Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:26 pm BST

PDB ID	:	2A6K
Title	:	Crystal Structure Analysis of the germline antibody 36-65 Fab in complex with the dodecapeptide SLGDNLTNHNLR
Authors	:	Sethi, D.K.; Agarwal, A.; Manivel, V.; Rao, K.V.; Salunke, D.M.
Deposited on	:	2005-07-03
Resolution	:	3.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

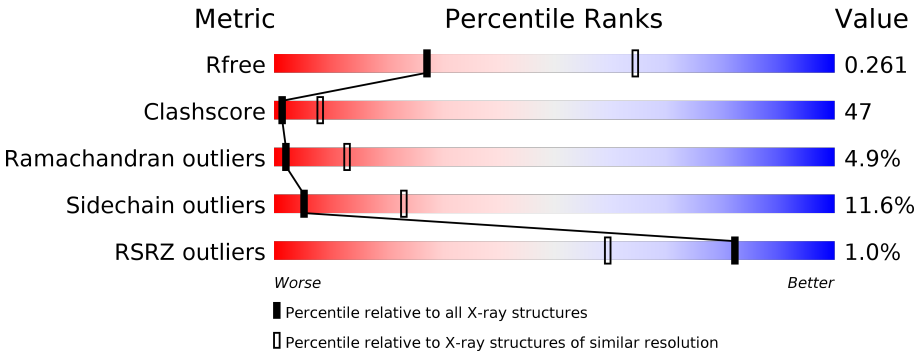
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	214	37% 53% 10%
1	L	214	41% 48% 10%
2	B	222	% 41% 49% 8%
2	H	222	39% 49% 9%
3	P	12	42% 8% 33% 25% 17% 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6764 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 Germline antibody 36-65 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1651	1021	283	340	7			
1	L	214	Total	C	N	O	S	0	0	0
			1658	1024	283	344	7			

- Molecule 2 is a protein called Germline antibody 36-65 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1634	1036	267	324	7			
2	H	216	Total	C	N	O	S	0	0	0
			1637	1039	267	324	7			

- Molecule 3 is a protein called DODECAPEPTIDE: SLGDNLTNHNLR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	0	0	0
			81	46	18	17			

- Molecule 4 is water.

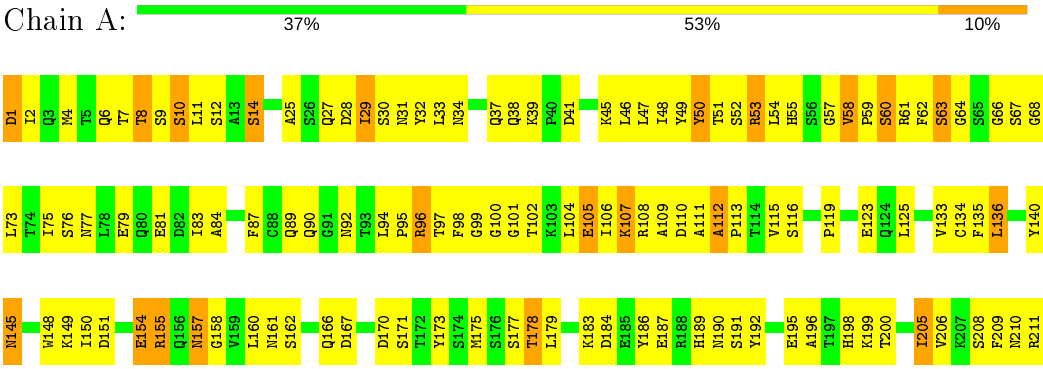
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	B	21	Total	O	0	0
			21	21		
4	L	20	Total	O	0	0
			20	20		
4	H	26	Total	O	0	0
			26	26		
4	P	3	Total	O	0	0
			3	3		

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 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.

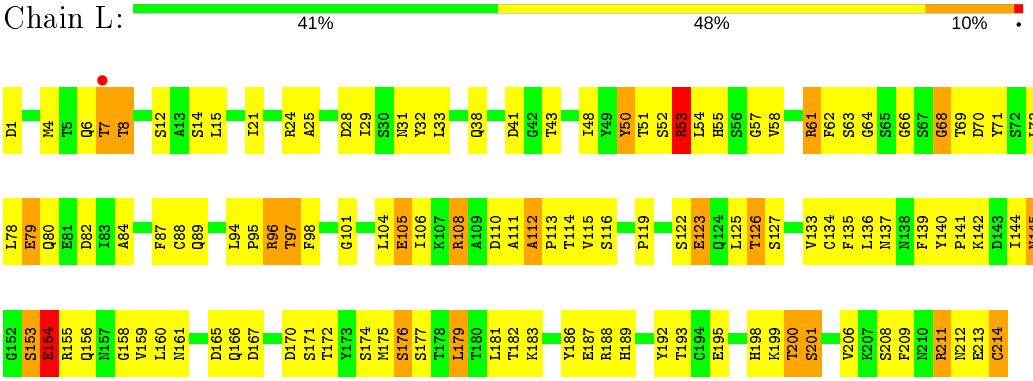
- Molecule 1: Germline antibody 36-65 Fab light chain

Chain A:



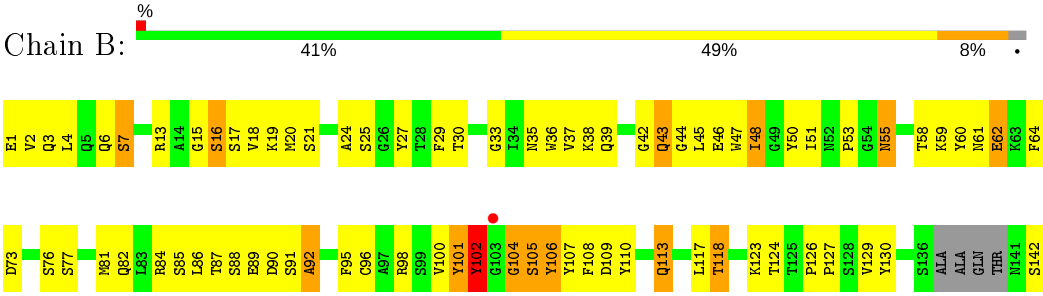
- Molecule 1: Germline antibody 36-65 Fab light chain

