806	1	-	0/6/23/26	0/1/1/1
2	NAG	A	807	1	-	0/6/23/26	0/1/1/1
2	NAG	A	808	1	-	0/6/23/26	0/1/1/1
2	NAG	A	809	1	-	0/6/23/26	0/1/1/1
2	NAG	A	810	1	-	0/6/23/26	0/1/1/1
2	NAG	A	811	1	-	0/6/23/26	0/1/1/1
2	NAG	B	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	802	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	803	2	-	0/2/19/22	0/1/1/1
2	NAG	B	804	1	-	0/6/23/26	0/1/1/1
2	NAG	B	805	1	-	0/6/23/26	0/1/1/1
2	NAG	B	806	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	807	2	-	0/6/23/26	0/1/1/1
2	NAG	B	808	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	809	2	-	0/6/23/26	0/1/1/1
2	NAG	B	810	1	-	0/6/23/26	0/1/1/1
2	NAG	B	811	1	-	0/6/23/26	0/1/1/1
2	NAG	B	812	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	813	2	-	0/6/23/26	0/1/1/1
2	NAG	C	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	802	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	803	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	804	3	-	0/2/19/22	0/1/1/1
4	MAN	C	805	3	-	0/2/19/22	0/1/1/1
2	NAG	C	806	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	807	2	-	0/6/23/26	0/1/1/1
2	NAG	C	808	1	-	0/6/23/26	0/1/1/1
2	NAG	C	809	1	-	0/6/23/26	0/1/1/1
2	NAG	C	810	1	-	0/6/23/26	0/1/1/1
2	NAG	C	811	1	-	0/6/23/26	0/1/1/1
2	NAG	C	812	1	-	0/6/23/26	0/1/1/1
2	NAG	C	813	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	814	2	-	0/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	806	NAG	O5-C1	-2.95	1.38	1.43
4	C	804	MAN	O5-C1	-2.70	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	NAG	O5-C1	-2.36	1.39	1.43
2	A	807	NAG	O5-C1	-2.27	1.40	1.43
2	C	812	NAG	O5-C1	-2.03	1.40	1.43
3	A	803	BMA	C1-C2	2.10	1.57	1.52
2	B	809	NAG	C1-C2	2.14	1.55	1.52
4	A	804	MAN	C1-C2	2.20	1.57	1.52
4	C	805	MAN	C1-C2	2.40	1.58	1.52
2	A	811	NAG	O5-C1	2.51	1.47	1.43
4	A	804	MAN	C2-C3	2.56	1.56	1.52
2	B	813	NAG	O5-C1	2.82	1.48	1.43
2	C	813	NAG	O5-C1	2.89	1.48	1.43
2	C	808	NAG	C1-C2	3.23	1.57	1.52
3	B	803	BMA	C4-C5	3.39	1.60	1.53
4	C	805	MAN	C2-C3	3.73	1.57	1.52
2	B	813	NAG	C1-C2	3.82	1.57	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	803	BMA	O5-C5-C4	-2.91	105.31	110.13
2	C	801	NAG	O4-C4-C5	-2.42	102.86	109.23
2	C	812	NAG	C1-O5-C5	-2.40	108.61	112.14
3	B	803	BMA	O5-C1-C2	-2.10	107.54	110.89
4	C	804	MAN	O2-C2-C3	-2.07	106.02	110.19
3	A	803	BMA	O2-C2-C3	-2.02	106.12	110.19
3	C	803	BMA	C6-C5-C4	2.04	118.11	112.99
2	B	802	NAG	C1-O5-C5	2.06	115.17	112.14
4	C	805	MAN	C1-O5-C5	2.08	115.19	112.14
2	B	806	NAG	C3-C4-C5	2.29	114.31	110.23
2	B	812	NAG	O4-C4-C3	2.30	115.55	110.36
2	C	807	NAG	O5-C5-C4	2.39	114.09	110.13
4	A	804	MAN	C1-C2-C3	2.48	112.56	109.55
3	A	803	BMA	O5-C1-C2	2.50	114.89	110.89
2	C	806	NAG	C1-O5-C5	2.87	116.36	112.14
3	A	803	BMA	C1-O5-C5	3.17	116.80	112.14
4	A	804	MAN	C1-O5-C5	3.58	117.40	112.14
2	C	807	NAG	C3-C4-C5	3.84	117.08	110.23
3	A	803	BMA	C1-C2-C3	3.94	114.32	109.55
2	B	813	NAG	C2-N2-C7	4.52	128.99	123.11
2	C	813	NAG	C1-O5-C5	4.55	118.82	112.14
2	C	808	NAG	C2-N2-C7	4.55	129.03	123.11
2	C	813	NAG	C2-N2-C7	4.66	129.17	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	812	NAG	C2-N2-C7	4.69	129.20	123.11
2	B	807	NAG	C2-N2-C7	4.76	129.29	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	810	NAG	1	0
2	B	802	NAG	1	0
3	B	803	BMA	1	0
2	B	804	NAG	1	0
2	B	805	NAG	1	0
2	B	806	NAG	1	0
2	B	807	NAG	1	0
2	B	808	NAG	1	0
2	B	809	NAG	1	0
2	B	811	NAG	1	0
2	B	812	NAG	1	0
2	B	813	NAG	1	0
2	C	806	NAG	2	0
2	C	808	NAG	2	0
2	C	813	NAG	2	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	562/630 (89%)	-0.07	4 (0%) 89 81	66, 116, 152, 183	0
1	B	570/630 (90%)	-0.10	3 (0%) 91 86	65, 108, 149, 166	0
1	C	576/630 (91%)	-0.08	0 100 100	64, 102, 145, 176	0
All	All	1708/1890 (90%)	-0.08	7 (0%) 93 88	64, 109, 151, 183	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	320	ARG	2.3
1	B	242	HIS	2.3
1	A	259	SER	2.2
1	A	193	ILE	2.2
1	A	430	PHE	2.2
1	B	309	PHE	2.1
1	A	191	ARG	2.1

