Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 12:55 PM EDT

PDB ID	:	4K3J
Title	:	Crystal structure of Onartuzumab Fab in complex with MET and HGF-beta
Authors	:	Ma, X.; Starovasnik, M.A.
Deposited on	:	2013-04-10
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

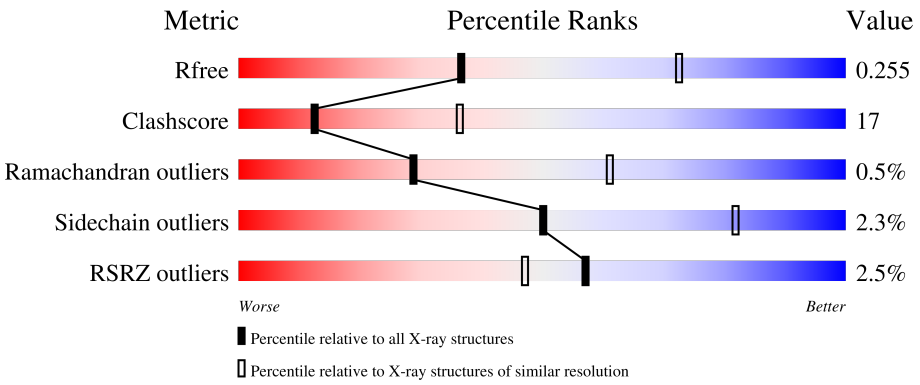
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	233	76% 21% •
2	B	534	4% 63% 29% • 7%
3	H	224	% 73% 22% • •
4	L	220	% 75% 22% ••

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9281 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 Hepatocyte growth factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	227	1766	1123	314	315	14	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	604	SER	CYS	engineered mutation	UNP P14210
A	722	HIS	-	expression tag	UNP P14210
A	723	HIS	-	expression tag	UNP P14210
A	724	HIS	-	expression tag	UNP P14210
A	725	HIS	-	expression tag	UNP P14210
A	726	HIS	-	expression tag	UNP P14210
A	727	HIS	-	expression tag	UNP P14210

- Molecule 2 is a protein called Hepatocyte growth factor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	499	3958	2516	672	740	30	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	565	HIS	-	expression tag	UNP P08581
B	566	HIS	-	expression tag	UNP P08581
B	567	HIS	-	expression tag	UNP P08581
B	568	HIS	-	expression tag	UNP P08581
B	569	HIS	-	expression tag	UNP P08581
B	570	HIS	-	expression tag	UNP P08581
B	571	HIS	-	expression tag	UNP P08581
B	572	HIS	-	expression tag	UNP P08581

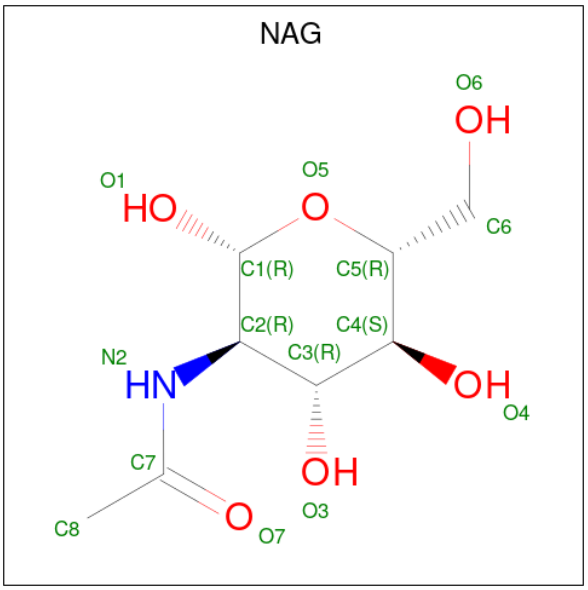
- Molecule 3 is a protein called Onartuzumab Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	221	1665	1053	277	329	6	0	0	0

- Molecule 4 is a protein called Onartuzumab Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	217	1695	1069	280	341	5	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	52	52	52	0	0
6	B	80	80	80	0	0
6	H	19	19	19	0	0

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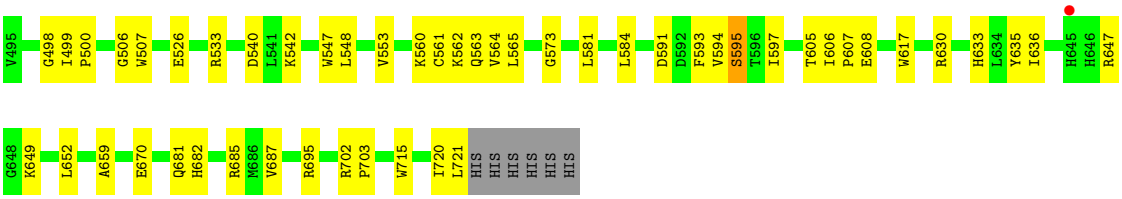
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	L	32	32	32	0	0

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.

