Full wwPDB X-ray Structure Validation Report

Apr 8, 2024 – 12:29 PM EDT

PDB ID	:	8SIC
Title	:	Crystal structure of Epstein-Barr virus glycoprotein 350 (gp350) in complex with Cy137C02, a monoclonal antibody isolated from macaques immunized with a gp350 nanoparticle vaccine
Authors	:	Joyce, M.G.; Jensen, J.L.; Chen, W.H.; Kanekiyo, M.
Deposited on	:	2023-04-14
Resolution	:	2.76 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:

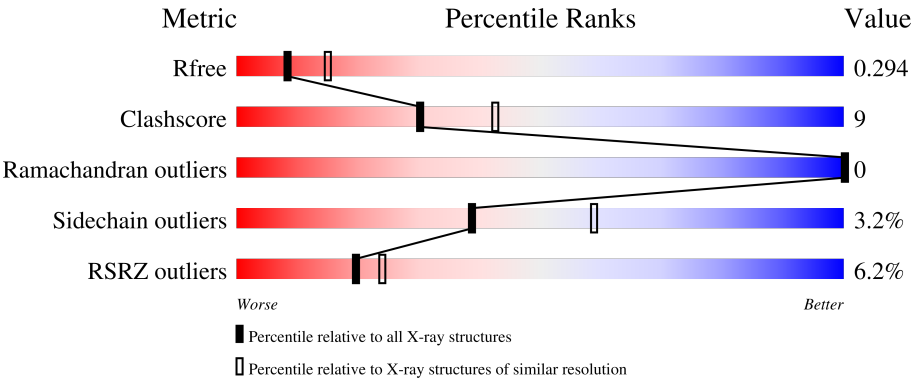
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 2.76 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	222	7% 75% 24%
1	H	222	5% 84% 15%
2	B	215	2% 86% 13%
2	L	215	3% 88% 12%
3	E	431	10% 63% 28% 6%

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Mol	Chain	Length	Quality of chain
3	G	431	6% 82% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	E	504	-	-	-	X
4	NAG	E	508	-	-	-	X
4	NAG	G	501	-	-	-	X
4	NAG	G	502	-	-	-	X
4	NAG	G	508	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13230 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 Cy137C02 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1678	1068	281	325	4			
1	H	221	Total	C	N	O	S	0	0	0
			1671	1064	280	323	4			

- Molecule 2 is a protein called Cy137C02 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1604	1003	268	328	5			
2	L	215	Total	C	N	O	S	0	0	0
			1604	1003	268	328	5			

- Molecule 3 is a protein called Envelope glycoprotein gp350.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	404	Total	C	N	O	S	0	1	0
			3111	1964	512	618	17			
3	G	419	Total	C	N	O	S	0	0	0
			3206	2024	525	640	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	426	HIS	-	expression tag	UNP P03200
E	427	HIS	-	expression tag	UNP P03200
E	428	HIS	-	expression tag	UNP P03200
E	429	HIS	-	expression tag	UNP P03200
E	430	HIS	-	expression tag	UNP P03200
E	431	HIS	-	expression tag	UNP P03200
G	426	HIS	-	expression tag	UNP P03200
G	427	HIS	-	expression tag	UNP P03200

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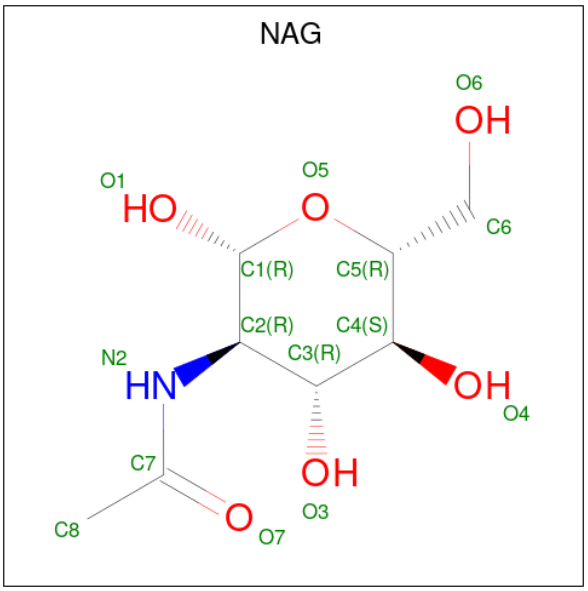
Chain	Residue	Modelled	Actual	Comment	Reference
G	428	HIS	-	expression tag	UNP P03200
G	429	HIS	-	expression tag	UNP P03200
G	430	HIS	-	expression tag	UNP P03200
G	431	HIS	-	expression tag	UNP P03200

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total Zn 1 1	0	0
5	G	1	Total Zn 1 1	0	0

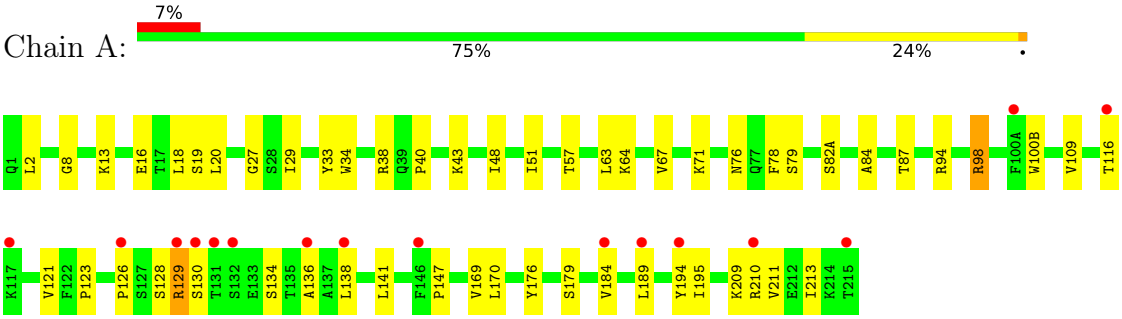
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	5	Total O 5 5	0	0
6	B	8	Total O 8 8	0	0
6	E	22	Total O 22 22	0	0
6	G	37	Total O 37 37	0	0
6	H	26	Total O 26 26	0	0
6	L	18	Total O 18 18	0	0