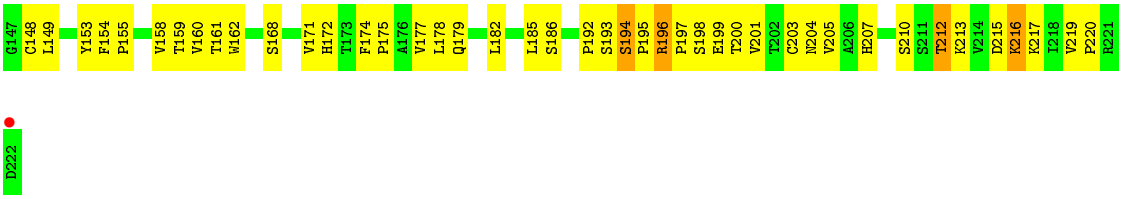
Chain L:



- Molecule 2: Germline antibody 36-65 Fab heavy chain

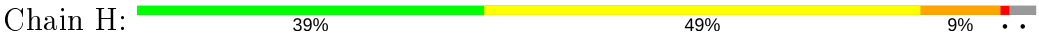
Chain B:

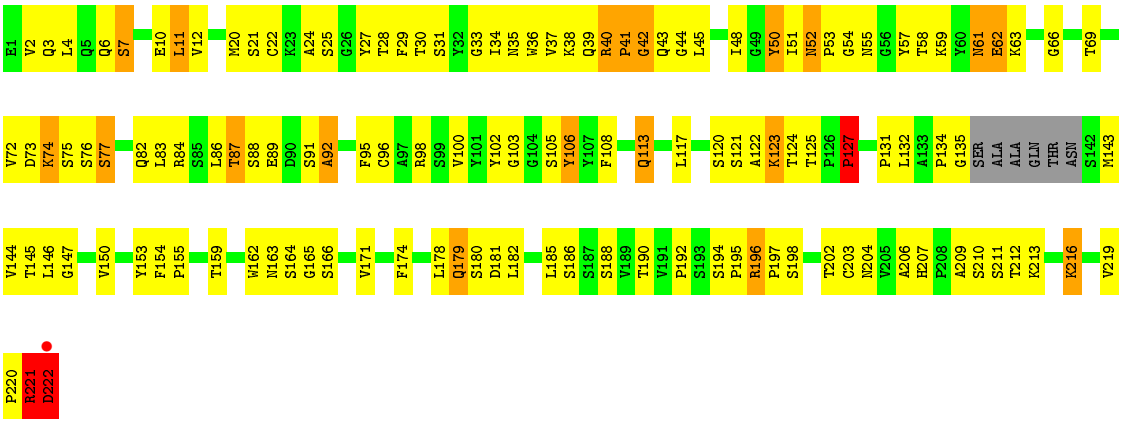




• Molecule 2: Germline antibody 36-65 Fab heavy chain

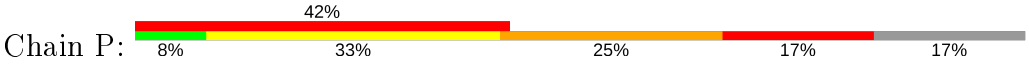
Chain H:

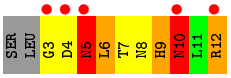




• Molecule 3: DODECAPEPTIDE: SLGDNLTNHNLR

Chain P:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.13Å 144.92Å 70.99Å 90.00° 104.35° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 17.52 – 2.89	Depositor EDS
% Data completeness (in resolution range)	88.6 (50.00-3.00) 88.4 (17.52-2.89)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.43 (at 2.87Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.264 0.244 , 0.261	Depositor DCC
R_{free} test set	1813 reflections (8.24%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6764	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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

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	0.46	0/1684	0.73	0/2284
1	L	0.52	1/1691 (0.1%)	0.80	2/2293 (0.1%)
2	B	0.60	4/1677 (0.2%)	0.81	2/2289 (0.1%)
2	H	0.49	0/1680	0.78	2/2290 (0.1%)
3	P	1.16	0/81	1.93	2/107 (1.9%)
All	All	0.53	5/6813 (0.1%)	0.80	8/9263 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	102	TYR	CB-CG	7.40	1.62	1.51
1	L	154	GLU	CB-CG	6.79	1.65	1.52
2	B	101	TYR	CB-CG	5.70	1.60	1.51
2	B	101	TYR	CA-C	5.62	1.67	1.52
2	B	102	TYR	N-CA	5.55	1.57	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	101	TYR	N-CA-C	9.06	135.46	111.00
2	H	222	ASP	N-CA-C	7.86	132.23	111.00
1	L	154	GLU	N-CA-CB	-7.04	97.94	110.60
2	B	101	TYR	CA-CB-CG	6.79	126.30	113.40
3	P	5	ASN	CA-C-N	-6.59	102.69	117.20
1	L	153	SER	CA-C-N	-5.30	105.55	117.20
2	H	103	GLY	N-CA-C	-5.28	99.91	113.10
3	P	6	LEU	N-CA-C	5.26	125.21	111.00

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	1651	0	1569	164	1
1	L	1658	0	1581	151	2
2	B	1634	0	1565	141	1
2	H	1637	0	1589	165	0
3	P	81	0	73	41	0
4	A	33	0	0	13	0
4	B	21	0	0	6	0
4	H	26	0	0	1	0
4	L	20	0	0	5	0
4	P	3	0	0	2	0
All	All	6764	0	6377	618	2

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 47.