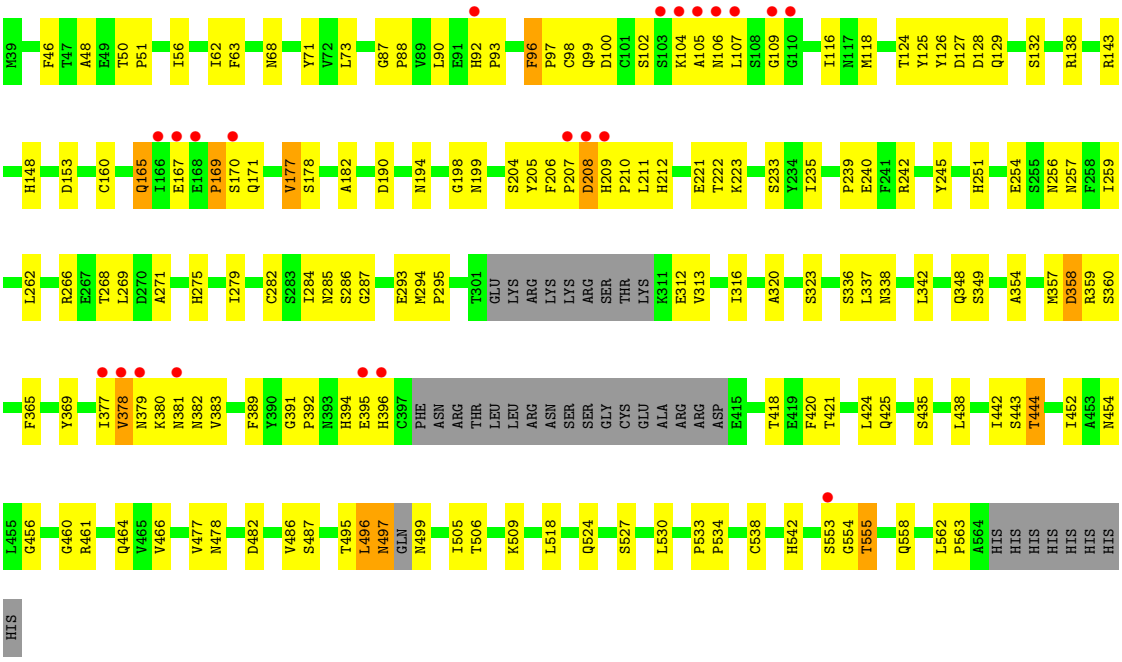
• Molecule 1: Hepatocyte growth factor

Chain A:



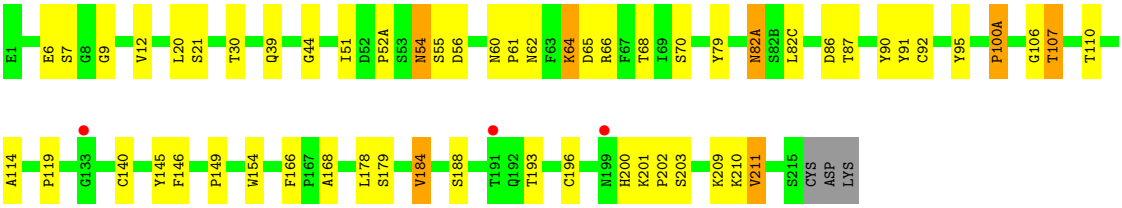
• Molecule 2: Hepatocyte growth factor beta chain

Chain B:



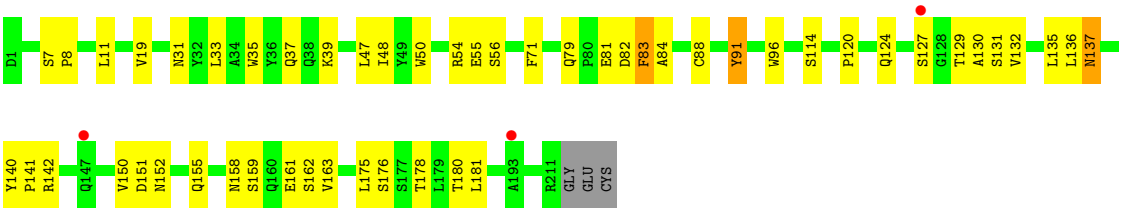
• Molecule 3: Onartuzumab Fab heavy chain

Chain H:



• Molecule 4: Onartuzumab Fab light chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	128.19Å 192.23Å 65.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-2.80) 98.9 (49.90-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.211 , 0.253 0.212 , 0.255	Depositor DCC
R_{free} test set	2027 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	54.2	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9281	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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 (i)

5.1 Standard geometry (i)

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

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	0.39	0/1808	0.53	0/2449
2	B	0.40	0/4057	0.56	0/5508
3	H	0.36	0/1709	0.50	0/2335
4	L	0.36	0/1736	0.50	0/2359
All	All	0.39	0/9310	0.53	0/12651

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1766	0	1764	54	0
2	B	3958	0	3817	186	0
3	H	1665	0	1620	38	0
4	L	1695	0	1643	32	0
5	B	14	0	13	1	0
6	A	52	0	0	4	0
6	B	80	0	0	4	0
6	H	19	0	0	2	0
6	L	32	0	0	1	0
All	All	9281	0	8857	301	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 17.