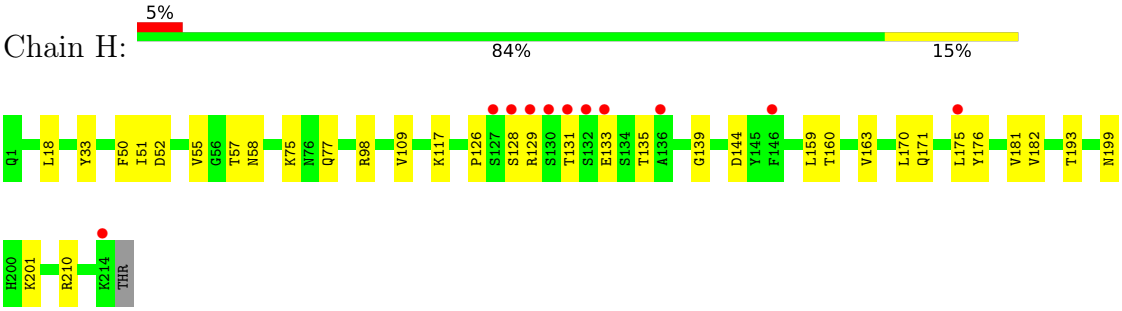
3 Residue-property plots (i)

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.

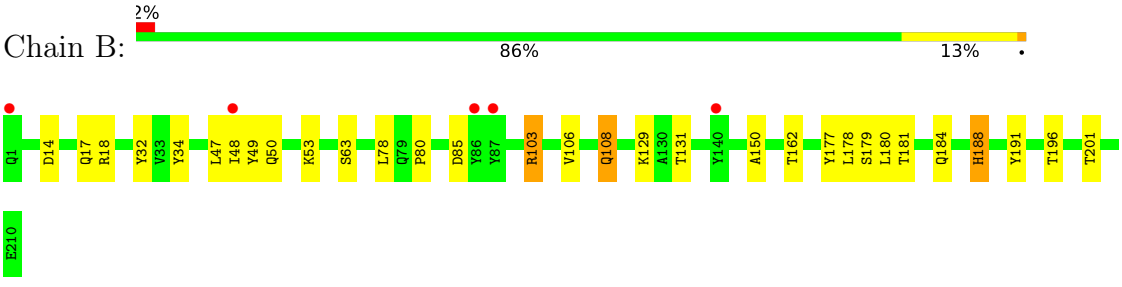
• Molecule 1: Cy137C02 Fab heavy chain



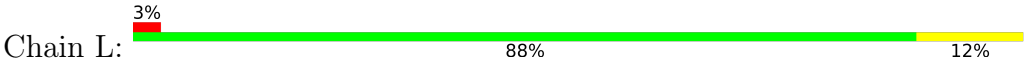
• Molecule 1: Cy137C02 Fab heavy chain

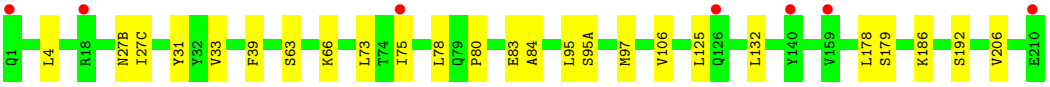


• Molecule 2: Cy137C02 Fab light chain

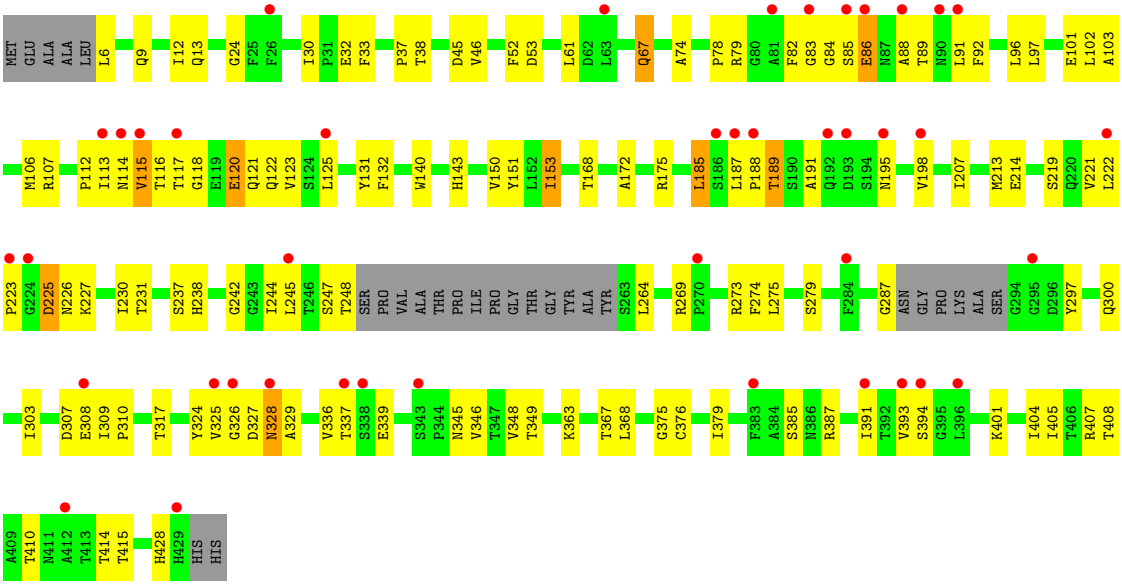


• Molecule 2: Cy137C02 Fab light chain

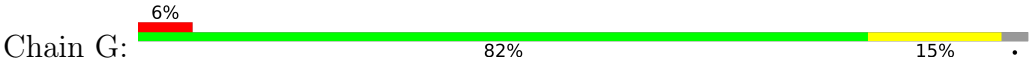


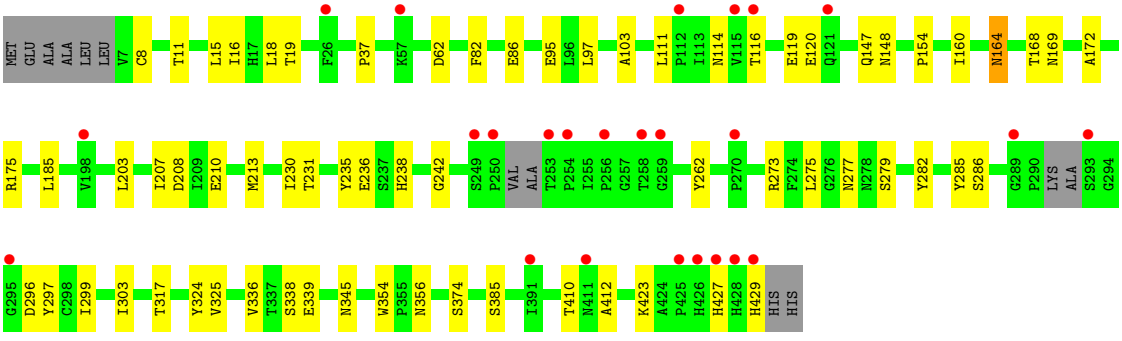


• Molecule 3: Envelope glycoprotein gp350



• Molecule 3: Envelope glycoprotein gp350





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	69.05Å 71.38Å 395.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.38 – 2.76 71.38 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.5 (71.38-2.76) 99.5 (71.38-2.76)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.245 , 0.295 0.250 , 0.294	Depositor DCC
R_{free} test set	2611 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	75.8	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13230	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% 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: NAG, ZN

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	0.31	0/1723	0.58	0/2355
1	H	0.31	0/1716	0.52	0/2345
2	B	0.29	0/1643	0.49	0/2240
2	L	0.27	0/1643	0.53	0/2240
3	E	0.37	0/3188	0.60	0/4356
3	G	0.30	0/3286	0.53	0/4495
All	All	0.32	0/13199	0.55	0/18031

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	1678	0	1667	40	0
1	H	1671	0	1660	24	0
2	B	1604	0	1546	23	0
2	L	1604	0	1546	15	0
3	E	3111	0	2978	102	0
3	G	3206	0	3054	46	0
4	E	112	0	104	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	126	0	117	7	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	A	5	0	0	0	0
6	B	8	0	0	0	0
6	E	22	0	0	1	0
6	G	37	0	0	1	0
6	H	26	0	0	0	0
6	L	18	0	0	0	0
All	All	13230	0	12672	239	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 9.

