Full wwPDB X-ray Structure Validation Report (i)

Nov 23, 2016 – 10:48 AM EST

PDB ID	:	1UWG
Title	:	Molecular Mechanism of Enantioselective Proton Transfer to Carbon in Catalytic Antibody 14D9
Authors	:	Baumann, U.; Reymond, J.L.
Deposited on	:	2004-02-05
Resolution	:	2.79 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 (i) symbol.

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

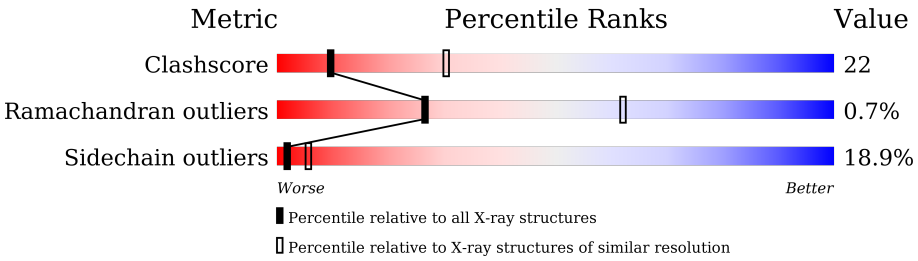
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	225	59% 25% 9% 7%
1	Y	225	51% 36% 6% 7%
2	L	213	52% 38% 9%
2	X	213	55% 31% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6499 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.

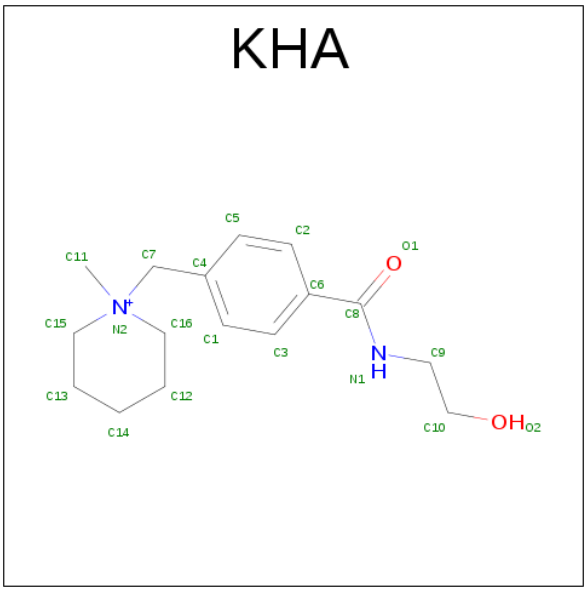
- Molecule 1 is a protein called ANTIBODY 14D9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	209	Total	C	N	O	S	0	0	1
			1535	981	248	301	5			
1	Y	209	Total	C	N	O	S	0	0	1
			1535	981	248	301	5			

- Molecule 2 is a protein called ANTIBODY 14D9.

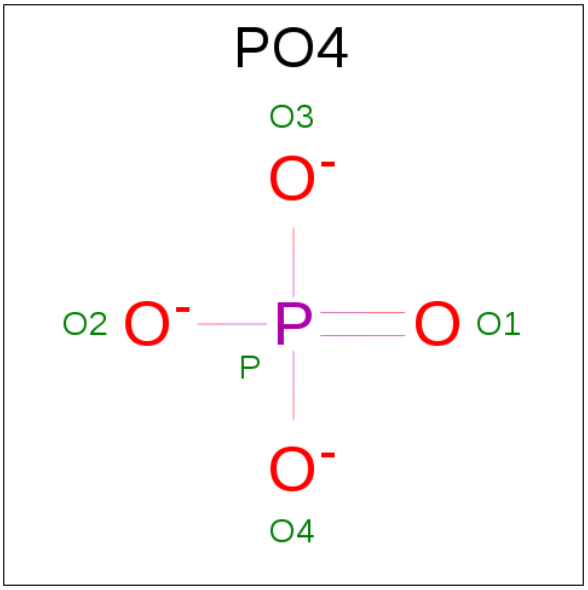
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1637	1024	274	333	6			
2	X	213	Total	C	N	O	S	0	0	0
			1637	1024	274	333	6			

- Molecule 3 is 1-(4-{[(2-HYDROXYETHYL)AMINO]CARBONYL}BENZYL)-1-METHYL PIPERIDINIUM (three-letter code: KHA) (formula: $C_{16}H_{25}N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C N O 20 16 2 2	0	0
3	Y	1	Total C N O 20 16 2 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total O P 5 4 1	0	0
4	L	1	Total O P 5 4 1	0	0
4	L	1	Total O P 5 4 1	0	0
4	L	1	Total O P 5 4 1	0	0
4	L	1	Total O P 5 4 1	0	0
4	X	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	19	Total O 19 19	0	0
5	L	23	Total O 23 23	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	X	20	Total O 20 20	0	0
5	Y	23	Total O 23 23	0	0

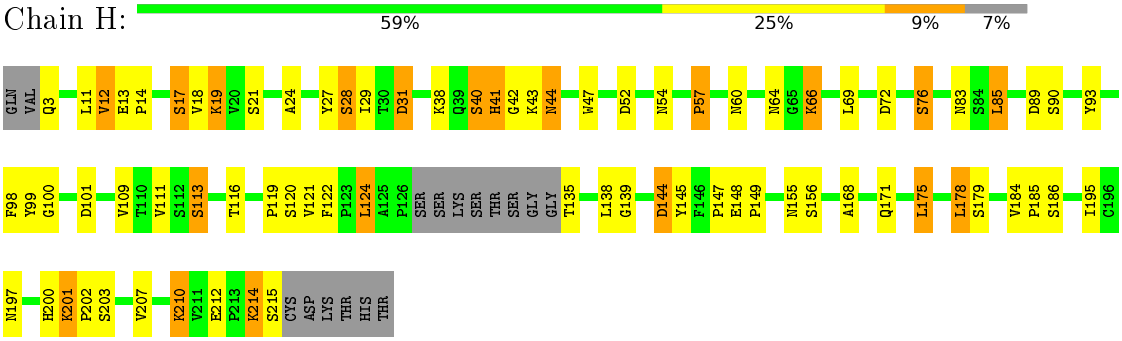
3 Residue-property plots (i)

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.