All (301) 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)
2:B:204:SER:C	2:B:205:TYR:HD1	1.42	1.22
2:B:167:GLU:O	2:B:169:PRO:HD3	1.46	1.15
1:A:647:ARG:NH2	2:B:148:HIS:ND1	1.92	1.15
2:B:378:VAL:HG13	2:B:379:ASN:H	1.00	1.12
2:B:165:GLN:HB3	2:B:169:PRO:HG2	1.13	1.11
2:B:377:ILE:O	2:B:378:VAL:HG12	1.50	1.11
2:B:206:PHE:HB2	2:B:208:ASP:O	1.53	1.06
2:B:496:LEU:C	2:B:497:ASN:HD22	1.58	1.04
2:B:204:SER:O	2:B:205:TYR:HD1	1.42	1.02
2:B:204:SER:C	2:B:205:TYR:CD1	2.35	1.00
2:B:204:SER:O	2:B:205:TYR:CD1	2.14	0.99
2:B:378:VAL:HG13	2:B:379:ASN:N	1.75	0.98
2:B:138:ARG:HA	2:B:209:HIS:NE2	1.87	0.90
2:B:378:VAL:CG1	2:B:379:ASN:H	1.84	0.89
2:B:495:THR:O	2:B:499:ASN:O	1.91	0.87
2:B:165:GLN:HB3	2:B:169:PRO:CG	2.01	0.85
2:B:68:ASN:OD1	2:B:87:GLY:C	2.15	0.84
2:B:496:LEU:C	2:B:497:ASN:ND2	2.31	0.83
1:A:606:ILE:HD12	1:A:607:PRO:HD2	1.60	0.82
2:B:206:PHE:HB3	2:B:207:PRO:HD2	1.62	0.81
3:H:87:THR:HG23	3:H:110:THR:HA	1.61	0.81
4:L:180:THR:O	4:L:181:LEU:HD23	1.82	0.80
2:B:379:ASN:ND2	2:B:381:ASN:HB2	1.96	0.79
1:A:647:ARG:HH21	2:B:148:HIS:CE1	2.02	0.78
1:A:647:ARG:NH2	2:B:148:HIS:CE1	2.52	0.77
1:A:608:GLU:O	1:A:636:ILE:O	2.03	0.77
2:B:167:GLU:C	2:B:169:PRO:HD3	2.04	0.77
3:H:66:ARG:O	3:H:82(A):ASN:ND2	2.18	0.77
2:B:165:GLN:CB	2:B:169:PRO:HG2	2.06	0.76
2:B:268:THR:HB	2:B:271:ALA:HB2	1.68	0.76
2:B:365:PHE:HE2	2:B:424:LEU:HD22	1.50	0.76
2:B:118:MET:HB2	2:B:177:VAL:HG11	1.65	0.75
2:B:495:THR:HB	2:B:499:ASN:O	1.87	0.74
2:B:394:HIS:HD2	2:B:396:HIS:H	1.34	0.74
2:B:357:MET:O	2:B:358:ASP:HB2	1.87	0.74
2:B:56:ILE:HG22	2:B:63:PHE:HB2	1.70	0.73
2:B:377:ILE:O	2:B:378:VAL:CG1	2.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:PHE:CG	2:B:97:PRO:HD2	2.24	0.72
2:B:92:HIS:CG	2:B:93:PRO:HD2	2.24	0.72
2:B:99:GLN:HG2	2:B:100:ASP:N	2.04	0.71
2:B:380:LYS:HG3	2:B:381:ASN:N	2.06	0.71
2:B:497:ASN:HD22	2:B:497:ASN:N	1.88	0.71
1:A:591:ASP:HB3	1:A:593:PHE:H	1.56	0.70
2:B:129:GLN:HE21	2:B:143:ARG:HH11	1.37	0.70
2:B:129:GLN:NE2	2:B:143:ARG:HH11	1.89	0.70
2:B:383:VAL:HG13	2:B:418:THR:CG2	2.21	0.70
1:A:591:ASP:HB2	1:A:594:VAL:H	1.56	0.70
1:A:533:ARG:NH2	2:B:190:ASP:OD1	2.25	0.69
1:A:540:ASP:OD1	1:A:542:LYS:HG3	1.93	0.69
2:B:206:PHE:CB	2:B:208:ASP:O	2.39	0.68
2:B:206:PHE:CD2	2:B:209:HIS:HB3	2.28	0.68
2:B:106:ASN:O	2:B:107:LEU:HB3	1.93	0.68
1:A:681:GLN:HG2	1:A:682:HIS:CD2	2.29	0.67
1:A:561:CYS:HB3	1:A:593:PHE:CD1	2.29	0.67
2:B:497:ASN:C	2:B:499:ASN:HA	2.15	0.67
2:B:383:VAL:HG13	2:B:418:THR:HG23	1.75	0.67
1:A:681:GLN:HE21	1:A:682:HIS:H	1.43	0.67
2:B:165:GLN:HA	2:B:165:GLN:OE1	1.94	0.67
3:H:95:TYR:HB3	3:H:100(A):PRO:O	1.96	0.66
2:B:107:LEU:HD13	2:B:107:LEU:O	1.96	0.65
2:B:323:SER:OG	2:B:444:THR:HG22	1.97	0.65
2:B:464:GLN:HB2	2:B:477:VAL:HB	1.77	0.65