All (239) 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)
3:E:363:LYS:HD3	3:E:375:GLY:HA3	1.24	1.15
1:A:138:LEU:HD13	1:A:211:VAL:HG11	1.17	1.09
3:E:363:LYS:CD	3:E:375:GLY:HA3	1.91	1.00
3:G:338:SER:HB2	3:G:412:ALA:HA	1.48	0.93
3:E:125:LEU:H	3:E:150:VAL:HG22	1.34	0.92
3:E:13:GLN:HG2	3:E:143:HIS:HB3	1.53	0.89
3:E:38:THR:HG23	3:E:404:ILE:HD11	1.51	0.89
2:B:78:LEU:HD21	2:B:106:VAL:HG22	1.58	0.84
1:A:129:ARG:HA	1:A:129:ARG:NE	1.93	0.80
1:H:126:PRO:HA	1:H:129:ARG:HH21	1.47	0.80
3:E:37:PRO:HG3	3:E:317:THR:HG21	1.64	0.80
3:G:37:PRO:HG3	3:G:317:THR:HG21	1.69	0.74
3:E:297:TYR:HD1	4:E:509:NAG:H5	1.52	0.74
3:E:324:TYR:HD2	3:E:326:GLY:O	1.69	0.74
3:E:297:TYR:CD1	4:E:509:NAG:H5	2.25	0.71
3:E:24:GLY:HA3	3:E:207:ILE:HG22	1.73	0.71
3:E:61:LEU:HA	3:E:83:GLY:HA3	1.72	0.70
2:B:80:PRO:HA	2:B:106:VAL:HG21	1.72	0.70
3:G:86:GLU:HB2	4:G:504:NAG:H82	1.72	0.70
3:E:12:ILE:HD11	3:E:32:GLU:HG3	1.73	0.69
3:G:207:ILE:HD11	3:G:275:LEU:HG	1.72	0.69
3:E:74:ALA:HA	3:E:96:LEU:HD12	1.74	0.69
1:A:138:LEU:HD13	1:A:211:VAL:CG1	2.10	0.69
3:E:391:ILE:HD12	3:E:405:ILE:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:285:TYR:HE1	3:G:299:ILE:HD13	1.59	0.68
3:E:175:ARG:NH2	3:E:308:GLU:OE1	2.26	0.68
3:E:348:VAL:HG22	3:E:407:ARG:HG3	1.76	0.68
1:H:159:LEU:HD21	1:H:182:VAL:HG21	1.76	0.67
3:E:237:SER:HB3	3:E:269:ARG:CG	2.26	0.65
1:A:129:ARG:NE	1:A:136:ALA:HB2	2.11	0.65
1:A:129:ARG:HE	1:A:136:ALA:HB2	1.60	0.64
3:E:336:VAL:HG23	3:E:415:THR:HG22	1.80	0.63
3:E:214:GLU:HG2	3:E:231:THR:HG23	1.80	0.63
2:B:50:GLN:HB2	2:B:53:LYS:HD2	1.80	0.63
3:E:238:HIS:HD2	3:G:429:HIS:HB3	1.62	0.63
3:E:191:ALA:HB1	3:E:221:VAL:HG11	1.79	0.63
3:E:222:LEU:HD23	3:E:226:ASN:HB3	1.81	0.63
2:B:196:THR:HG23	2:B:201:THR:HG22	1.80	0.62
3:G:286:SER:HA	3:G:296:ASP:HB2	1.82	0.61
3:E:337:THR:HG23	3:E:339:GLU:HG3	1.80	0.61
3:G:116:THR:HG23	3:G:116:THR:O	2.00	0.61
1:A:38:ARG:HD3	1:A:48:ILE:HD11	1.83	0.61
3:E:85:SER:HB2	3:E:112:PRO:O	2.01	0.61
1:A:33:TYR:CZ	1:A:98:ARG:HB3	2.37	0.59
3:E:85:SER:HB3	3:E:88:ALA:HB2	1.82	0.59
3:G:210:GLU:OE1	1:H:98:ARG:NH1	2.35	0.59
1:A:169:VAL:HG22	2:B:162:THR:HG22	1.85	0.59
3:E:117:THR:H	3:E:120:GLU:CD	2.06	0.59
3:G:374:SER:HB3	6:G:619:HOH:O	2.01	0.59
2:L:83:GLU:HG3	2:L:106:VAL:HG23	1.85	0.58
1:A:18:LEU:HD12	1:A:109:VAL:HG11	1.85	0.58
1:A:126:PRO:HB2	1:A:129:ARG:H	1.68	0.58
3:E:237:SER:HB3	3:E:269:ARG:HG3	1.85	0.58
3:E:385:SER:HB2	4:E:503:NAG:H82	1.85	0.58
1:H:193:THR:HA	1:H:210:ARG:NH2	2.19	0.58
3:E:195:ASN:H	3:E:219:SER:HA	1.69	0.58
3:E:84:GLY:HA3	3:E:114:ASN:HB3	1.85	0.57
3:E:185:LEU:HD11	3:E:248:THR:OG1	2.04	0.57
2:B:184:GLN:O	2:B:191:TYR:OH	2.21	0.57
3:E:230:ILE:HG23	3:E:242:GLY:HA2	1.87	0.57
3:E:346:VAL:HG21	3:E:387:ARG:HH11	1.68	0.57
3:E:368:LEU:HD11	3:E:387:ARG:NH1	2.20	0.57
3:E:225:ASP:HB3	3:E:244:ILE:HG12	1.87	0.56