All (618) 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:P:4:ASP:OD1	3:P:5:ASN:N	1.76	1.16
1:L:31:ASN:HD22	1:L:51:THR:HG21	1.10	1.10
2:H:192:PRO:HD2	2:H:195:PRO:HG2	1.35	1.07
1:L:136:LEU:HD23	1:L:144:ILE:HD13	1.34	1.06
2:H:220:PRO:O	2:H:221:ARG:C	1.92	1.06
2:H:106:TYR:OH	3:P:9:HIS:HA	1.55	1.05
1:A:133:VAL:HG22	1:A:178:THR:HG23	1.38	1.04
3:P:12:ARG:HG3	3:P:12:ARG:NH1	1.63	1.04
1:L:25:ALA:HB2	1:L:29:ILE:HD11	1.41	1.03
1:L:112:ALA:HB2	1:L:200:THR:HG21	1.41	1.02
2:B:6:GLN:H	2:B:113:GLN:HE22	1.08	1.01
1:L:166:GLN:HE21	1:L:171:SER:HB3	1.22	1.00
3:P:12:ARG:HG3	3:P:12:ARG:HH11	0.85	1.00
1:L:166:GLN:NE2	1:L:171:SER:HB3	1.78	0.98
3:P:12:ARG:CG	3:P:12:ARG:HH11	1.76	0.98
1:A:46:LEU:HD13	2:B:108:PHE:O	1.65	0.96
2:B:64:PHE:O	2:B:68:THR:HG22	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:4:ASP:O	3:P:5:ASN:CG	2.05	0.95
1:A:150:ILE:HD12	1:A:155:ARG:HD3	1.49	0.95
2:H:106:TYR:OH	3:P:9:HIS:CA	2.16	0.94
2:B:1:GLU:CD	2:B:3:GLN:HE21	1.70	0.94
1:L:108:ARG:NH1	1:L:172:THR:HG23	1.83	0.92
1:A:14:SER:HA	1:A:107:LYS:HD2	1.50	0.91
1:L:108:ARG:HH11	1:L:172:THR:HG23	1.34	0.91
2:H:59:LYS:HZ3	3:P:5:ASN:HA	1.35	0.90
1:L:112:ALA:CB	1:L:200:THR:HG21	2.02	0.90
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.52	0.90
2:H:6:GLN:HE22	2:H:95:PHE:HA	1.36	0.88
1:L:31:ASN:HD22	1:L:51:THR:CG2	1.86	0.88
2:B:192:PRO:O	2:B:195:PRO:HD2	1.75	0.86
2:B:82:GLN:HE21	2:B:84:ARG:HH11	1.21	0.86
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.56	0.86
1:L:31:ASN:ND2	1:L:51:THR:HG21	1.90	0.86
1:A:29:ILE:HG22	1:A:32:TYR:H	1.39	0.86
1:L:108:ARG:NH1	1:L:172:THR:CG2	2.39	0.85
2:B:33:GLY:HA3	2:B:50:TYR:HE1	1.41	0.85
2:H:192:PRO:O	2:H:195:PRO:HD2	1.76	0.85
3:P:4:ASP:O	3:P:5:ASN:ND2	2.10	0.84
3:P:4:ASP:O	3:P:5:ASN:CB	2.25	0.83
2:H:40:ARG:HG3	2:H:92:ALA:HB2	1.59	0.83
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.59	0.82
2:B:6:GLN:H	2:B:113:GLN:NE2	1.75	0.82
1:A:6:GLN:NE2	1:A:101:GLY:H	1.78	0.82
2:H:113:GLN:H	2:H:113:GLN:HE21	1.26	0.82
2:B:86:LEU:HD23	2:B:90:ASP:OD2	1.78	0.81
2:H:220:PRO:O	2:H:222:ASP:N	2.12	0.81
2:H:194:SER:O	2:H:198:SER:HB3	1.81	0.81
2:H:52:ASN:HB2	3:P:8:ASN:HD21	1.43	0.81
2:H:143:MET:CE	2:H:190:THR:HG22	2.10	0.81
1:A:31:ASN:ND2	1:A:51:THR:HG21	1.97	0.80
1:A:151:ASP:OD2	1:A:189:HIS:HB3	1.82	0.79
1:A:31:ASN:CA	1:A:51:THR:OG1	2.30	0.79
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.65	0.79
2:B:37:VAL:CG1	2:B:45:LEU:HB3	2.13	0.79
3:P:4:ASP:CG	3:P:5:ASN:H	1.85	0.78
2:B:37:VAL:HG11	2:B:45:LEU:HB3	1.64	0.78
1:A:14:SER:CA	1:A:107:LYS:HD2	2.13	0.78
2:B:35:ASN:CG	2:B:108:PHE:HE1	1.87	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:THR:OG1	2:B:204:ASN:HB2	1.83	0.78
1:L:53:ARG:HD3	1:L:53:ARG:C	2.04	0.78
1:A:107:LYS:HD3	1:A:107:LYS:H	1.48	0.77
1:L:31:ASN:O	1:L:51:THR:HB	1.85	0.77
1:A:115:VAL:HG22	1:A:136:LEU:HD23	1.65	0.77
1:A:100:GLY:HA2	4:A:225:HOH:O	1.84	0.77
2:H:131:PRO:HD3	2:H:216:LYS:HD3	1.66	0.76
2:H:143:MET:HE2	2:H:190:THR:HG22	1.67	0.76
2:H:29:PHE:CD2	2:H:77:SER:HA	2.21	0.76