Note EDS was not executed.

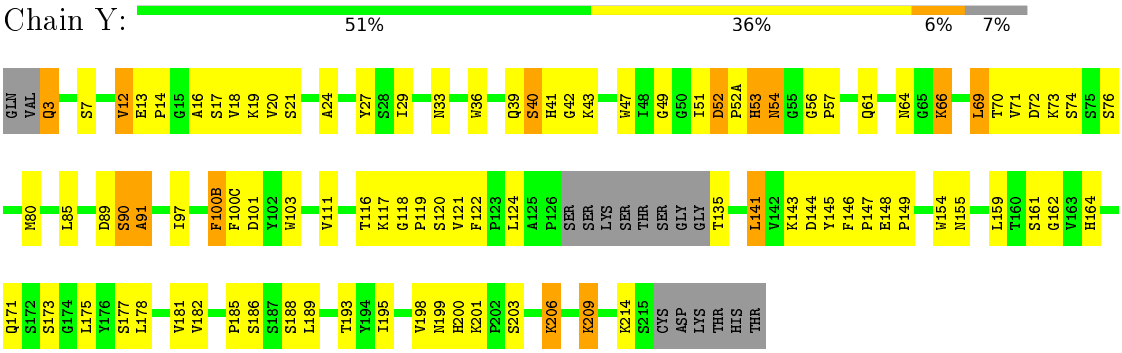
- Molecule 1: ANTIBODY 14D9

Chain H:



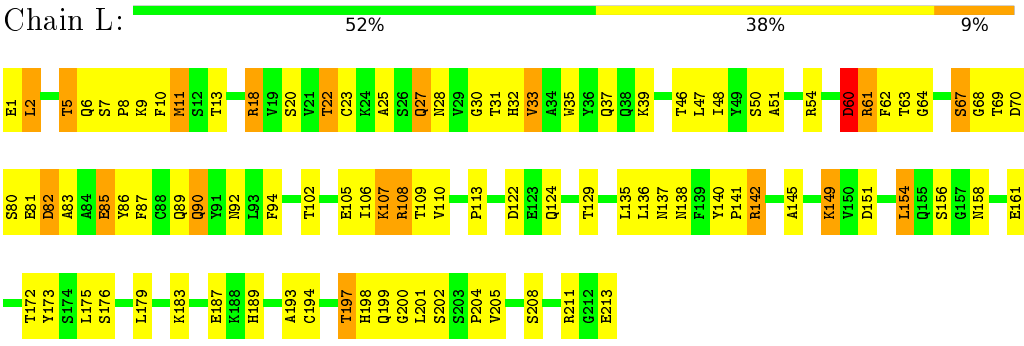
- Molecule 1: ANTIBODY 14D9

Chain Y:



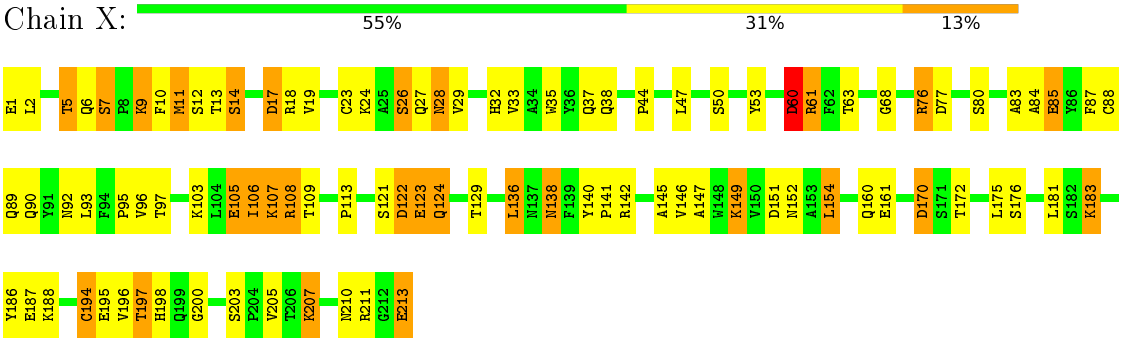
- Molecule 2: ANTIBODY 14D9

Chain L:



• Molecule 2: ANTIBODY 14D9

Chain X:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.47Å 97.92Å 70.88Å 90.00° 99.28° 90.00°	Depositor
Resolution (Å)	20.00 – 2.79	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.79)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.204 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6499	wwPDB-VP
Average B, all atoms (Å^2)	7.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KHA, PO4