2:B:282:CYS:O	6:B:908:HOH:O	2.13	0.65
3:H:9:GLY:HA3	3:H:107:THR:CG2	2.27	0.65
2:B:118:MET:CB	2:B:177:VAL:HG11	2.26	0.65
2:B:378:VAL:CG1	2:B:379:ASN:N	2.48	0.65
2:B:424:LEU:HD23	2:B:424:LEU:C	2.17	0.65
2:B:358:ASP:HA	2:B:438:LEU:HB2	1.78	0.64
2:B:316:ILE:HD12	2:B:349:SER:HB3	1.79	0.64
1:A:633:HIS:HB3	6:A:851:HOH:O	1.97	0.64
2:B:100:ASP:OD1	2:B:102:SER:HB2	1.98	0.64
1:A:695:ARG:HD2	2:B:125:TYR:O	1.97	0.64
2:B:394:HIS:CD2	2:B:395:GLU:HG2	2.32	0.64
1:A:533:ARG:NH1	2:B:190:ASP:OD1	2.31	0.63
2:B:124:THR:HG22	2:B:128:ASP:OD1	1.97	0.63
1:A:560:LYS:O	1:A:560:LYS:HG2	1.97	0.63
2:B:461:ARG:NH1	2:B:478:ASN:OD1	2.30	0.63
2:B:68:ASN:OD1	2:B:87:GLY:CA	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:HIS:N	2:B:210:PRO:CD	2.62	0.63
1:A:681:GLN:H	1:A:681:GLN:CD	2.02	0.63
1:A:507:TRP:CH2	1:A:685:ARG:HD3	2.34	0.62
2:B:208:ASP:C	2:B:210:PRO:HD3	2.20	0.62
2:B:104:LYS:C	2:B:106:ASN:H	2.03	0.62
2:B:553:SER:O	2:B:554:GLY:C	2.39	0.61
2:B:496:LEU:O	2:B:497:ASN:ND2	2.34	0.61
2:B:68:ASN:OD1	2:B:88:PRO:N	2.34	0.60
2:B:256:ASN:O	2:B:257:ASN:HB2	2.00	0.60
2:B:365:PHE:CE2	2:B:424:LEU:HD22	2.33	0.60
1:A:687:VAL:HG13	1:A:687:VAL:O	2.02	0.60
1:A:548:LEU:HD12	1:A:548:LEU:N	2.17	0.59
2:B:50:THR:HB	2:B:51:PRO:CD	2.31	0.59
4:L:31:ASN:O	4:L:50:TRP:HA	2.02	0.59
2:B:100:ASP:OD2	2:B:102:SER:HB2	2.02	0.59
2:B:382:ASN:O	2:B:421:THR:N	2.35	0.58
2:B:239:PRO:HA	2:B:242:ARG:HD2	1.84	0.58
4:L:55:GLU:HG3	4:L:56:SER:N	2.17	0.58
2:B:138:ARG:HG2	2:B:209:HIS:HD2	1.67	0.58
4:L:155:GLN:OE1	4:L:158:ASN:ND2	2.37	0.58
1:A:649:LYS:HD3	2:B:124:THR:O	2.03	0.58
2:B:279:ILE:HG12	2:B:293:GLU:HG2	1.86	0.58
3:H:64:LYS:HG2	3:H:65:ASP:N	2.18	0.57
2:B:359:ARG:HA	2:B:435:SER:O	2.04	0.57
2:B:269:LEU:HD12	2:B:392:PRO:HG3	1.86	0.57
2:B:391:GLY:HA3	6:B:933:HOH:O	2.03	0.57
4:L:33:LEU:HD13	4:L:71:PHE:CD1	2.38	0.57
2:B:336:SER:C	2:B:338:ASN:H	2.07	0.57
4:L:135:LEU:HD21	4:L:137:ASN:HD22	1.70	0.57
2:B:284:ILE:HG22	2:B:286:SER:H	1.70	0.57
2:B:496:LEU:H	2:B:496:LEU:CD2	2.18	0.57
4:L:124:GLN:HE22	4:L:131:SER:HB2	1.69	0.57
4:L:11:LEU:HD11	4:L:19:VAL:HG13	1.86	0.57
2:B:487:SER:HB3	2:B:505:ILE:HB	1.85	0.56
2:B:424:LEU:HD23	2:B:425:GLN:N	2.21	0.56
2:B:50:THR:HB	2:B:51:PRO:HD2	1.87	0.56
2:B:336:SER:C	2:B:338:ASN:N	2.56	0.56
3:H:6:GLU:HA	3:H:21:SER:O	2.05	0.56
3:H:168:ALA:HA	3:H:178:LEU:HB3	1.86	0.56
2:B:382:ASN:HA	2:B:421:THR:HB	1.88	0.55
3:H:114:ALA:HB3	3:H:146:PHE:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ASP:CG	2:B:102:SER:HB2	2.27	0.55
3:H:9:GLY:HA3	3:H:107:THR:HG21	1.87	0.55
2:B:178:SER:HB2	2:B:211:LEU:HD13	1.88	0.55
1:A:498:GLY:O	1:A:499:ILE:HD13	2.07	0.54
1:A:606:ILE:HD12	1:A:607:PRO:CD	2.34	0.54
2:B:165:GLN:HG3	2:B:171:GLN:O	2.07	0.54
4:L:91:TYR:HA	4:L:96:TRP:CD1	2.42	0.54