1:L:123:GLU:O	1:L:126:THR:HG23	1.86	0.76
1:L:53:ARG:HD2	1:L:54:LEU:HD23	1.66	0.76
2:H:6:GLN:H	2:H:113:GLN:NE2	1.83	0.76
1:L:136:LEU:HD23	1:L:144:ILE:CD1	2.15	0.76
1:L:189:HIS:O	1:L:211:ARG:NH1	2.19	0.76
1:A:48:ILE:CG2	1:A:52:SER:HA	2.16	0.76
1:L:66:GLY:HA3	1:L:71:TYR:HA	1.66	0.76
1:A:105:GLU:OE2	1:A:173:TYR:OH	2.04	0.75
1:L:6:GLN:HE22	1:L:87:PHE:HA	1.51	0.75
2:H:124:THR:HG21	2:H:209:ALA:O	1.87	0.74
1:L:48:ILE:HG21	1:L:52:SER:HA	1.69	0.74
1:A:51:THR:O	1:A:51:THR:HG22	1.86	0.74
2:B:106:TYR:HD2	2:B:106:TYR:H	1.35	0.74
2:B:35:ASN:ND2	2:B:108:PHE:CE1	2.56	0.74
1:A:198:HIS:ND1	1:A:200:THR:HB	2.02	0.74
2:B:100:VAL:HB	2:B:107:TYR:CE1	2.22	0.74
1:A:190:ASN:HD21	1:A:212:ASN:H	1.36	0.73
1:L:12:SER:OG	1:L:105:GLU:OE1	2.05	0.73
1:A:150:ILE:CD1	1:A:155:ARG:HD3	2.17	0.73
2:B:196:ARG:HG3	2:B:201:VAL:CG2	2.18	0.73
1:L:41:ASP:OD1	1:L:43:THR:HG23	1.89	0.73
1:A:192:TYR:O	1:A:208:SER:HB2	1.89	0.73
1:A:52:SER:O	1:A:53:ARG:HB3	1.89	0.73
2:B:35:ASN:CB	2:B:108:PHE:HE1	2.02	0.72
1:L:119:PRO:HB3	1:L:209:PHE:CZ	2.25	0.72
1:A:94:LEU:HD12	2:B:59:LYS:HE3	1.70	0.72
2:H:192:PRO:C	2:H:195:PRO:HD2	2.11	0.72
2:B:192:PRO:C	2:B:195:PRO:HD2	2.10	0.71
2:B:7:SER:OG	2:B:21:SER:N	2.22	0.71
2:B:100:VAL:O	2:B:106:TYR:HA	1.91	0.70
1:A:27:GLN:O	1:A:69:THR:HG22	1.89	0.70
2:B:88:SER:C	2:B:90:ASP:H	1.94	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:6:GLN:H	2:H:113:GLN:HE22	1.38	0.70
1:A:31:ASN:CB	1:A:51:THR:OG1	2.40	0.70
2:B:86:LEU:CD2	2:B:90:ASP:OD2	2.40	0.70
2:H:24:ALA:HB1	2:H:27:TYR:CE2	2.27	0.70
1:L:111:ALA:O	1:L:112:ALA:HB3	1.92	0.69
2:H:30:THR:HG23	2:H:54:GLY:HA2	1.72	0.69
1:L:31:ASN:CB	1:L:51:THR:HB	2.22	0.69
1:A:111:ALA:O	1:A:112:ALA:HB3	1.93	0.69
1:L:31:ASN:HB3	1:L:51:THR:HB	1.74	0.69
1:A:190:ASN:ND2	1:A:212:ASN:H	1.91	0.69
1:A:4:MET:HA	1:A:4:MET:HE3	1.74	0.69
1:A:48:ILE:HG21	1:A:52:SER:HA	1.74	0.69
1:L:108:ARG:HH11	1:L:172:THR:CG2	2.04	0.68
1:A:161:ASN:HD22	1:A:177:SER:HA	1.59	0.68
2:B:15:GLY:O	2:B:85:SER:HA	1.93	0.68
1:A:157:ASN:HD22	1:A:157:ASN:N	1.92	0.68
1:L:167:ASP:HB3	1:L:170:ASP:OD1	1.93	0.68
1:A:29:ILE:HA	1:A:92:ASN:HD22	1.58	0.68
2:H:11:LEU:HD21	2:H:154:PHE:CZ	2.29	0.68
2:B:35:ASN:HB2	2:B:108:PHE:CE1	2.30	0.67
2:B:58:THR:HG1	2:B:60:TYR:HE1	1.41	0.67
2:B:82:GLN:HE21	2:B:84:ARG:NH1	1.92	0.67
1:L:161:ASN:HB3	1:L:175:MET:HE3	1.76	0.67
2:H:202:THR:HG23	2:H:216:LYS:O	1.95	0.67
2:H:12:VAL:HG22	2:H:117:LEU:HD11	1.77	0.66
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.76	0.66
1:L:198:HIS:ND1	1:L:200:THR:HB	2.11	0.66
2:H:52:ASN:HB2	3:P:8:ASN:ND2	2.10	0.66
2:H:51:ILE:HD11	2:H:72:VAL:HG12	1.76	0.66
1:A:167:ASP:HB3	1:A:170:ASP:O	1.96	0.66
1:A:4:MET:HE3	1:A:25:ALA:HA	1.78	0.66
1:A:39:LYS:NZ	1:A:81:GLU:O	2.26	0.66
1:A:30:SER:HA	4:A:222:HOH:O	1.96	0.66
2:B:42:GLY:O	2:B:43:GLN:O	2.14	0.65
1:A:14:SER:CB	1:A:107:LYS:HD2	2.26	0.65
2:B:87:THR:O	2:B:90:ASP:HB2	1.96	0.65
2:H:52:ASN:ND2	2:H:54:GLY:H	1.93	0.65
1:L:29:ILE:HB	1:L:71:TYR:OH	1.96	0.65
2:B:55:ASN:OD1	2:B:55:ASN:N	2.29	0.65
2:H:212:THR:C	2:H:213:LYS:HD2	2.16	0.65