3:E:328:ASN:HA	3:E:394:SER:CB	2.35	0.56
3:G:325:VAL:HG21	3:G:427:HIS:CG	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:237:SER:HB3	3:E:269:ARG:HG2	1.87	0.56
3:G:172:ALA:HB3	3:G:303:ILE:HG22	1.88	0.56
1:A:129:ARG:HG3	1:A:213:ILE:HG12	1.87	0.55
3:E:198:VAL:H	3:E:213:MET:HE3	1.71	0.55
3:G:230:ILE:HG23	3:G:242:GLY:HA2	1.88	0.55
1:A:179:SER:HG	2:B:177:TYR:HH	1.54	0.55
3:E:297:TYR:HA	4:E:509:NAG:H62	1.88	0.55
2:L:186:LYS:O	2:L:186:LYS:HD3	2.07	0.55
1:A:2:LEU:HD12	1:A:27:GLY:HA3	1.89	0.55
1:A:170:LEU:HG	1:A:176:TYR:CE1	2.41	0.55
1:A:129:ARG:HG3	1:A:213:ILE:CG1	2.37	0.54
2:B:32:TYR:HD1	2:B:50:GLN:HA	1.73	0.54
3:E:387:ARG:HB3	3:E:407:ARG:HH22	1.72	0.54
3:E:38:THR:CG2	3:E:404:ILE:HD11	2.32	0.53
3:E:408:THR:HB	3:E:414:THR:HG23	1.89	0.53
1:H:33:TYR:CD2	1:H:52:ASP:HA	2.44	0.53
3:E:187:LEU:HD11	3:E:287:GLY:C	2.28	0.53
3:E:172:ALA:HB3	3:E:303:ILE:HG22	1.91	0.52
3:E:207:ILE:HG13	3:E:275:LEU:HD23	1.91	0.52
3:G:185:LEU:HD12	3:G:262:TYR:HB2	1.90	0.52
1:H:163:VAL:HG12	1:H:182:VAL:HB	1.91	0.52
2:B:47:LEU:O	2:B:48:ILE:HD13	2.10	0.52
3:E:191:ALA:HB1	3:E:221:VAL:CG1	2.39	0.52
3:G:325:VAL:HG21	3:G:427:HIS:CD2	2.45	0.52
2:B:78:LEU:CD2	2:B:106:VAL:HG22	2.36	0.51
3:E:33:PHE:HD2	3:E:102:LEU:HD21	1.75	0.51
3:E:85:SER:CB	3:E:88:ALA:HB2	2.39	0.51
1:H:18:LEU:HD13	1:H:109:VAL:HG11	1.92	0.51
3:E:84:GLY:CA	3:E:114:ASN:HB3	2.40	0.51
3:E:92:PHE:CE1	3:E:106:MET:HG3	2.45	0.51
3:G:285:TYR:CE1	3:G:299:ILE:HD13	2.43	0.51
3:G:169:ASN:HD22	4:G:502:NAG:C7	2.22	0.51
3:G:338:SER:CB	3:G:412:ALA:HA	2.32	0.51
2:L:95:LEU:HD12	2:L:97:MET:SD	2.50	0.51
3:E:345:ASN:HB2	3:E:410:THR:HG23	1.92	0.51
4:G:505:NAG:H81	1:H:55:VAL:HG21	1.92	0.51
1:A:123:PRO:HD3	1:A:209:LYS:HE3	1.93	0.51
3:E:84:GLY:C	3:E:114:ASN:HB3	2.31	0.51
3:E:346:VAL:HG21	3:E:387:ARG:NH1	2.25	0.51
3:G:19:THR:HG21	3:G:236:GLU:HG3	1.92	0.50
3:G:336:VAL:HG12	3:G:339:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:THR:HA	1:A:147:PRO:HD3	1.94	0.50
3:E:9:GLN:HG2	4:E:502:NAG:H61	1.92	0.50
3:G:62:ASP:HB2	3:G:82:PHE:HB3	1.94	0.50
1:A:8:GLY:HA3	1:A:20:LEU:HD12	1.94	0.50
3:G:168:THR:O	3:G:169:ASN:HB2	2.11	0.50
3:E:223:PRO:HA	3:E:247:SER:OG	2.12	0.50
2:B:50:GLN:CB	2:B:53:LYS:HD2	2.41	0.49
3:G:18:LEU:HB2	3:G:235:TYR:CZ	2.47	0.49
2:L:27(C):ILE:HD12	2:L:33:VAL:HG21	1.94	0.49
3:E:363:LYS:HD2	3:E:375:GLY:HA3	1.87	0.49
3:G:114:ASN:HD22	4:G:504:NAG:H83	1.78	0.49
1:A:100(B):TRP:HB3	2:B:34:TYR:CE1	2.47	0.49
3:G:8:CYS:SG	3:G:11:THR:HG22	2.52	0.49
3:E:221:VAL:HA	3:E:226:ASN:HD21	1.78	0.49
3:G:208:ASP:OD1	1:H:98:ARG:NH2	2.46	0.49
3:G:116:THR:HG23	3:G:120:GLU:HA	1.94	0.48
2:B:106:VAL:HB	2:B:108:GLN:OE1	2.13	0.48
3:E:191:ALA:O	3:E:221:VAL:HB	2.13	0.48
3:G:160:ILE:O	3:G:203:LEU:HD23	2.13	0.48
1:A:40:PRO:HG2	1:A:43:LYS:HB2	1.95	0.48
2:B:131:THR:HG22	2:B:179:SER:HA	1.96	0.48