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	H	0.42	0/1577	0.73	4/2157 (0.2%)
1	Y	0.40	0/1577	0.75	4/2157 (0.2%)
2	L	0.43	0/1673	0.76	5/2271 (0.2%)
2	X	0.39	0/1673	0.75	6/2271 (0.3%)
All	All	0.41	0/6500	0.75	19/8856 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	72	ASP	CB-CG-OD2	6.34	124.00	118.30
2	L	77	ASP	CB-CG-OD2	6.26	123.94	118.30
1	Y	89	ASP	CB-CG-OD2	5.89	123.60	118.30
2	L	122	ASP	CB-CG-OD2	5.87	123.58	118.30
2	X	60	ASP	CB-CG-OD2	5.57	123.31	118.30
2	X	151	ASP	CB-CG-OD2	5.49	123.24	118.30
1	Y	101	ASP	CB-CG-OD2	5.48	123.23	118.30
2	L	70	ASP	CB-CG-OD2	5.44	123.19	118.30
1	H	101	ASP	CB-CG-OD2	5.36	123.12	118.30
2	L	82	ASP	CB-CG-OD2	5.30	123.07	118.30
2	X	122	ASP	CB-CG-OD2	5.29	123.06	118.30
1	H	31	ASP	CB-CG-OD2	5.29	123.06	118.30
2	X	170	ASP	CB-CG-OD2	5.27	123.04	118.30
1	H	144	ASP	CB-CG-OD2	5.25	123.03	118.30
2	X	77	ASP	CB-CG-OD2	5.24	123.02	118.30
2	X	17	ASP	CB-CG-OD2	5.19	122.97	118.30
2	L	60	ASP	CB-CG-OD2	5.17	122.95	118.30
1	Y	72	ASP	CB-CG-OD2	5.04	122.84	118.30
1	Y	52	ASP	CB-CG-OD2	5.02	122.82	118.30

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	H	1535	0	1468	67	0
1	Y	1535	0	1468	73	0
2	L	1637	0	1574	79	0
2	X	1637	0	1574	68	0
3	H	20	0	25	5	0
3	Y	20	0	25	3	0
4	H	5	0	0	1	0
4	L	20	0	0	2	0
4	X	5	0	0	1	0
5	H	19	0	0	5	0
5	L	23	0	0	7	0
5	X	20	0	0	1	0
5	Y	23	0	0	3	0
All	All	6499	0	6134	281	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 22.