1:L:78:LEU:HG	1:L:79:GLU:N	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:25:ALA:CB	1:L:29:ILE:HD11	2.23	0.65
1:A:52:SER:HB3	1:A:64:GLY:HA3	1.78	0.65
2:B:13:ARG:HH11	2:B:13:ARG:HG2	1.61	0.65
2:B:113:GLN:HE21	2:B:113:GLN:H	1.45	0.64
2:B:113:GLN:NE2	2:B:113:GLN:H	1.95	0.64
1:A:7:THR:O	1:A:8:THR:HB	1.96	0.64
2:B:6:GLN:N	2:B:113:GLN:HE22	1.88	0.64
2:B:16:SER:O	2:B:85:SER:N	2.30	0.64
1:L:112:ALA:HB2	1:L:200:THR:CG2	2.24	0.64
1:A:49:TYR:CE2	1:A:54:LEU:HD12	2.33	0.64
2:B:33:GLY:HA3	2:B:50:TYR:CE1	2.29	0.64
2:B:1:GLU:OE2	2:B:3:GLN:NE2	2.30	0.64
2:H:219:VAL:HG23	2:H:222:ASP:HA	1.77	0.64
1:L:108:ARG:NH1	1:L:170:ASP:HB2	2.13	0.64
1:L:48:ILE:CG2	1:L:52:SER:HA	2.27	0.63
2:H:113:GLN:NE2	2:H:113:GLN:H	1.96	0.63
2:H:220:PRO:C	2:H:222:ASP:N	2.48	0.63
1:A:69:THR:HG23	4:A:231:HOH:O	1.99	0.63
2:B:7:SER:HG	2:B:21:SER:H	1.44	0.63
1:A:6:GLN:HE22	1:A:87:PHE:HA	1.64	0.63
2:H:53:PRO:O	2:H:74:LYS:HD2	1.99	0.63
1:L:94:LEU:HD13	3:P:6:LEU:CD1	2.28	0.63
2:B:106:TYR:CD2	2:B:106:TYR:N	2.66	0.63
1:L:119:PRO:HB3	1:L:209:PHE:CE1	2.34	0.63
2:H:7:SER:HB3	2:H:21:SER:H	1.64	0.62
2:B:87:THR:HG22	2:B:88:SER:N	2.13	0.62
2:B:51:ILE:HD11	2:B:72:VAL:HG12	1.80	0.62
4:A:225:HOH:O	2:B:44:GLY:HA2	1.99	0.62
1:A:95:PRO:HB3	2:B:61:ASN:HD22	1.64	0.62
2:H:6:GLN:HB2	2:H:113:GLN:HE22	1.64	0.62
1:L:75:ILE:O	1:L:77:ASN:N	2.33	0.62
3:P:9:HIS:CD2	3:P:10:ASN:H	2.17	0.62
1:L:153:SER:HB2	1:L:154:GLU:HG2	1.81	0.62
2:B:192:PRO:HD2	2:B:195:PRO:HG2	1.82	0.62
1:L:115:VAL:HA	1:L:135:PHE:O	2.00	0.62
3:P:6:LEU:HG	3:P:7:THR:H	1.64	0.62
1:A:151:ASP:OD2	1:A:189:HIS:CB	2.48	0.62
2:B:196:ARG:HG3	2:B:201:VAL:HG23	1.81	0.62
2:H:11:LEU:HD21	2:H:154:PHE:HZ	1.65	0.61
1:A:6:GLN:NE2	1:A:101:GLY:N	2.48	0.61
2:B:58:THR:OG1	2:B:60:TYR:HE1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:73:ASP:C	2:H:75:SER:H	2.03	0.61
1:A:61:ARG:HD2	1:A:77:ASN:O	2.01	0.61
2:H:220:PRO:O	2:H:221:ARG:O	2.16	0.61
1:A:148:TRP:O	1:A:154:GLU:O	2.19	0.61
2:H:206:ALA:HB1	2:H:213:LYS:HE3	1.82	0.61
2:H:30:THR:HG23	2:H:54:GLY:CA	2.30	0.61
1:L:31:ASN:ND2	1:L:51:THR:OG1	2.34	0.61
1:A:166:GLN:NE2	1:A:171:SER:HB3	2.16	0.61
1:A:31:ASN:HA	1:A:51:THR:OG1	2.01	0.61
2:B:35:ASN:ND2	2:B:108:PHE:HE1	1.93	0.61
2:B:88:SER:O	2:B:90:ASP:N	2.32	0.61
1:L:111:ALA:O	1:L:112:ALA:CB	2.48	0.61
1:L:52:SER:HB3	1:L:64:GLY:C	2.21	0.61
2:H:106:TYR:CZ	3:P:9:HIS:HA	2.35	0.60
1:L:31:ASN:ND2	1:L:51:THR:CB	2.64	0.60
1:L:151:ASP:OD2	1:L:189:HIS:HB3	2.02	0.60
1:L:192:TYR:O	1:L:208:SER:HB2	2.01	0.60
1:A:31:ASN:C	1:A:51:THR:HG1	2.03	0.60
1:L:200:THR:HG23	1:L:200:THR:O	2.00	0.60
1:A:107:LYS:HD3	1:A:107:LYS:N	2.12	0.60
2:H:12:VAL:HG21	2:H:86:LEU:CD1	2.31	0.60
2:H:59:LYS:NZ	3:P:5:ASN:HA	2.13	0.60
1:A:31:ASN:C	1:A:51:THR:OG1	2.40	0.60
2:H:132:LEU:HD12	2:H:147:GLY:HA3	1.84	0.60
1:A:48:ILE:HG22	1:A:52:SER:HA	1.83	0.59
2:B:213:LYS:N	4:B:224:HOH:O	2.35	0.59
2:B:200:THR:HG23	2:B:217:LYS:HD2	1.83	0.59
2:B:35:ASN:CB	2:B:108:PHE:CE1	2.82	0.59
1:A:52:SER:O	1:A:53:ARG:CB	2.50	0.59
1:L:33:LEU:HD11	1:L:88:CYS:HB2	1.84	0.59