1:H:144:ASP:HB3	1:H:175:LEU:HD13	1.96	0.48
1:A:18:LEU:CD1	1:A:109:VAL:HG11	2.44	0.48
2:B:14:ASP:HB2	2:B:17:GLN:HG3	1.96	0.47
2:L:80:PRO:HA	2:L:106:VAL:HG21	1.95	0.47
3:E:221:VAL:HA	3:E:226:ASN:ND2	2.29	0.47
3:E:225:ASP:HB2	3:E:227:LYS:HE2	1.97	0.47
3:E:30:ILE:HG21	3:E:33:PHE:CE2	2.49	0.47
1:H:75:LYS:HB2	1:H:77:GLN:HG2	1.96	0.47
1:A:71:LYS:HA	1:A:78:PHE:HA	1.96	0.47
2:B:181:THR:HG23	2:B:184:GLN:H	1.78	0.47
3:E:225:ASP:HB3	3:E:244:ILE:CD1	2.44	0.46
3:E:52:PHE:CG	3:E:113:ILE:HD11	2.50	0.46
3:E:91:LEU:HD11	3:E:112:PRO:HB3	1.97	0.46
1:H:133:GLU:CD	1:H:133:GLU:H	2.18	0.46
1:H:160:THR:O	1:H:163:VAL:HG22	2.16	0.46
3:E:78:PRO:HG2	3:E:89:THR:HA	1.98	0.46
3:E:117:THR:HG23	3:E:120:GLU:OE2	2.15	0.46
3:E:225:ASP:HB3	3:E:244:ILE:CG1	2.45	0.46
3:E:401:LYS:HA	3:E:401:LYS:HD3	1.65	0.46
1:H:33:TYR:CE1	1:H:98:ARG:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:39:PHE:CE1	2:L:84:ALA:HB2	2.50	0.46
2:L:75:ILE:HG21	2:L:78:LEU:HD13	1.98	0.46
1:A:195:ILE:HD12	1:A:210:ARG:HD3	1.97	0.46
2:L:27(B):ASN:O	2:L:31:TYR:HB2	2.16	0.46
1:A:126:PRO:HB2	1:A:129:ARG:N	2.30	0.46
3:G:97:LEU:HD11	3:G:103:ALA:HB2	1.98	0.46
1:A:29:ILE:HG12	1:A:76:ASN:OD1	2.16	0.46
3:E:187:LEU:HD22	3:E:188:PRO:HD2	1.97	0.46
1:H:129:ARG:CD	2:L:206:VAL:HG23	2.45	0.46
3:E:225:ASP:HB3	3:E:244:ILE:HD11	1.98	0.45
2:L:63:SER:O	2:L:73:LEU:HD12	2.17	0.45
2:L:66:LYS:HG2	2:L:66:LYS:O	2.16	0.45
1:H:199:ASN:HD21	1:H:201:LYS:HE2	1.81	0.45
1:A:121:VAL:HG23	1:A:209:LYS:CD	2.46	0.45
3:E:132:PHE:HB3	3:E:140:TRP:HB2	1.99	0.45
3:E:107:ARG:NH2	3:E:274:PHE:O	2.50	0.45
3:E:101:GLU:OE2	3:G:429:HIS:CE1	2.70	0.45
3:G:210:GLU:HB2	1:H:98:ARG:HH12	1.82	0.45
2:L:4:LEU:HG	2:L:97:MET:CE	2.46	0.45
3:E:97:LEU:HD11	3:E:103:ALA:HB2	1.98	0.44
1:A:121:VAL:HG23	1:A:209:LYS:HD2	1.98	0.44
2:B:150:ALA:HB1	2:B:188:HIS:HD2	1.82	0.44
3:G:95:GLU:OE2	3:G:273:ARG:NH1	2.50	0.44
3:E:245:LEU:HB2	3:E:264:LEU:HD12	1.98	0.44
3:G:296:ASP:HB3	3:G:297:TYR:CD2	2.53	0.44
3:G:231:THR:HG23	3:G:236:GLU:OE2	2.17	0.44
3:E:168:THR:HG22	3:E:300:GLN:O	2.18	0.44
3:E:79:ARG:HH11	3:E:79:ARG:HG3	1.81	0.44
3:E:309:ILE:HG13	3:E:310:PRO:HD2	1.98	0.44
1:A:184:VAL:HG21	1:A:194:TYR:CE1	2.52	0.44
3:G:164:ASN:O	4:G:505:NAG:H82	2.18	0.44
3:E:79:ARG:HG3	3:E:79:ARG:NH1	2.33	0.44
1:A:129:ARG:HE	1:A:136:ALA:CB	2.28	0.43
2:B:129:LYS:HD3	2:B:129:LYS:HA	1.79	0.43
3:G:111:LEU:HD21	3:G:154:PRO:HG3	1.99	0.43
3:E:114:ASN:OD1	3:E:115:VAL:N	2.51	0.43
1:A:51:ILE:HD12	1:A:57:THR:HG22	2.00	0.43
3:G:203:LEU:HD22	3:G:282:TYR:CE2	2.52	0.43
3:E:153:ILE:H	3:E:153:ILE:HG13	1.66	0.43
1:H:50:PHE:CE1	1:H:58:ASN:HB3	2.54	0.43
3:G:345:ASN:H	3:G:410:THR:HG23	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:185:LEU:HD12	3:E:185:LEU:O	2.19	0.42
3:E:187:LEU:HD13	3:E:189:THR:H	1.83	0.42
3:E:367:THR:HG22	3:E:368:LEU:H	1.84	0.42