All (281) 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:H:3:GLN:HB3	5:H:2001:HOH:O	1.49	1.11
1:Y:200:HIS:HD2	1:Y:203:SER:OG	1.36	1.08
1:Y:148:GLU:HG3	1:Y:149:PRO:HA	1.37	1.05
2:L:33:VAL:HG11	2:L:71:PHE:CE1	1.93	1.02
2:L:183:LYS:HD2	5:L:2017:HOH:O	0.84	1.01
1:H:148:GLU:HG3	1:H:149:PRO:HA	1.43	1.01
1:H:148:GLU:HG3	1:H:149:PRO:CA	1.96	0.95
1:Y:24:ALA:HB2	1:Y:29:ILE:HG23	1.51	0.93
1:Y:3:GLN:HA	1:Y:3:GLN:NE2	1.84	0.90
2:L:79:GLN:O	2:L:82:ASP:HB2	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:197:THR:HG22	2:L:204:PRO:HG3	1.56	0.87
2:X:108:ARG:HG2	2:X:109:THR:N	1.89	0.87
2:X:60:ASP:N	2:X:60:ASP:OD1	2.08	0.86
1:H:147:PRO:O	1:H:200:HIS:HE1	1.58	0.85
2:L:201:LEU:HD13	2:L:205:VAL:HG13	1.58	0.85
1:H:122:PHE:CE2	2:L:124:GLN:HG3	2.12	0.83
1:Y:200:HIS:CD2	1:Y:203:SER:OG	2.27	0.82
1:Y:148:GLU:HG3	1:Y:149:PRO:CA	2.09	0.81
2:L:77:ASP:O	2:L:79:GLN:NE2	2.12	0.81
2:L:33:VAL:HG11	2:L:71:PHE:CD1	2.17	0.79
2:X:85:GLU:HG2	2:X:87:PHE:CZ	2.18	0.79
1:H:214:LYS:HZ2	1:H:215:SER:N	1.81	0.78
2:L:83:ALA:HB1	5:L:2014:HOH:O	1.82	0.78
2:X:207:LYS:HE3	2:X:207:LYS:HA	1.63	0.78
2:X:136:LEU:HD21	2:X:146:VAL:HG22	1.67	0.77
2:L:7:SER:HB2	2:L:8:PRO:HA	1.65	0.76
1:H:214:LYS:HD2	1:H:215:SER:N	2.00	0.76
2:L:197:THR:CG2	2:L:204:PRO:HG3	2.17	0.75
2:L:33:VAL:CG1	2:L:71:PHE:CE1	2.69	0.74
2:X:136:LEU:HD21	2:X:146:VAL:CG2	2.18	0.73
1:H:13:GLU:OE2	1:H:113:SER:HB3	1.87	0.73
1:H:214:LYS:NZ	1:H:215:SER:N	2.34	0.73
2:L:32:HIS:HB2	2:L:92:ASN:HB2	1.70	0.73
2:L:60:ASP:N	2:L:60:ASP:OD1	2.22	0.72
1:H:13:GLU:HG3	1:H:14:PRO:HD2	1.72	0.72
2:X:175:LEU:HD23	2:X:176:SER:N	2.05	0.72
1:Y:199:ASN:CB	1:Y:206:LYS:NZ	2.53	0.71
3:H:1215:KHA:C1	3:H:1215:KHA:C11	2.67	0.71
1:H:121:VAL:HG21	1:H:207:VAL:HG11	1.73	0.71
2:X:183:LYS:O	2:X:187:GLU:HG2	1.92	0.70
2:L:158:ASN:O	2:L:179:LEU:HD12	1.91	0.70
2:X:2:LEU:HD21	2:X:27:GLN:NE2	2.07	0.70
1:Y:52:ASP:OD1	1:Y:52(A):PRO:HD2	1.92	0.69
3:H:1215:KHA:C1	3:H:1215:KHA:H113	2.22	0.69
2:L:201:LEU:HD13	2:L:205:VAL:CG1	2.22	0.69
1:H:40:SER:O	1:H:42:GLY:O	2.11	0.68
1:Y:148:GLU:CG	1:Y:149:PRO:HA	2.20	0.68
1:Y:206:LYS:HG2	5:Y:2021:HOH:O	1.92	0.68
1:Y:90:SER:O	1:Y:91:ALA:HB2	1.93	0.68
1:H:155:ASN:ND2	1:H:195:ILE:H	1.92	0.68
2:X:175:LEU:HD23	2:X:175:LEU:C	2.14	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:189:HIS:O	2:L:211:ARG:NH1	2.28	0.67
1:Y:40:SER:O	1:Y:42:GLY:O	2.13	0.67
1:Y:24:ALA:HB3	1:Y:27:TYR:O	1.95	0.66
1:H:214:LYS:CE	1:H:215:SER:N	2.59	0.66
1:Y:121:VAL:O	1:Y:209:LYS:HD3	1.97	0.65
1:H:148:GLU:CG	1:H:149:PRO:HA	2.23	0.65
2:L:183:LYS:CD	5:L:2017:HOH:O	1.65	0.65
2:L:154:LEU:HD23	2:L:154:LEU:N	2.12	0.65
1:H:155:ASN:HD21	1:H:195:ILE:H	1.43	0.65
2:L:83:ALA:CB	5:L:2014:HOH:O	2.42	0.65
1:H:76:SER:OG	1:H:76:SER:O	2.14	0.64
2:X:152:ASN:HB3	5:X:2014:HOH:O	1.94	0.64
1:H:19:LYS:HE2	5:H:2003:HOH:O	1.97	0.64
2:L:2:LEU:HD21	2:L:27:GLN:NE2	2.13	0.64
2:L:80:SER:HB2	2:L:168:SER:O	1.98	0.64
1:Y:7:SER:OG	1:Y:20:VAL:HG13	1.98	0.64
1:H:178:LEU:C	1:H:178:LEU:HD12	2.18	0.63
1:H:214:LYS:CD	1:H:215:SER:N	2.60	0.63
1:Y:12:VAL:O	1:Y:111:VAL:HA	1.98	0.63
1:H:122:PHE:CD2	2:L:124:GLN:HG3	2.34	0.63
1:H:147:PRO:O	1:H:200:HIS:CE1	2.48	0.63
2:X:1:GLU:HG3	2:X:97:THR:HG21	1.80	0.63
1:H:121:VAL:HG21	1:H:207:VAL:CG1	2.29	0.62
1:Y:3:GLN:CA	1:Y:3:GLN:NE2	2.56	0.62
1:H:178:LEU:HD12	1:H:178:LEU:O	2.00	0.62
1:Y:199:ASN:CB	1:Y:206:LYS:HZ2	2.12	0.62
2:X:138:ASN:HD22	2:X:138:ASN:N	1.97	0.62
2:X:207:LYS:HE3	2:X:207:LYS:CA	2.26	0.62
1:H:214:LYS:CE	5:H:2019:HOH:O	2.47	0.62
2:X:113:PRO:HD3	2:X:198:HIS:CD2	2.35	0.61
1:Y:24:ALA:HB2	1:Y:29:ILE:CG2	2.29	0.61
2:L:142:ARG:HB3	2:L:173:TYR:CE2	2.35	0.61
1:H:24:ALA:HB2	1:H:29:ILE:CG2	2.31	0.61
1:Y:100(B):PHE:N	1:Y:100(B):PHE:CD2	2.70	0.60
1:Y:155:ASN:ND2	1:Y:195:ILE:H	2.00	0.60
1:Y:3:GLN:CA	1:Y:3:GLN:HE21	2.15	0.60
1:H:11:LEU:HB2	1:H:147:PRO:HG3	1.85	0.59
1:H:201:LYS:HE2	5:H:2017:HOH:O	2.02	0.59
1:Y:36:TRP:CE3	1:Y:80:MET:HE2	2.37	0.59
2:L:31:THR:HG22	2:L:67:SER:HB2	1.85	0.59
2:L:61:ARG:NH2	2:L:82:ASP:OD1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:18:VAL:HG13	1:Y:18:VAL:O	2.03	0.58
1:Y:39:GLN:O	1:Y:91:ALA:HB1	2.03	0.58
2:X:136:LEU:N	2:X:136:LEU:HD12	2.18	0.58