2:B:316:ILE:CD1	2:B:349:SER:HB3	2.37	0.54
1:A:605:THR:HG22	1:A:606:ILE:N	2.23	0.54
2:B:337:LEU:CD1	2:B:337:LEU:H	2.21	0.54
1:A:565:LEU:HD12	1:A:584:LEU:HD13	1.89	0.54
4:L:124:GLN:HE22	4:L:131:SER:CB	2.21	0.54
2:B:235:ILE:HG23	2:B:389:PHE:CD1	2.43	0.54
3:H:54:ASN:O	3:H:55:SER:HB2	2.08	0.54
2:B:312:GLU:HG3	2:B:348:GLN:NE2	2.23	0.54
1:A:681:GLN:NE2	1:A:682:HIS:H	2.05	0.54
2:B:323:SER:OG	2:B:444:THR:CG2	2.55	0.53
1:A:606:ILE:CD1	1:A:607:PRO:HD2	2.35	0.53
2:B:194:ASN:OD1	2:B:285:ASN:HB3	2.08	0.53
1:A:591:ASP:HB3	1:A:593:PHE:N	2.22	0.53
4:L:48:ILE:HD13	4:L:54:ARG:HA	1.91	0.53
2:B:92:HIS:HD2	2:B:109:GLY:C	2.13	0.52
2:B:68:ASN:OD1	2:B:87:GLY:HA3	2.09	0.52
4:L:140:TYR:CG	4:L:141:PRO:HA	2.45	0.52
1:A:563:GLN:NE2	1:A:594:VAL:HG21	2.24	0.52
2:B:337:LEU:CD1	2:B:337:LEU:N	2.72	0.52
2:B:100:ASP:OD1	2:B:102:SER:CB	2.58	0.52
2:B:337:LEU:N	2:B:337:LEU:HD12	2.24	0.52
4:L:120:PRO:HD3	4:L:132:VAL:HG22	1.93	0.51
1:A:507:TRP:CE2	1:A:597:ILE:HD12	2.46	0.51
3:H:184:VAL:HG13	3:H:188:SER:OG	2.10	0.51
2:B:268:THR:HG22	2:B:269:LEU:N	2.26	0.51
2:B:383:VAL:CG1	2:B:418:THR:CG2	2.89	0.51
4:L:161:GLU:HA	4:L:176:SER:O	2.11	0.51
3:H:119:PRO:HB3	3:H:145:TYR:HB3	1.93	0.51
1:A:560:LYS:O	1:A:560:LYS:CG	2.59	0.51
1:A:565:LEU:CD1	1:A:584:LEU:HD13	2.41	0.51
2:B:92:HIS:CD2	2:B:93:PRO:HD2	2.46	0.51
2:B:199:ASN:HB2	2:B:212:HIS:O	2.10	0.51
1:A:670:GLU:HG2	6:A:836:HOH:O	2.11	0.51
3:H:211:VAL:HA	6:H:316:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:555:THR:HG22	2:B:555:THR:O	2.11	0.50
3:H:6:GLU:OE2	3:H:92:CYS:N	2.37	0.50
2:B:379:ASN:HD21	2:B:381:ASN:HB2	1.71	0.50
2:B:209:HIS:N	2:B:210:PRO:HD2	2.25	0.50
2:B:394:HIS:CD2	2:B:396:HIS:H	2.21	0.50
2:B:46:PHE:O	2:B:509:LYS:HA	2.12	0.50
2:B:129:GLN:HE21	2:B:143:ARG:NH1	2.09	0.50
4:L:136:LEU:HB2	4:L:175:LEU:HB3	1.94	0.50
2:B:233:SER:HA	2:B:287:GLY:HA2	1.94	0.49
4:L:155:GLN:HB3	4:L:158:ASN:HD21	1.78	0.49
2:B:383:VAL:CG1	2:B:418:THR:HG23	2.43	0.49
1:A:533:ARG:CZ	2:B:190:ASP:OD1	2.59	0.49
5:B:801:NAG:H81	6:B:957:HOH:O	2.12	0.49
2:B:424:LEU:C	2:B:424:LEU:CD2	2.81	0.49
3:H:60:ASN:O	3:H:62:ASN:N	2.46	0.49
3:H:193:THR:HG23	3:H:210:LYS:NZ	2.27	0.49
3:H:201:LYS:N	3:H:202:PRO:CD	2.76	0.49
2:B:206:PHE:C	2:B:208:ASP:O	2.52	0.48
2:B:208:ASP:C	2:B:210:PRO:CD	2.81	0.48
2:B:138:ARG:CG	2:B:209:HIS:HD2	2.27	0.48
2:B:443:SER:HG	2:B:454:ASN:HD22	1.61	0.48
2:B:456:GLY:HA3	2:B:486:VAL:HG11	1.96	0.48
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.95	0.48
2:B:269:LEU:HD23	2:B:269:LEU:HA	1.76	0.47
1:A:561:CYS:HB3	1:A:593:PHE:CE1	2.49	0.47
1:A:605:THR:CG2	1:A:606:ILE:N	2.77	0.47
2:B:460:GLY:HA3	2:B:482:ASP:O	2.14	0.47
2:B:90:LEU:CD2	2:B:105:ALA:HA	2.45	0.47
2:B:268:THR:HB	2:B:271:ALA:CB	2.43	0.47