3:E:227:LYS:HD2	3:E:244:ILE:HD13	2.01	0.42
3:G:324:TYR:O	3:G:423:LYS:HA	2.19	0.42
3:G:345:ASN:HD22	4:G:507:NAG:H83	1.85	0.42
3:E:337:THR:O	3:E:339:GLU:HG3	2.20	0.42
1:A:189:LEU:HD11	1:A:213:ILE:HD11	2.02	0.42
1:H:193:THR:HG22	1:H:210:ARG:HH21	1.84	0.42
3:E:376:CYS:SG	3:E:379:ILE:HB	2.60	0.42
2:B:150:ALA:HB1	2:B:188:HIS:CD2	2.55	0.42
2:B:178:LEU:HD21	2:B:180:LEU:HD11	2.00	0.42
3:E:84:GLY:O	3:E:114:ASN:N	2.52	0.42
3:E:122:GLN:O	3:E:122:GLN:HG3	2.19	0.42
1:A:100(B):TRP:HB3	2:B:34:TYR:CD1	2.55	0.42
3:E:86:GLU:H	3:E:86:GLU:HG3	1.57	0.42
3:G:119:GLU:HA	3:G:119:GLU:OE1	2.19	0.42
3:G:147:GLN:HG3	3:G:148:ASN:N	2.34	0.42
1:A:13:LYS:HB2	1:A:16:GLU:HG3	2.02	0.41
3:G:15:LEU:O	3:G:16:ILE:HD13	2.19	0.41
3:G:423:LYS:HB2	3:G:423:LYS:HE2	1.78	0.41
1:H:117:LYS:HE3	1:H:144:ASP:HB3	2.02	0.41
3:E:45:ASP:OD1	3:E:67:GLN:HG3	2.20	0.41
3:E:273:ARG:NH1	3:E:307:ASP:OD1	2.51	0.41
1:A:84:ALA:O	1:A:87:THR:HG22	2.20	0.41
3:E:118:GLY:HA3	6:E:601:HOH:O	2.20	0.41
3:E:226:ASN:N	3:E:244:ILE:HD11	2.35	0.41
1:H:129:ARG:HD2	2:L:206:VAL:HG23	2.02	0.41
1:H:139:GLY:HA3	1:H:181:VAL:HG12	2.02	0.41
1:A:129:ARG:CZ	1:A:136:ALA:HB2	2.51	0.41
2:B:85:ASP:OD1	2:B:103:ARG:HD3	2.21	0.41
1:A:34:TRP:CZ3	1:A:94:ARG:HB2	2.55	0.41
2:B:49:TYR:CD2	2:B:50:GLN:HG2	2.56	0.41
1:A:121:VAL:HA	1:A:141:LEU:O	2.21	0.41
1:A:170:LEU:HG	1:A:176:TYR:HE1	1.84	0.41
3:E:46:VAL:HA	3:E:131:TYR:O	2.20	0.41
1:H:51:ILE:HG13	1:H:57:THR:HG22	2.03	0.41
2:L:125:LEU:HD23	2:L:125:LEU:HA	1.97	0.41
2:L:132:LEU:HB2	2:L:178:LEU:HB3	2.02	0.41
1:A:19:SER:O	1:A:20:LEU:HD13	2.20	0.41
3:E:6:LEU:HD23	3:E:6:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:9:GLN:HA	4:E:502:NAG:H4	2.02	0.40
3:E:297:TYR:HA	4:E:509:NAG:C6	2.50	0.40
3:E:195:ASN:N	3:E:219:SER:HA	2.36	0.40
3:E:226:ASN:N	3:E:226:ASN:OD1	2.53	0.40
3:G:213:MET:H	3:G:213:MET:HG2	1.65	0.40
3:G:354:TRP:HB2	4:G:508:NAG:H4	2.03	0.40
1:H:170:LEU:HD13	1:H:176:TYR:CE1	2.57	0.40
1:A:63:LEU:O	1:A:67:VAL:HG23	2.21	0.40
3:E:85:SER:HB3	3:E:88:ALA:N	2.36	0.40
3:E:329:ALA:HB3	3:E:393:VAL:HG12	2.04	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	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
1	H	219/222 (99%)	212 (97%)	7 (3%)	0	100	100
2	B	213/215 (99%)	206 (97%)	7 (3%)	0	100	100
2	L	213/215 (99%)	206 (97%)	7 (3%)	0	100	100
3	E	399/431 (93%)	378 (95%)	21 (5%)	0	100	100
3	G	413/431 (96%)	396 (96%)	17 (4%)	0	100	100
All	All	1677/1736 (97%)	1613 (96%)	64 (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	193/193 (100%)	185 (96%)	8 (4%)	30 50
1	H	192/193 (100%)	188 (98%)	4 (2%)	53 71
2	B	178/178 (100%)	173 (97%)	5 (3%)	43 63
2	L	178/178 (100%)	175 (98%)	3 (2%)	60 76
3	E	355/373 (95%)	335 (94%)	20 (6%)	21 36
3	G	365/373 (98%)	358 (98%)	7 (2%)	57 73
All	All	1461/1488 (98%)	1414 (97%)	47 (3%)	39 59