2:L:6:GLN:HB2	2:L:23:CYS:SG	2.43	0.58
2:X:6:GLN:O	2:X:9:LYS:HE3	2.02	0.58
1:Y:119:PRO:HB3	1:Y:145:TYR:HB3	1.86	0.58
2:L:151:ASP:OD2	2:L:189:HIS:HB3	2.03	0.58
2:L:198:HIS:CD2	2:L:200:GLY:H	2.22	0.58
2:X:108:ARG:CG	2:X:109:THR:N	2.64	0.58
2:X:122:ASP:OD1	1:Y:214:LYS:HE2	2.04	0.58
1:H:148:GLU:HG3	1:H:149:PRO:CB	2.34	0.57
1:H:17:SER:OG	1:H:83:ASN:HA	2.03	0.57
2:L:28:ASN:OD1	2:L:30:GLY:N	2.32	0.57
2:L:183:LYS:CE	5:L:2017:HOH:O	2.27	0.57
2:L:175:LEU:HD23	2:L:175:LEU:C	2.25	0.57
2:X:147:ALA:HB1	2:X:154:LEU:HD21	1.87	0.57
2:X:108:ARG:HG2	2:X:109:THR:O	2.05	0.56
1:Y:199:ASN:CB	1:Y:206:LYS:HZ1	2.18	0.56
2:L:108:ARG:HG2	2:L:109:THR:O	2.06	0.56
2:X:136:LEU:N	2:X:136:LEU:CD1	2.69	0.56
1:Y:206:LYS:CG	5:Y:2021:HOH:O	2.53	0.56
2:L:137:ASN:HB3	4:L:1216:PO4:O3	2.06	0.55
1:Y:53:HIS:O	1:Y:54:ASN:CB	2.53	0.55
2:L:149:LYS:HG3	2:L:193:ALA:HB3	1.87	0.55
1:H:168:ALA:HA	1:H:178:LEU:HB3	1.88	0.55
2:X:80:SER:HA	2:X:106:ILE:HD13	1.89	0.55
2:X:27:GLN:O	2:X:29:VAL:HG13	2.07	0.55
2:L:54:ARG:HH12	2:L:63:THR:HG22	1.72	0.54
2:X:13:THR:HG21	2:X:19:VAL:HG11	1.89	0.54
2:L:2:LEU:HD21	2:L:27:GLN:HE22	1.73	0.54
2:X:2:LEU:CD2	2:X:27:GLN:NE2	2.70	0.54
1:Y:51:ILE:CD1	1:Y:71:VAL:HG13	2.37	0.54
1:H:11:LEU:CD2	1:H:116:THR:HG22	2.38	0.54
2:X:198:HIS:CD2	2:X:200:GLY:H	2.26	0.54
1:H:121:VAL:CG2	1:H:207:VAL:HG11	2.37	0.54
1:H:200:HIS:HD2	1:H:203:SER:OG	1.91	0.54
2:L:54:ARG:NH1	2:L:62:PHE:O	2.40	0.54
2:X:83:ALA:O	2:X:84:ALA:HB2	2.06	0.54
2:L:61:ARG:HH21	2:L:82:ASP:CG	2.12	0.53
1:Y:155:ASN:HD21	1:Y:195:ILE:H	1.56	0.53
1:H:214:LYS:NZ	5:H:2019:HOH:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1215:KHA:HB	3:H:1215:KHA:H112	1.90	0.53
2:X:28:ASN:OD1	2:X:68:GLY:HA2	2.08	0.53
2:X:32:HIS:HB2	2:X:92:ASN:HB2	1.91	0.53
2:L:136:LEU:N	2:L:136:LEU:HD12	2.23	0.53
1:H:178:LEU:C	1:H:178:LEU:CD1	2.77	0.52
2:L:175:LEU:HD23	2:L:176:SER:N	2.25	0.52
2:X:5:THR:HG23	2:X:24:LYS:HB3	1.90	0.52
1:Y:117:LYS:NZ	1:Y:118:GLY:O	2.42	0.52
1:Y:178:LEU:HD12	1:Y:178:LEU:C	2.31	0.51
2:X:50:SER:HB3	2:X:53:TYR:HD2	1.76	0.51
2:L:113:PRO:HD3	2:L:198:HIS:CD2	2.45	0.51
1:Y:47:TRP:CZ2	1:Y:49:GLY:HA2	2.46	0.51
1:Y:100(B):PHE:O	1:Y:100(C):PHE:HB3	2.10	0.51
3:Y:1215:KHA:C1	3:Y:1215:KHA:C11	2.86	0.50
1:Y:100(B):PHE:N	1:Y:100(B):PHE:HD2	2.08	0.50
1:Y:90:SER:O	1:Y:91:ALA:CB	2.59	0.50
2:X:10:PHE:HB2	4:X:1214:PO4:O2	2.11	0.50
1:Y:61:GLN:O	1:Y:64:ASN:HB2	2.11	0.50
2:L:5:THR:HA	5:L:2001:HOH:O	2.11	0.50
2:X:38:GLN:O	2:X:84:ALA:HB1	2.12	0.50
2:L:37:GLN:HB2	2:L:86:TYR:CE1	2.46	0.50
1:H:57:PRO:HG3	4:H:1216:PO4:O1	2.12	0.49
1:Y:24:ALA:CB	1:Y:29:ILE:HG23	2.32	0.49
1:Y:146:PHE:CG	1:Y:147:PRO:HA	2.48	0.49
1:Y:3:GLN:HA	1:Y:3:GLN:HE21	1.66	0.49
1:H:64:ASN:OD1	1:H:64:ASN:C	2.49	0.49
2:X:61:ARG:HA	2:X:76:ARG:NH1	2.28	0.49
2:X:33:VAL:HA	2:X:89:GLN:O	2.12	0.49
2:X:121:SER:HB2	2:X:123:GLU:OE1	2.13	0.49
1:H:11:LEU:HD23	1:H:116:THR:HG22	1.95	0.49
1:H:90:SER:HA	1:H:109:VAL:O	2.13	0.49
1:H:44:ASN:C	1:H:44:ASN:OD1	2.51	0.49
1:H:24:ALA:HB2	1:H:29:ILE:HG23	1.94	0.48
1:H:184:VAL:HB	1:H:185:PRO:CD	2.43	0.48
2:L:140:TYR:CG	2:L:141:PRO:HA	2.48	0.48
2:X:107:LYS:NZ	2:X:107:LYS:HB2	2.29	0.48
2:X:95:PRO:O	2:X:97:THR:HG23	2.14	0.48
2:L:145:ALA:HB3	2:L:197:THR:OG1	2.13	0.48
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.94	0.48
2:L:8:PRO:O	2:L:102:THR:HG23	2.14	0.48
1:H:12:VAL:O	1:H:111:VAL:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:201:LYS:HB2	1:H:202:PRO:HD3	1.95	0.48
1:Y:198:VAL:O	1:Y:206:LYS:HE3	2.14	0.48
1:Y:51:ILE:HD12	1:Y:71:VAL:CG1	2.44	0.48
1:Y:12:VAL:HG23	1:Y:16:ALA:HB3	1.95	0.48
1:Y:51:ILE:HD12	1:Y:71:VAL:HG13	1.96	0.48
2:L:165:GLU:HA	2:L:165:GLU:OE1	2.13	0.47
1:Y:51:ILE:HG12	1:Y:57:PRO:HB3	1.97	0.47
2:L:135:LEU:HD12	2:L:136:LEU:N	2.30	0.47
1:H:85:LEU:HA	1:H:89:ASP:OD2	2.14	0.47
2:L:10:PHE:HB2	4:L:1217:PO4:O2	2.15	0.47
1:H:28:SER:OG	1:H:76:SER:HB2	2.14	0.47
2:L:193:ALA:HB2	2:L:208:SER:HB3	1.96	0.47
2:X:210:ASN:HB2	2:X:213:GLU:HG3	1.97	0.46
1:Y:122:PHE:HB2	1:Y:141:LEU:HB3	1.97	0.46
2:X:96:VAL:HB	1:Y:47:TRP:CG	2.50	0.46
1:Y:18:VAL:CG1	1:Y:18:VAL:O	2.63	0.46
1:H:98:PHE:CD1	3:H:1215:KHA:H161	2.51	0.46