2:H:52:ASN:ND2	2:H:54:GLY:N	2.51	0.59
2:H:24:ALA:HB1	2:H:27:TYR:HE2	1.66	0.59
1:L:211:ARG:O	1:L:214:CYS:HB2	2.03	0.59
1:L:25:ALA:HB2	1:L:29:ILE:CD1	2.25	0.59
1:L:51:THR:O	1:L:52:SER:HB2	2.02	0.59
1:A:55:HIS:HE1	1:A:62:PHE:O	1.86	0.59
1:L:21:ILE:HD11	1:L:104:LEU:HD21	1.85	0.58
1:A:158:GLY:O	1:A:179:LEU:HA	2.04	0.58
2:H:210:SER:O	2:H:211:SER:OG	2.16	0.58
1:A:96:ARG:NH1	2:B:35:ASN:HD21	2.00	0.58
2:H:37:VAL:CG1	2:H:45:LEU:HB3	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:179:LEU:HD11	1:L:181:LEU:HD21	1.85	0.58
2:H:52:ASN:CB	3:P:8:ASN:HD21	2.15	0.58
1:L:160:LEU:C	1:L:161:ASN:HD22	2.06	0.58
2:H:73:ASP:O	2:H:75:SER:N	2.36	0.58
1:A:94:LEU:CD1	2:B:59:LYS:HE3	2.33	0.58
2:H:113:GLN:N	2:H:113:GLN:HE21	1.99	0.58
2:H:194:SER:O	2:H:198:SER:CB	2.52	0.58
2:H:212:THR:O	2:H:213:LYS:HD2	2.03	0.58
1:L:31:ASN:ND2	1:L:51:THR:CG2	2.59	0.58
1:L:75:ILE:HG22	1:L:75:ILE:O	2.02	0.58
1:L:38:GLN:O	1:L:84:ALA:HB1	2.04	0.58
1:A:195:GLU:HG2	1:A:206:VAL:HG13	1.85	0.58
2:B:212:THR:HG23	4:B:224:HOH:O	2.03	0.58
2:H:53:PRO:O	2:H:74:LYS:CD	2.52	0.58
2:B:64:PHE:C	2:B:68:THR:HG22	2.24	0.57
3:P:10:ASN:ND2	4:P:87:HOH:O	2.36	0.57
1:A:29:ILE:CG2	1:A:32:TYR:H	2.15	0.57
4:A:225:HOH:O	2:B:44:GLY:CA	2.51	0.57
1:L:137:ASN:OD1	1:L:174:SER:HB3	2.03	0.57
1:A:186:TYR:CE2	1:A:211:ARG:HD2	2.40	0.57
1:A:29:ILE:HD12	1:A:92:ASN:HB3	1.86	0.57
1:L:200:THR:O	1:L:200:THR:CG2	2.52	0.57
1:A:79:GLU:HG3	4:A:216:HOH:O	2.03	0.56
2:B:123:LYS:O	2:B:124:THR:C	2.43	0.56
1:A:160:LEU:HD13	2:B:177:VAL:HG21	1.87	0.56
1:A:31:ASN:O	1:A:50:TYR:CD1	2.58	0.56
2:B:196:ARG:HG3	2:B:201:VAL:HG21	1.87	0.56
2:H:222:ASP:OXT	2:H:222:ASP:CG	2.39	0.56
1:L:53:ARG:HH11	1:L:54:LEU:CD2	2.18	0.56
2:B:35:ASN:ND2	2:B:108:PHE:CZ	2.73	0.56
1:L:110:ASP:OD1	1:L:141:PRO:HD3	2.05	0.56
2:H:28:THR:HG21	2:H:31:SER:OG	2.05	0.56
2:H:28:THR:HG22	2:H:31:SER:H	1.69	0.56
1:L:29:ILE:HG22	1:L:29:ILE:O	2.05	0.56
1:A:161:ASN:ND2	1:A:177:SER:OG	2.38	0.56
2:B:35:ASN:OD1	2:B:50:TYR:HD1	1.88	0.56
1:A:55:HIS:CE1	1:A:62:PHE:O	2.60	0.55
2:B:204:ASN:ND2	2:B:215:ASP:OD1	2.36	0.55
2:B:88:SER:C	2:B:90:ASP:N	2.60	0.55
1:A:108:ARG:HB2	1:A:171:SER:HB2	1.89	0.55
1:A:37:GLN:HB2	1:A:47:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:108:ARG:HB2	1:L:171:SER:HB2	1.88	0.55
1:L:112:ALA:CA	1:L:200:THR:HG21	2.37	0.55
1:L:135:PHE:CE1	1:L:176:SER:HB2	2.40	0.55
2:H:150:VAL:HG12	2:H:153:TYR:CD1	2.41	0.55
1:L:50:TYR:O	1:L:52:SER:O	2.24	0.55
2:H:40:ARG:HD2	2:H:89:GLU:O	2.06	0.55
1:L:159:VAL:O	1:L:160:LEU:HD23	2.06	0.55
1:L:135:PHE:CE1	2:H:174:PHE:CE2	2.94	0.55
1:L:55:HIS:CE1	1:L:62:PHE:O	2.60	0.55
2:H:106:TYR:OH	3:P:9:HIS:N	2.39	0.55
2:B:51:ILE:O	2:B:53:PRO:HD3	2.07	0.55
2:H:4:LEU:HD23	2:H:24:ALA:HA	1.89	0.55
2:B:194:SER:O	2:B:198:SER:HB3	2.07	0.54
1:L:136:LEU:CD2	1:L:144:ILE:HD13	2.22	0.54
1:A:66:GLY:HA3	1:A:71:TYR:CD2	2.42	0.54
2:H:6:GLN:CB	2:H:113:GLN:HE22	2.21	0.54
1:A:151:ASP:OD2	1:A:189:HIS:CD2	2.60	0.54
1:A:113:PRO:HG2	1:A:205:ILE:HD12	1.88	0.54
2:B:72:VAL:CG2	2:B:73:ASP:N	2.71	0.54