2:B:316:ILE:CD1	2:B:354:ALA:HA	2.44	0.47
3:H:70:SER:HB3	6:H:307:HOH:O	2.13	0.47
2:B:369:TYR:HE2	2:B:424:LEU:HD21	1.80	0.47
3:H:66:ARG:NH2	3:H:86:ASP:OD2	2.48	0.47
1:A:547:TRP:C	1:A:548:LEU:HD12	2.35	0.47
3:H:200:HIS:CE1	3:H:203:SER:HB3	2.51	0.46
2:B:138:ARG:HG2	2:B:209:HIS:CD2	2.50	0.46
3:H:6:GLU:OE2	3:H:91:TYR:HA	2.15	0.46
1:A:573:GLY:HA2	1:A:715:TRP:CZ2	2.50	0.46
2:B:129:GLN:NE2	2:B:143:ARG:NH1	2.62	0.46
3:H:168:ALA:HB2	3:H:178:LEU:HD23	1.98	0.46
2:B:254:GLU:HG2	2:B:259:ILE:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:496:LEU:CD2	2:B:496:LEU:N	2.79	0.46
1:A:561:CYS:CB	1:A:593:PHE:CD1	2.98	0.46
1:A:553:VAL:HB	1:A:617:TRP:CD1	2.51	0.46
2:B:182:ALA:HA	2:B:198:GLY:O	2.16	0.46
2:B:380:LYS:CG	2:B:381:ASN:N	2.78	0.46
2:B:48:ALA:HB1	2:B:71:TYR:CE2	2.51	0.46
2:B:495:THR:O	2:B:496:LEU:C	2.53	0.46
2:B:496:LEU:N	2:B:496:LEU:HD22	2.31	0.45
1:A:591:ASP:CB	1:A:594:VAL:H	2.24	0.45
2:B:294:MET:HA	2:B:295:PRO:HD3	1.83	0.45
2:B:92:HIS:CG	2:B:93:PRO:CD	2.97	0.45
2:B:153:ASP:OD1	2:B:153:ASP:C	2.54	0.45
2:B:251:HIS:HB3	2:B:262:LEU:HD12	1.97	0.45
2:B:126:TYR:O	2:B:127:ASP:C	2.55	0.45
2:B:92:HIS:ND1	2:B:93:PRO:HD2	2.31	0.45
2:B:206:PHE:CB	2:B:207:PRO:HD2	2.39	0.45
4:L:142:ARG:HE	4:L:163:VAL:HG11	1.82	0.45
1:A:670:GLU:CG	6:A:836:HOH:O	2.65	0.45
3:H:39:GLN:HG3	3:H:44:GLY:O	2.15	0.45
2:B:357:MET:O	2:B:358:ASP:CB	2.56	0.45
2:B:206:PHE:HD2	2:B:209:HIS:HB3	1.76	0.45
2:B:138:ARG:HA	2:B:209:HIS:CD2	2.50	0.44
1:A:500:PRO:HD3	1:A:630:ARG:CZ	2.46	0.44
2:B:116:ILE:HB	2:B:118:MET:HE2	1.97	0.44
1:A:526:GLU:H	1:A:526:GLU:CD	2.20	0.44
2:B:524:GLN:OE1	2:B:524:GLN:HA	2.18	0.44
4:L:35:TRP:CZ3	4:L:88:CYS:HB3	2.53	0.44
2:B:138:ARG:CB	2:B:209:HIS:CD2	3.01	0.44
1:A:681:GLN:CD	1:A:681:GLN:N	2.70	0.44
3:H:193:THR:HG23	3:H:210:LYS:HZ3	1.81	0.44
3:H:20:LEU:O	3:H:79:TYR:HA	2.18	0.44
4:L:79:GLN:O	4:L:82:ASP:HB2	2.18	0.44
3:H:9:GLY:HA3	3:H:107:THR:HG22	1.99	0.43
2:B:313:VAL:O	2:B:348:GLN:HG2	2.18	0.43
3:H:12:VAL:HG11	3:H:82(C):LEU:HD13	1.99	0.43
3:H:140:CYS:O	3:H:179:SER:HA	2.19	0.43
4:L:150:VAL:C	4:L:152:ASN:N	2.69	0.43
2:B:106:ASN:O	2:B:107:LEU:CB	2.61	0.43
2:B:533:PRO:HA	2:B:534:PRO:HD3	1.84	0.43
2:B:205:TYR:CD1	2:B:205:TYR:N	2.77	0.43
2:B:316:ILE:HD11	2:B:354:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:THR:CG2	2:B:269:LEU:N	2.81	0.43
4:L:129:THR:CG2	4:L:130:ALA:N	2.81	0.43
1:A:562:LYS:HE2	1:A:564:VAL:CG2	2.49	0.43
2:B:104:LYS:C	2:B:106:ASN:N	2.72	0.43
2:B:452:ILE:HD13	2:B:466:VAL:HG22	2.01	0.43
4:L:39:LYS:HE2	6:L:309:HOH:O	2.18	0.43
1:A:702:ARG:HA	1:A:703:PRO:HD3	1.85	0.42
2:B:486:VAL:HA	2:B:506:THR:HG22	2.01	0.42
2:B:208:ASP:OD1	2:B:209:HIS:N	2.51	0.42
2:B:245:TYR:CE1	2:B:266:ARG:HB2	2.55	0.42
2:B:538:CYS:N	6:B:936:HOH:O	2.35	0.42