1:H:144:ASP:HA	1:H:175:LEU:HB3	1.97	0.46
1:H:148:GLU:HG3	1:H:149:PRO:HB3	1.97	0.46
2:L:33:VAL:HA	2:L:89:GLN:O	2.16	0.46
1:Y:154:TRP:HB3	1:Y:159:LEU:HD23	1.98	0.46
1:H:66:LYS:HE2	1:H:66:LYS:HB2	1.57	0.45
2:X:12:SER:HB2	2:X:105:GLU:HG2	1.97	0.45
1:Y:162:GLY:O	1:Y:182:VAL:HA	2.16	0.45
2:X:26:SER:O	2:X:27:GLN:HG3	2.16	0.45
2:L:28:ASN:C	2:L:28:ASN:OD1	2.54	0.45
1:Y:143:LYS:O	1:Y:144:ASP:HB2	2.16	0.45
2:L:136:LEU:CD1	2:L:136:LEU:N	2.80	0.45
1:H:124:LEU:HB2	1:H:139:GLY:C	2.37	0.45
1:H:47:TRP:CH2	2:L:94:PHE:CD1	3.05	0.45
2:X:140:TYR:CG	2:X:141:PRO:HA	2.51	0.45
2:X:44:PRO:HD2	1:Y:103:TRP:CE3	2.51	0.45
1:Y:42:GLY:O	5:Y:2001:HOH:O	2.21	0.45
1:H:184:VAL:HB	1:H:185:PRO:HD2	1.99	0.45
2:X:186:TYR:CZ	2:X:211:ARG:HG3	2.52	0.45
1:Y:69:LEU:CD1	1:Y:80:MET:HG3	2.47	0.45
2:L:27:GLN:O	2:L:28:ASN:C	2.55	0.44
2:L:80:SER:C	2:L:82:ASP:H	2.21	0.44
2:X:145:ALA:HB3	2:X:197:THR:HG23	1.99	0.44
2:X:136:LEU:HG	2:X:196:VAL:HG21	2.00	0.44
2:L:138:ASN:HD22	2:L:138:ASN:N	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:13:GLU:HG3	1:H:14:PRO:CD	2.47	0.43
2:L:25:ALA:HB3	2:L:69:THR:HA	2.01	0.43
2:L:51:ALA:O	2:L:64:GLY:HA3	2.19	0.43
1:Y:147:PRO:O	1:Y:200:HIS:HE1	2.02	0.43
1:H:99:TYR:O	1:H:100:GLY:C	2.56	0.43
2:X:149:LYS:HB3	2:X:149:LYS:HE2	1.62	0.43
1:Y:69:LEU:HD11	1:Y:80:MET:HG3	1.99	0.43
2:X:170:ASP:OD1	2:X:172:THR:HG23	2.18	0.43
2:X:2:LEU:HD21	2:X:27:GLN:HE21	1.81	0.43
2:L:154:LEU:CD2	2:L:154:LEU:N	2.81	0.43
3:Y:1215:KHA:H113	3:Y:1215:KHA:C1	2.44	0.43
1:Y:13:GLU:HG3	1:Y:14:PRO:HD2	2.01	0.43
2:L:37:GLN:HB2	2:L:47:LEU:HD11	2.01	0.43
2:L:8:PRO:HB3	2:X:11:MET:HG3	2.01	0.43
2:X:14:SER:N	2:X:17:ASP:OD2	2.52	0.43
1:H:47:TRP:CH2	2:L:94:PHE:HD1	2.36	0.42
2:L:107:LYS:HB2	2:L:107:LYS:HE2	1.26	0.42
3:Y:1215:KHA:C5	3:Y:1215:KHA:H162	2.49	0.42
1:Y:164:HIS:HB2	1:Y:181:VAL:CG2	2.49	0.42
2:X:140:TYR:CD2	2:X:141:PRO:HA	2.54	0.42
2:L:35:TRP:HB2	2:L:48:ILE:HB	2.00	0.42
2:L:7:SER:HB2	2:X:13:THR:OG1	2.19	0.42
2:X:37:GLN:HB2	2:X:47:LEU:HD11	2.01	0.42
1:Y:66:LYS:HG3	1:Y:66:LYS:O	2.16	0.42
2:L:18:ARG:O	2:X:7:SER:HB2	2.20	0.42
1:Y:56:GLY:HA2	1:Y:57:PRO:HD3	1.83	0.42
1:Y:33:ASN:O	1:Y:97:ILE:HA	2.19	0.42
1:H:135:THR:HG23	1:H:135:THR:O	2.20	0.42
2:X:32:HIS:ND1	2:X:92:ASN:HA	2.34	0.42
1:H:210:LYS:HD2	1:H:212:GLU:OE1	2.20	0.42
2:L:172:THR:H	2:L:172:THR:HG1	1.66	0.42
2:X:27:GLN:O	2:X:28:ASN:C	2.58	0.42
3:H:1215:KHA:HB	3:H:1215:KHA:C11	2.44	0.42
2:X:138:ASN:N	2:X:138:ASN:ND2	2.65	0.42
1:Y:201:LYS:HE3	1:Y:201:LYS:HB3	1.74	0.42
1:H:24:ALA:CB	1:H:29:ILE:HG23	2.50	0.42
2:L:7:SER:OG	2:X:18:ARG:O	2.38	0.41
1:Y:189:LEU:HA	1:Y:189:LEU:HD23	1.83	0.41
1:Y:200:HIS:CD2	1:Y:203:SER:CB	3.02	0.41
1:H:40:SER:HB2	1:H:41:HIS:H	1.51	0.41
2:X:35:TRP:CZ3	2:X:88:CYS:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:146:PHE:CE1	1:Y:147:PRO:HB3	2.55	0.41
1:H:38:LYS:HD2	1:H:93:TYR:CZ	2.55	0.41
2:L:22:THR:HG21	2:X:18:ARG:HD2	2.03	0.41
1:Y:143:LYS:NZ	1:Y:171:GLN:HE22	2.18	0.41
1:Y:36:TRP:CE3	1:Y:80:MET:CE	3.03	0.41
1:H:171:GLN:H	1:H:171:GLN:HG3	1.57	0.41
1:H:60:ASN:OD1	1:H:60:ASN:C	2.59	0.41
2:X:175:LEU:CD2	2:X:175:LEU:C	2.84	0.41
2:L:85:GLU:HG2	2:L:87:PHE:CE2	2.56	0.41
2:X:194:CYS:SG	2:X:194:CYS:O	2.79	0.41
2:L:22:THR:CG2	2:L:23:CYS:N	2.84	0.41
1:Y:185:PRO:HB2	1:Y:188:SER:OG	2.21	0.41
2:L:28:ASN:HA	2:L:68:GLY:O	2.20	0.41
2:L:39:LYS:HE2	2:L:81:GLU:O	2.21	0.41
2:L:90:GLN:OE1	2:L:92:ASN:N	2.52	0.41
1:H:11:LEU:HD23	1:H:116:THR:CG2	2.51	0.40
2:L:162:SER:HA	5:L:2012:HOH:O	2.20	0.40
2:X:61:ARG:O	2:X:76:ARG:HG3	2.21	0.40
1:Y:76:SER:O	1:Y:76:SER:OG	2.34	0.40
2:L:7:SER:HA	2:L:8:PRO:C	2.41	0.40
2:X:12:SER:HB2	2:X:105:GLU:CG	2.51	0.40
1:H:24:ALA:HB3	1:H:27:TYR:O	2.22	0.40
2:L:11:MET:HB2	2:L:11:MET:HE2	1.88	0.40
1:Y:100(B):PHE:HD2	1:Y:100(B):PHE:H	1.67	0.40
2:X:124:GLN:HB2	1:Y:122:PHE:CE2	2.56	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	H	205/225 (91%)	189 (92%)	14 (7%)	2 (1%)	19 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Y	205/225 (91%)	185 (90%)	17 (8%)	3 (2%)	13 40
2	L	211/213 (99%)	200 (95%)	10 (5%)	1 (0%)	34 69
2	X	211/213 (99%)	204 (97%)	7 (3%)	0	100 100
All	All	832/876 (95%)	778 (94%)	48 (6%)	6 (1%)	26 62