1:A:28:ASP:OD2	1:A:30:SER:N	2.38	0.54
2:B:192:PRO:HB2	2:B:195:PRO:CD	2.37	0.54
2:H:143:MET:HE1	2:H:190:THR:HG22	1.88	0.54
1:L:89:GLN:HG2	1:L:97:THR:O	2.07	0.54
2:H:106:TYR:OH	3:P:8:ASN:C	2.45	0.54
2:B:24:ALA:HB1	2:B:27:TYR:CE2	2.42	0.54
2:H:29:PHE:CG	2:H:77:SER:HB3	2.43	0.54
1:A:157:ASN:N	1:A:157:ASN:ND2	2.55	0.54
1:A:50:TYR:O	1:A:52:SER:O	2.25	0.54
2:B:13:ARG:HG2	2:B:13:ARG:NH1	2.22	0.54
2:H:219:VAL:CG2	2:H:222:ASP:HA	2.38	0.54
2:H:38:LYS:CB	2:H:48:ILE:HD11	2.34	0.54
2:H:61:ASN:O	2:H:63:LYS:N	2.41	0.54
2:H:106:TYR:CZ	3:P:8:ASN:O	2.61	0.54
1:A:111:ALA:O	1:A:112:ALA:CB	2.56	0.53
2:H:135:GLY:HA2	2:H:221:ARG:CD	2.38	0.53
1:L:94:LEU:HD13	3:P:6:LEU:HD11	1.88	0.53
3:P:4:ASP:O	3:P:5:ASN:HB2	2.07	0.53
1:A:4:MET:CE	1:A:25:ALA:HA	2.39	0.53
2:B:72:VAL:HG22	2:B:73:ASP:N	2.23	0.53
1:A:108:ARG:HH11	1:A:108:ARG:HG3	1.74	0.53
1:L:160:LEU:CD1	2:H:179:GLN:HG2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:NH2	4:A:237:HOH:O	2.39	0.53
1:A:33:LEU:H	1:A:51:THR:H	1.57	0.53
2:B:46:GLU:OE1	2:B:64:PHE:CZ	2.61	0.53
1:A:8:THR:HG22	1:A:102:THR:HG23	1.90	0.53
2:B:46:GLU:OE1	2:B:64:PHE:HZ	1.92	0.53
2:H:59:LYS:NZ	3:P:5:ASN:HD22	2.07	0.53
1:L:1:ASP:OD1	1:L:95:PRO:HD2	2.08	0.53
2:H:106:TYR:OH	3:P:9:HIS:CB	2.57	0.53
2:H:87:THR:OG1	2:H:88:SER:N	2.37	0.53
2:H:51:ILE:HD11	2:H:72:VAL:CG1	2.39	0.52
2:H:83:LEU:HB3	2:H:86:LEU:HD21	1.91	0.52
1:A:133:VAL:HG12	1:A:134:CYS:N	2.23	0.52
1:A:140:TYR:HD2	1:A:173:TYR:HE1	1.56	0.52
2:H:29:PHE:CE2	2:H:77:SER:HA	2.44	0.52
2:H:82:GLN:OE1	2:H:84:ARG:NH1	2.42	0.52
1:L:182:THR:HB	4:L:219:HOH:O	2.09	0.52
2:B:126:PRO:HG3	2:B:210:SER:HB2	1.92	0.52
1:A:45:LYS:HG2	1:A:46:LEU:N	2.25	0.52
1:L:6:GLN:NE2	1:L:101:GLY:H	2.07	0.52
1:L:48:ILE:HD12	1:L:73:LEU:HD12	1.92	0.52
2:H:150:VAL:HG12	2:H:153:TYR:HD1	1.75	0.52
1:A:107:LYS:O	1:A:107:LYS:HG2	2.10	0.52
1:A:2:ILE:HG21	1:A:29:ILE:HD11	1.92	0.52
1:A:31:ASN:HB3	1:A:51:THR:OG1	2.09	0.52
1:A:51:THR:HG23	1:A:71:TYR:CE2	2.45	0.52
1:A:51:THR:HG23	1:A:71:TYR:CD2	2.45	0.51
2:B:127:PRO:CB	2:B:153:TYR:HB3	2.34	0.51
2:H:106:TYR:CE1	3:P:8:ASN:O	2.64	0.51
1:L:4:MET:HG2	1:L:97:THR:HB	1.92	0.51
1:A:112:ALA:HA	1:A:200:THR:HG21	1.92	0.51
1:A:46:LEU:HD22	2:B:109:ASP:HA	1.91	0.51
2:H:83:LEU:CB	2:H:86:LEU:HD21	2.41	0.51
3:P:9:HIS:O	3:P:10:ASN:HB2	2.10	0.51
1:A:123:GLU:OE2	2:B:216:LYS:HE2	2.10	0.51
1:A:191:SER:HB2	4:A:240:HOH:O	2.09	0.51
1:A:31:ASN:O	1:A:50:TYR:CE1	2.64	0.51
2:H:106:TYR:OH	3:P:9:HIS:HB3	2.10	0.51
2:H:143:MET:HE1	2:H:190:THR:CG2	2.40	0.51
2:H:194:SER:HB2	2:H:195:PRO:HD3	1.92	0.51
1:L:52:SER:O	1:L:53:ARG:CB	2.58	0.51
1:A:8:THR:HG23	1:A:10:SER:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:143:MET:CE	2:H:190:THR:CG2	2.84	0.51
2:H:192:PRO:HB2	2:H:195:PRO:CD	2.41	0.51
1:A:115:VAL:CG2	1:A:136:LEU:HD23	2.38	0.51
1:A:140:TYR:CD2	1:A:173:TYR:HE1	2.28	0.51
2:H:159:THR:HB	2:H:206:ALA:HB3	1.91	0.51
2:H:106:TYR:N	2:H:106:TYR:CD2	2.79	0.51
1:L:167:ASP:HB3	1:L:170:ASP:O	2.11	0.51
2:H:154:PHE:CE2	2:H:155:PRO:HB3	2.46	0.50