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LYS
1	A	79	SER
1	A	82(A)	SER
1	A	98	ARG
1	A	128	SER
1	A	129	ARG
1	A	130	SER
1	A	134	SER
2	B	18	ARG
2	B	63	SER
2	B	103	ARG
2	B	108	GLN
2	B	188	HIS
3	E	53	ASP
3	E	67	GLN
3	E	82	PHE
3	E	86	GLU
3	E	115	VAL
3	E	116	THR
3	E	120	GLU
3	E	121	GLN
3	E	123	VAL

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Mol	Chain	Res	Type
3	E	151	TYR
3	E	153	ILE
3	E	185	LEU
3	E	189	THR
3	E	225	ASP
3	E	279	SER
3	E	325	VAL
3	E	327	ASP
3	E	328	ASN
3	E	349	THR
3	E	428	HIS
3	G	164	ASN
3	G	175	ARG
3	G	238	HIS
3	G	277	ASN
3	G	279	SER
3	G	356	ASN
3	G	385	SER
1	H	128	SER
1	H	131	THR
1	H	135	THR
1	H	171	GLN
2	L	95(A)	SER
2	L	179	SER
2	L	192	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	195	ASN

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 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
4	NAG	G	505	3	14,14,15	0.39	0	17,19,21	1.03	1 (5%)
4	NAG	G	507	3	14,14,15	0.26	0	17,19,21	0.67	1 (5%)
4	NAG	E	505	3	14,14,15	0.31	0	17,19,21	0.73	0
4	NAG	E	502	3	14,14,15	0.29	0	17,19,21	0.81	0
4	NAG	G	508	3	14,14,15	0.30	0	17,19,21	0.83	1 (5%)
4	NAG	E	504	3	14,14,15	0.37	0	17,19,21	0.52	0
4	NAG	G	502	3	14,14,15	0.25	0	17,19,21	0.69	0
4	NAG	E	503	3	14,14,15	0.37	0	17,19,21	0.82	1 (5%)
4	NAG	E	509	3	14,14,15	0.30	0	17,19,21	1.03	2 (11%)
4	NAG	G	501	3	14,14,15	0.35	0	17,19,21	0.99	2 (11%)
4	NAG	E	501	3	14,14,15	0.30	0	17,19,21	0.60	0
4	NAG	G	504	3	14,14,15	0.30	0	17,19,21	0.69	0
4	NAG	G	503	3	14,14,15	0.34	0	17,19,21	0.58	0
4	NAG	G	509	3	14,14,15	0.39	0	17,19,21	0.68	0
4	NAG	E	508	3	14,14,15	0.29	0	17,19,21	0.58	0
4	NAG	E	506	3	14,14,15	0.26	0	17,19,21	0.74	0
4	NAG	G	506	3	14,14,15	0.31	0	17,19,21	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	505	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	507	3	-	3/6/23/26	0/1/1/1
4	NAG	E	505	3	-	3/6/23/26	0/1/1/1
4	NAG	E	502	3	-	3/6/23/26	0/1/1/1
4	NAG	G	508	3	-	5/6/23/26	0/1/1/1
4	NAG	E	504	3	-	2/6/23/26	0/1/1/1
4	NAG	G	502	3	-	3/6/23/26	0/1/1/1
4	NAG	E	503	3	-	3/6/23/26	0/1/1/1
4	NAG	E	509	3	-	3/6/23/26	0/1/1/1
4	NAG	G	501	3	-	2/6/23/26	0/1/1/1
4	NAG	E	501	3	-	2/6/23/26	0/1/1/1
4	NAG	G	504	3	-	3/6/23/26	0/1/1/1
4	NAG	G	503	3	-	2/6/23/26	0/1/1/1
4	NAG	G	509	3	-	0/6/23/26	0/1/1/1
4	NAG	E	508	3	-	1/6/23/26	0/1/1/1
4	NAG	E	506	3	-	3/6/23/26	0/1/1/1
4	NAG	G	506	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	509	NAG	C1-O5-C5	2.85	116.05	112.19
4	G	508	NAG	C1-O5-C5	2.69	115.83	112.19
4	G	501	NAG	C2-N2-C7	-2.39	119.49	122.90
4	E	503	NAG	C4-C3-C2	-2.27	107.69	111.02
4	G	505	NAG	C2-N2-C7	-2.23	119.73	122.90
4	E	509	NAG	C1-C2-N2	-2.19	106.75	110.49
4	G	501	NAG	C1-O5-C5	2.10	115.03	112.19
4	G	507	NAG	C1-O5-C5	2.10	115.03	112.19