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	41	HIS
1	Y	54	ASN
1	H	41	HIS
1	H	54	ASN
1	Y	91	ALA
2	L	78	VAL

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	H	170/193 (88%)	141 (83%)	29 (17%)	2 7
1	Y	170/193 (88%)	141 (83%)	29 (17%)	2 7
2	L	184/184 (100%)	148 (80%)	36 (20%)	1 5
2	X	184/184 (100%)	144 (78%)	40 (22%)	1 3
All	All	708/754 (94%)	574 (81%)	134 (19%)	2 5

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	VAL
1	H	17	SER
1	H	18	VAL
1	H	19	LYS
1	H	21	SER

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Mol	Chain	Res	Type
1	H	28	SER
1	H	31	ASP
1	H	40	SER
1	H	43	LYS
1	H	44	ASN
1	H	52	ASP
1	H	57	PRO
1	H	66	LYS
1	H	69	LEU
1	H	76	SER
1	H	85	LEU
1	H	113	SER
1	H	120	SER
1	H	124	LEU
1	H	138	LEU
1	H	156	SER
1	H	175	LEU
1	H	178	LEU
1	H	179	SER
1	H	186	SER
1	H	197	ASN
1	H	201	LYS
1	H	210	LYS
1	H	214	LYS
2	L	1	GLU
2	L	2	LEU
2	L	5	THR
2	L	9	LYS
2	L	11	MET
2	L	13	THR
2	L	18	ARG
2	L	20	SER
2	L	22	THR
2	L	27	GLN
2	L	33	VAL
2	L	46	THR
2	L	50	SER
2	L	60	ASP
2	L	61	ARG
2	L	67	SER
2	L	85	GLU
2	L	90	GLN