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

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	805	14/15	0.87	0.23	0.32	162,167,177,185	0
2	NAG	A	810	14/15	0.72	0.23	0.25	144,160,170,171	0
2	NAG	B	801	14/15	0.91	0.24	-0.66	104,111,122,126	0
2	NAG	B	811	14/15	0.89	0.14	-1.00	109,125,134,134	0
2	NAG	C	801	14/15	0.90	0.20	-1.14	80,89,99,105	0
2	NAG	A	801	14/15	0.93	0.15	-1.45	105,114,124,126	0
5	CA	A	812	1/1	0.95	0.10	-3.36	94,94,94,94	0
4	MAN	C	805	11/12	0.90	0.19	-	127,135,151,156	0
2	NAG	C	813	14/15	0.83	0.17	-	153,165,177,180	0
2	NAG	C	811	14/15	0.82	0.42	-	162,169,175,178	0
2	NAG	C	806	14/15	0.80	0.18	-	144,161,172,173	0
2	NAG	C	809	14/15	0.77	0.40	-	149,162,165,170	0
2	NAG	A	811	14/15	0.62	0.25	-	147,171,175,178	0
2	NAG	B	808	14/15	0.81	0.21	-	176,180,186,188	0
2	NAG	B	806	14/15	0.81	0.33	-	155,171,184,190	0
4	MAN	C	804	11/12	0.72	0.26	-	135,143,148,148	0
2	NAG	B	805	14/15	0.83	0.17	-	134,145,157,163	0
2	NAG	C	807	14/15	0.85	0.14	-	163,176,182,184	0
2	NAG	B	804	14/15	0.66	0.30	-	157,181,185,188	0
2	NAG	B	807	14/15	0.71	0.47	-	169,184,193,193	0
3	BMA	C	803	11/12	0.85	0.16	-	106,117,130,136	0
3	BMA	B	803	11/12	0.81	0.22	-	120,133,138,139	0
2	NAG	C	802	14/15	0.94	0.18	-	87,95,106,110	0
2	NAG	B	802	14/15	0.92	0.22	-	109,114,121,122	0
2	NAG	C	812	14/15	0.76	0.39	-	163,172,176,178	0
2	NAG	C	810	14/15	0.74	0.41	-	160,163,171,173	0
4	MAN	A	804	11/12	0.79	0.20	-	145,169,176,177	0
2	NAG	B	809	14/15	0.79	0.26	-	177,188,192,192	0
2	NAG	A	809	14/15	0.75	0.19	-	164,175,183,184	0
2	NAG	B	810	14/15	0.84	0.21	-	146,166,174,174	0
2	NAG	C	808	14/15	0.73	0.23	-	143,171,174,176	0
2	NAG	B	813	14/15	0.80	0.29	-	167,181,186,187	0
2	NAG	A	802	14/15	0.85	0.18	-	109,114,131,131	0
3	BMA	A	803	11/12	0.80	0.17	-	133,144,153,158	0
2	NAG	A	806	14/15	0.72	0.26	-	160,166,169,176	0
2	NAG	A	808	14/15	0.81	0.19	-	169,175,178,179	0
2	NAG	A	807	14/15	0.81	0.27	-	156,167,171,171	0
2	NAG	B	812	14/15	0.84	0.17	-	141,165,180,182	0
2	NAG	C	814	14/15	0.83	0.19	-	180,183,188,189	0

6.5 Other polymers (i)

There are no such residues in this entry.