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	502	NAG	C8-C7-N2-C2
4	E	502	NAG	O7-C7-N2-C2
4	E	503	NAG	C8-C7-N2-C2
4	E	503	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	E	504	NAG	C8-C7-N2-C2
4	E	504	NAG	O7-C7-N2-C2
4	E	509	NAG	C3-C2-N2-C7
4	E	509	NAG	C8-C7-N2-C2
4	E	509	NAG	O7-C7-N2-C2
4	G	501	NAG	C8-C7-N2-C2
4	G	501	NAG	O7-C7-N2-C2
4	G	502	NAG	C8-C7-N2-C2
4	G	502	NAG	O7-C7-N2-C2
4	G	504	NAG	C8-C7-N2-C2
4	G	504	NAG	O7-C7-N2-C2
4	G	507	NAG	C8-C7-N2-C2
4	G	507	NAG	O7-C7-N2-C2
4	G	508	NAG	C8-C7-N2-C2
4	G	508	NAG	O7-C7-N2-C2
4	E	501	NAG	C8-C7-N2-C2
4	E	505	NAG	C8-C7-N2-C2
4	E	506	NAG	C8-C7-N2-C2
4	G	503	NAG	C8-C7-N2-C2
4	G	503	NAG	O7-C7-N2-C2
4	E	505	NAG	O7-C7-N2-C2
4	E	506	NAG	O7-C7-N2-C2
4	G	506	NAG	C8-C7-N2-C2
4	E	502	NAG	C1-C2-N2-C7
4	G	502	NAG	C1-C2-N2-C7
4	G	508	NAG	C1-C2-N2-C7
4	E	501	NAG	O7-C7-N2-C2
4	G	506	NAG	O7-C7-N2-C2
4	E	506	NAG	C1-C2-N2-C7
4	G	504	NAG	C1-C2-N2-C7
4	G	507	NAG	C1-C2-N2-C7
4	E	505	NAG	O5-C5-C6-O6
4	E	508	NAG	O5-C5-C6-O6
4	E	503	NAG	C3-C2-N2-C7
4	G	508	NAG	C4-C5-C6-O6
4	G	508	NAG	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	505	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	507	NAG	1	0
4	E	502	NAG	2	0
4	G	508	NAG	1	0
4	G	502	NAG	1	0
4	E	503	NAG	1	0
4	E	509	NAG	4	0
4	G	504	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	222/222 (100%)	0.46	16 (7%) 15 18	67, 90, 131, 245	0
1	H	221/222 (99%)	0.36	11 (4%) 28 35	45, 68, 119, 210	0
2	B	215/215 (100%)	0.21	5 (2%) 60 69	63, 92, 122, 166	0
2	L	215/215 (100%)	0.24	7 (3%) 46 54	48, 82, 119, 148	0
3	E	404/431 (93%)	0.67	42 (10%) 6 7	50, 89, 148, 208	0
3	G	419/431 (97%)	0.39	25 (5%) 21 26	47, 74, 131, 194	0
All	All	1696/1736 (97%)	0.42	106 (6%) 20 24	45, 83, 136, 245	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	293	SER	13.6
1	A	131	THR	13.1
3	G	253	THR	11.0
1	H	127	SER	10.7
1	H	129	ARG	9.6
3	G	289	GLY	7.7
1	A	129	ARG	7.2
3	E	396	LEU	6.7
3	E	86	GLU	6.6
3	G	259	GLY	6.2
3	G	116	THR	5.7
2	B	1	GLN	5.4
3	E	429	HIS	5.3
1	A	130	SER	5.0
1	H	132	SER	4.7
3	G	256	PRO	4.7
1	H	130	SER	4.4
2	L	140	TYR	4.2
1	H	146	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
3	G	258	THR	3.9
1	A	116	THR	3.8
3	E	391	ILE	3.8
3	E	338	SER	3.7
3	G	254	PRO	3.7
3	E	325	VAL	3.7
3	E	63	LEU	3.6
3	E	198	VAL	3.5
3	E	270	PRO	3.5
3	E	394	SER	3.4
2	B	140	TYR	3.3
1	H	131	THR	3.2
3	E	326	GLY	3.2
1	H	136	ALA	3.1
3	E	193	ASP	3.1
3	E	26	PHE	3.1
3	E	90	ASN	3.1
3	E	186	SER	3.0
3	G	115	VAL	3.0
3	E	115	VAL	2.9
3	E	393	VAL	2.9
3	E	91	LEU	2.9
3	E	192	GLN	2.8
3	G	198	VAL	2.8
1	A	100(A)	PHE	2.8
3	G	250	PRO	2.8
3	G	411	ASN	2.8
1	A	117	LYS	2.7
1	A	136	ALA	2.7
1	A	189	LEU	2.7
1	A	146	PHE	2.7
3	E	88	ALA	2.7
3	G	26	PHE	2.7
3	G	57	LYS	2.6
3	E	337	THR	2.6
3	E	343	SER	2.6
3	G	112	PRO	2.6
3	G	121	GLN	2.6
3	G	249	SER	2.6
2	L	126	GLN	2.5
3	E	284	PHE	2.5
3	G	429	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	245	LEU	2.5
3	E	187	LEU	2.5
3	E	114	ASN	2.5
3	E	188	PRO	2.5
3	G	427	HIS	2.5
3	E	224	GLY	2.4
3	E	81	ALA	2.4
2	B	86	TYR	2.4
1	A	215	THR	2.4
3	E	83	GLY	2.4
1	H	128	SER	2.4
3	E	125	LEU	2.4
1	A	138	LEU	2.3
2	L	18	ARG	2.3
3	E	223	PRO	2.3
2	L	159	VAL	2.3
3	G	426	HIS	2.2
3	E	85	SER	2.2
3	E	222	LEU	2.2
3	E	383	PHE	2.2
3	G	428	HIS	2.2
3	G	425	PRO	2.2
1	A	184	VAL	2.2
3	E	412	ALA	2.1
3	E	113	ILE	2.1
1	H	214	LYS	2.1
3	E	308	GLU	2.1
3	E	328	ASN	2.1
3	E	295	GLY	2.1
3	G	295	GLY	2.1
2	L	1	GLN	2.1
3	E	117	THR	2.1
1	A	210	ARG	2.1
1	A	194	TYR	2.1
2	B	48	ILE	2.1
1	H	133	GLU	2.1
3	E	195	ASN	2.1
1	A	132	SER	2.1
3	G	270	PRO	2.0
3	G	391	ILE	2.0
2	L	210	GLU	2.0
1	A	126	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
2	L	75	ILE	2.0
2	B	87	TYR	2.0
1	H	175	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
4	NAG	E	504	14/15	0.56	0.64	124,140,143,145	0
4	NAG	E	503	14/15	0.59	0.33	115,127,134,136	0
4	NAG	E	505	14/15	0.63	0.31	104,112,120,120	0
4	NAG	G	502	14/15	0.64	0.58	50,50,50,50	0
4	NAG	G	501	14/15	0.66	0.59	50,50,50,50	0
4	NAG	E	508	14/15	0.66	0.52	50,50,50,50	0
4	NAG	G	507	14/15	0.66	0.40	103,110,118,119	0
5	ZN	G	510	1/1	0.67	0.23	130,130,130,130	0
4	NAG	G	508	14/15	0.68	0.55	81,97,102,103	0
4	NAG	E	502	14/15	0.68	0.24	101,105,108,112	0
4	NAG	E	501	14/15	0.75	0.20	89,102,105,107	0
4	NAG	E	509	14/15	0.77	0.34	50,50,50,50	0
4	NAG	G	504	14/15	0.78	0.20	117,121,125,127	0
4	NAG	E	506	14/15	0.79	0.18	108,115,120,122	0
4	NAG	G	506	14/15	0.82	0.21	81,96,102,104	0
4	NAG	G	505	14/15	0.82	0.17	82,91,93,94	0
4	NAG	G	503	14/15	0.86	0.19	83,90,93,94	0
4	NAG	G	509	14/15	0.90	0.25	79,83,89,89	0
5	ZN	E	507	1/1	0.92	0.18	83,83,83,83	0

6.5 Other polymers (i)

There are no such residues in this entry.