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Mol	Chain	Res	Type
2	L	105	GLU
2	L	106	ILE
2	L	107	LYS
2	L	108	ARG
2	L	110	VAL
2	L	129	THR
2	L	142	ARG
2	L	149	LYS
2	L	154	LEU
2	L	156	SER
2	L	161	GLU
2	L	162	SER
2	L	187	GLU
2	L	194	CYS
2	L	197	THR
2	L	199	GLN
2	L	202	SER
2	L	213	GLU
2	X	5	THR
2	X	7	SER
2	X	9	LYS
2	X	11	MET
2	X	14	SER
2	X	23	CYS
2	X	26	SER
2	X	28	ASN
2	X	60	ASP
2	X	61	ARG
2	X	63	THR
2	X	76	ARG
2	X	85	GLU
2	X	90	GLN
2	X	93	LEU
2	X	103	LYS
2	X	105	GLU
2	X	106	ILE
2	X	107	LYS
2	X	108	ARG
2	X	123	GLU
2	X	124	GLN
2	X	129	THR
2	X	136	LEU

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Mol	Chain	Res	Type
2	X	138	ASN
2	X	142	ARG
2	X	149	LYS
2	X	154	LEU
2	X	160	GLN
2	X	161	GLU
2	X	181	LEU
2	X	183	LYS
2	X	188	LYS
2	X	194	CYS
2	X	195	GLU
2	X	197	THR
2	X	203	SER
2	X	205	VAL
2	X	207	LYS
2	X	213	GLU
1	Y	3	GLN
1	Y	12	VAL
1	Y	17	SER
1	Y	19	LYS
1	Y	21	SER
1	Y	40	SER
1	Y	43	LYS
1	Y	53	HIS
1	Y	66	LYS
1	Y	69	LEU
1	Y	70	THR
1	Y	73	LYS
1	Y	74	SER
1	Y	85	LEU
1	Y	90	SER
1	Y	100(B)	PHE
1	Y	116	THR
1	Y	120	SER
1	Y	124	LEU
1	Y	135	THR
1	Y	141	LEU
1	Y	161	SER
1	Y	173	SER
1	Y	175	LEU
1	Y	177	SER
1	Y	186	SER

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Mol	Chain	Res	Type
1	Y	193	THR
1	Y	206	LYS
1	Y	209	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	33	ASN
1	H	155	ASN
1	H	200	HIS
2	L	27	GLN
2	L	32	HIS
2	L	37	GLN
2	L	89	GLN
2	L	92	ASN
2	L	138	ASN
2	L	198	HIS
2	X	27	GLN
2	X	79	GLN
2	X	89	GLN
2	X	138	ASN
2	X	198	HIS
1	Y	3	GLN
1	Y	81	HIS
1	Y	155	ASN
1	Y	171	GLN
1	Y	200	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 (i)

8 ligands are 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	$\#\|Z\| > 2$
3	KHA	H	1215	-	21,21,21	0.67	0	27,28,28	1.35	4 (14%)
4	PO4	H	1216	-	4,4,4	0.61	0	6,6,6	0.26	0
4	PO4	L	1214	-	4,4,4	0.78	0	6,6,6	0.23	0
4	PO4	L	1215	-	4,4,4	0.90	0	6,6,6	0.24	0
4	PO4	L	1216	-	4,4,4	0.88	0	6,6,6	0.23	0
4	PO4	L	1217	-	4,4,4	0.72	0	6,6,6	0.25	0
4	PO4	X	1214	-	4,4,4	0.70	0	6,6,6	0.23	0
3	KHA	Y	1215	-	21,21,21	0.59	0	27,28,28	1.84	8 (29%)

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
3	KHA	H	1215	-	-	0/13/23/23	0/2/2/2
4	PO4	H	1216	-	-	0/0/0/0	0/0/0/0
4	PO4	L	1214	-	-	0/0/0/0	0/0/0/0
4	PO4	L	1215	-	-	0/0/0/0	0/0/0/0
4	PO4	L	1216	-	-	0/0/0/0	0/0/0/0
4	PO4	L	1217	-	-	0/0/0/0	0/0/0/0
4	PO4	X	1214	-	-	0/0/0/0	0/0/0/0
3	KHA	Y	1215	-	-	0/13/23/23	0/2/2/2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	1215	KHA	C10-C9-N1	-3.42	104.13	112.00
3	Y	1215	KHA	C11-N2-C16	-3.39	103.56	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1215	KHA	C11-N2-C16	-3.32	103.69	110.14
3	Y	1215	KHA	C11-N2-C15	-2.67	104.96	110.14
3	H	1215	KHA	C15-N2-C16	2.01	112.77	108.60
3	H	1215	KHA	C16-N2-C7	2.14	113.28	109.37
3	Y	1215	KHA	C9-N1-C8	2.57	127.90	122.21
3	Y	1215	KHA	C15-N2-C7	2.62	114.16	109.37
3	Y	1215	KHA	C15-N2-C16	2.70	114.19	108.60
3	Y	1215	KHA	C12-C16-N2	3.59	116.14	112.64
3	H	1215	KHA	C12-C16-N2	3.65	116.20	112.64
3	Y	1215	KHA	C13-C15-N2	4.32	116.86	112.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1215	KHA	5	0
4	H	1216	PO4	1	0
4	L	1216	PO4	1	0
4	L	1217	PO4	1	0
4	X	1214	PO4	1	0
3	Y	1215	KHA	3	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.