3:H:90:TYR:O	3:H:106:GLY:HA2	2.19	0.42
3:H:178:LEU:HD12	3:H:178:LEU:C	2.40	0.42
2:B:357:MET:O	2:B:357:MET:HG2	2.19	0.42
2:B:320:ALA:HB1	2:B:342:LEU:HD11	2.01	0.42
4:L:129:THR:HG22	4:L:130:ALA:N	2.33	0.42
2:B:209:HIS:O	2:B:209:HIS:ND1	2.51	0.42
1:A:647:ARG:CZ	2:B:148:HIS:CE1	3.03	0.42
6:A:807:HOH:O	2:B:221:GLU:HG3	2.19	0.42
2:B:562:LEU:HB3	2:B:563:PRO:HD2	2.02	0.42
2:B:383:VAL:CG1	2:B:418:THR:HG21	2.50	0.42
4:L:83:PHE:O	4:L:84:ALA:HB2	2.20	0.42
1:A:573:GLY:HA2	1:A:715:TRP:CH2	2.55	0.42
4:L:7:SER:HA	4:L:8:PRO:HA	1.89	0.42
4:L:135:LEU:HD21	4:L:137:ASN:ND2	2.34	0.42
2:B:382:ASN:O	2:B:420:PHE:HA	2.20	0.41
2:B:518:LEU:HD12	2:B:518:LEU:HA	1.85	0.41
3:H:82(A):ASN:ND2	3:H:82(A):ASN:N	2.68	0.41
2:B:97:PRO:CG	2:B:138:ARG:HE	2.32	0.41
2:B:138:ARG:CG	2:B:209:HIS:CD2	3.03	0.41
1:A:581:LEU:HD23	1:A:581:LEU:HA	1.90	0.41
4:L:159:SER:HA	4:L:178:THR:O	2.19	0.41
2:B:170:SER:HA	2:B:207:PRO:O	2.20	0.41
3:H:30:THR:HA	3:H:52(A):PRO:HB2	2.02	0.41
2:B:98:CYS:HB3	2:B:160:CYS:HB3	1.89	0.41
2:B:118:MET:HG3	2:B:177:VAL:CG1	2.51	0.41
2:B:336:SER:O	2:B:338:ASN:N	2.54	0.41
2:B:497:ASN:ND2	2:B:497:ASN:N	2.58	0.41
4:L:124:GLN:O	4:L:127:SER:HB2	2.21	0.41
3:H:166:PHE:HB3	4:L:162:SER:OG	2.21	0.41
4:L:39:LYS:HE2	4:L:81:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:530:LEU:HD22	2:B:558:GLN:C	2.41	0.41
1:A:635:TYR:O	1:A:659:ALA:HA	2.20	0.40
2:B:240:GLU:O	2:B:240:GLU:HG2	2.21	0.40
3:H:7:SER:HB2	3:H:21:SER:HB2	2.02	0.40
3:H:200:HIS:ND1	3:H:203:SER:HB3	2.36	0.40
2:B:92:HIS:CE1	2:B:93:PRO:HD2	2.55	0.40
2:B:222:THR:O	2:B:223:LYS:HB2	2.20	0.40
2:B:360:SER:OG	2:B:438:LEU:HA	2.22	0.40
1:A:506:GLY:HA3	1:A:595:SER:HB3	2.02	0.40
1:A:652:LEU:N	1:A:652:LEU:HD12	2.37	0.40
1:A:720:ILE:HG13	1:A:721:LEU:HD12	2.03	0.40
2:B:62:ILE:HB	2:B:73:LEU:HB2	2.04	0.40
2:B:442:ILE:HA	2:B:454:ASN:O	2.22	0.40
3:H:209:LYS:HD2	3:H:209:LYS:HA	1.97	0.40
4:L:150:VAL:O	4:L:151:ASP:C	2.60	0.40
2:B:99:GLN:CG	2:B:100:ASP:N	2.80	0.40
3:H:51:ILE:HA	3:H:56:ASP:O	2.22	0.40
3:H:154:TRP:CH2	3:H:196:CYS:HB3	2.57	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	225/233 (97%)	216 (96%)	9 (4%)	0	100	100
2	B	491/534 (92%)	459 (94%)	29 (6%)	3 (1%)	25	56
3	H	219/224 (98%)	208 (95%)	8 (4%)	3 (1%)	11	34
4	L	215/220 (98%)	206 (96%)	9 (4%)	0	100	100
All	All	1150/1211 (95%)	1089 (95%)	55 (5%)	6 (0%)	29	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	169	PRO
2	B	378	VAL
3	H	100(A)	PRO
2	B	542	HIS
3	H	61	PRO
3	H	149	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	191/197 (97%)	190 (100%)	1 (0%)	88 96
2	B	451/484 (93%)	439 (97%)	12 (3%)	44 78
3	H	188/191 (98%)	181 (96%)	7 (4%)	34 68
4	L	193/195 (99%)	189 (98%)	4 (2%)	53 84
All	All	1023/1067 (96%)	999 (98%)	24 (2%)	50 82

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	595	SER
2	B	96	PHE
2	B	132	SER
2	B	165	GLN
2	B	177	VAL
2	B	208	ASP
2	B	275	HIS
2	B	358	ASP
2	B	444	THR
2	B	496	LEU
2	B	497	ASN
2	B	527	SER
2	B	555	THR
3	H	54	ASN
3	H	64	LYS
3	H	68	THR

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Mol	Chain	Res	Type
3	H	82(A)	ASN
3	H	107	THR
3	H	184	VAL
3	H	211	VAL
4	L	83	PHE
4	L	91	TYR
4	L	114	SER
4	L	137	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	682	HIS
2	B	106	ASN
2	B	129	GLN
2	B	142	GLN
2	B	256	ASN
2	B	394	HIS
2	B	497	ASN
3	H	54	ASN
4	L	100	GLN
4	L	124	GLN
4	L	189	HIS

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)

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
5	NAG	B	801	2	14,14,15	0.53	0	17,19,21	0.89	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
5	NAG	B	801	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	801	NAG	C4-C5-C6-O6
5	B	801	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	801	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	227/233 (97%)	-0.01	1 (0%)	92	91	23, 42, 96, 134	0
2	B	499/534 (93%)	0.10	22 (4%)	34	24	21, 49, 92, 145	0
3	H	221/224 (98%)	-0.01	3 (1%)	75	70	40, 57, 71, 80	0
4	L	217/220 (98%)	-0.01	3 (1%)	75	70	37, 51, 77, 85	0
All	All	1164/1211 (96%)	0.04	29 (2%)	57	47	21, 51, 83, 145	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	168	GLU	6.2
2	B	104	LYS	5.3
2	B	378	VAL	4.4
1	A	645	HIS	3.7
2	B	207	PRO	3.4
2	B	107	LEU	3.4
4	L	147	GLN	3.3
2	B	381	ASN	3.2
2	B	105	ALA	3.1
2	B	208	ASP	2.9
2	B	106	ASN	2.9
4	L	127	SER	2.6
2	B	395	GLU	2.6
2	B	92	HIS	2.5
2	B	110	GLY	2.5
2	B	103	SER	2.5
2	B	166	ILE	2.5
2	B	109	GLY	2.3
3	H	133	GLY	2.3
2	B	377	ILE	2.3
3	H	191	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	170	SER	2.2
2	B	167	GLU	2.2
2	B	553	SER	2.2
2	B	209	HIS	2.2
2	B	379	ASN	2.1
3	H	199	ASN	2.1
2	B	396	HIS	2.1
4	L	193	ALA	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(Å^2)	Q<0.9
5	NAG	B	801	14/15	0.91	0.16	44,50,51,52	0

6.5 Other polymers (i)

There are no such residues in this entry.