2:H:178:LEU:HD12	2:H:182:LEU:O	2.10	0.50
1:L:108:ARG:HH12	1:L:170:ASP:HB2	1.76	0.50
2:B:185:LEU:HD12	2:B:185:LEU:C	2.31	0.50
2:H:196:ARG:HD2	2:H:197:PRO:HA	1.91	0.50
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.94	0.50
1:A:7:THR:O	1:A:8:THR:CB	2.59	0.50
2:B:35:ASN:O	2:B:96:CYS:HA	2.11	0.50
2:H:84:ARG:HG3	2:H:84:ARG:HH11	1.77	0.50
1:L:51:THR:O	1:L:52:SER:CB	2.60	0.50
1:L:61:ARG:HH21	1:L:82:ASP:CG	2.14	0.50
2:B:154:PHE:CE2	2:B:155:PRO:HB3	2.47	0.50
2:H:66:GLY:O	2:H:84:ARG:NH2	2.45	0.50
1:L:135:PHE:HE1	1:L:176:SER:HB2	1.76	0.50
1:A:161:ASN:HB3	1:A:175:MET:HE3	1.92	0.50
2:B:158:VAL:HG23	2:B:207:HIS:HD2	1.76	0.50
2:H:131:PRO:HD3	2:H:216:LYS:CD	2.39	0.50
2:H:61:ASN:HD22	2:H:61:ASN:C	2.15	0.50
1:L:199:LYS:C	1:L:201:SER:H	2.14	0.50
1:L:29:ILE:HD12	1:L:71:TYR:CE1	2.47	0.50
3:P:9:HIS:O	4:P:87:HOH:O	2.19	0.50
2:H:6:GLN:N	2:H:113:GLN:HE22	2.08	0.49
1:L:4:MET:HE1	1:L:29:ILE:HD11	1.94	0.49
1:A:63:SER:O	1:A:73:LEU:HD12	2.12	0.49
2:B:35:ASN:HB2	2:B:108:PHE:HE1	1.66	0.49
2:H:29:PHE:HB2	2:H:77:SER:HB3	1.92	0.49
1:L:38:GLN:HA	1:L:43:THR:O	2.12	0.49
1:L:105:GLU:HB2	1:L:166:GLN:OE1	2.11	0.49
1:L:52:SER:O	1:L:53:ARG:HB3	2.12	0.49
2:H:40:ARG:O	2:H:42:GLY:N	2.45	0.49
2:H:51:ILE:HB	2:H:58:THR:HG22	1.94	0.49
2:B:35:ASN:HD22	2:B:47:TRP:HE1	1.60	0.49
2:H:123:LYS:O	2:H:124:THR:C	2.51	0.49
2:H:162:TRP:O	2:H:163:ASN:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:GLU:CD	2:B:3:GLN:NE2	2.53	0.48
1:L:50:TYR:O	1:L:51:THR:HG22	2.13	0.48
1:L:153:SER:CA	1:L:154:GLU:HG2	2.40	0.48
1:A:183:LYS:O	1:A:187:GLU:HG3	2.13	0.48
2:B:215:ASP:HB2	4:B:236:HOH:O	2.13	0.48
2:B:148:CYS:HB2	2:B:162:TRP:CH2	2.48	0.48
2:B:91:SER:O	2:B:92:ALA:HB2	2.14	0.48
1:L:94:LEU:HD13	3:P:6:LEU:HD12	1.94	0.48
2:H:185:LEU:HD12	2:H:186:SER:N	2.29	0.48
2:H:207:HIS:ND1	2:H:210:SER:HB3	2.28	0.48
2:H:37:VAL:HG11	2:H:45:LEU:HB3	1.94	0.48
1:A:107:LYS:O	1:A:107:LYS:CG	2.60	0.48
2:B:146:LEU:HD12	2:B:201:VAL:HG11	1.95	0.48
1:A:210:ASN:HB2	1:A:213:GLU:HB2	1.95	0.48
1:A:38:GLN:O	1:A:84:ALA:HB1	2.14	0.48
1:A:123:GLU:OE2	2:B:216:LYS:CE	2.62	0.48
2:H:178:LEU:HD12	2:H:182:LEU:C	2.34	0.48
2:H:27:TYR:CE1	2:H:98:ARG:HD2	2.49	0.48
1:L:52:SER:HB3	1:L:64:GLY:HA3	1.96	0.48
1:L:79:GLU:HG2	4:L:229:HOH:O	2.13	0.48
1:A:48:ILE:HD12	1:A:73:LEU:HD13	1.95	0.48
1:L:96:ARG:HG2	1:L:96:ARG:H	1.41	0.48
1:A:32:TYR:CZ	2:B:104:GLY:O	2.67	0.47
1:L:123:GLU:H	1:L:123:GLU:HG2	1.38	0.47
1:L:31:ASN:CA	1:L:51:THR:HB	2.43	0.47
1:L:31:ASN:HD22	1:L:51:THR:CB	2.25	0.47
1:A:108:ARG:HG2	1:A:109:ALA:N	2.28	0.47
2:B:98:ARG:O	2:B:108:PHE:HA	2.14	0.47
1:L:4:MET:O	4:L:220:HOH:O	2.20	0.47
1:L:94:LEU:HD12	4:L:233:HOH:O	2.14	0.47
1:A:4:MET:HA	1:A:4:MET:CE	2.41	0.47
1:A:170:ASP:C	1:A:170:ASP:OD1	2.53	0.47
1:A:48:ILE:HD12	1:A:73:LEU:CD1	2.45	0.47
1:A:48:ILE:HG22	1:A:49:TYR:N	2.29	0.47
2:H:35:ASN:O	2:H:96:CYS:HA	2.15	0.47
1:A:144:ILE:HG12	1:A:145:ASN:H	1.80	0.47
1:A:96:ARG:NH1	2:B:35:ASN:ND2	2.62	0.47
2:B:130:TYR:HB2	2:B:149:LEU:HB3	1.96	0.47
1:L:161:ASN:HB3	1:L:175:MET:CE	2.42	0.47
3:P:8:ASN:OD1	3:P:8:ASN:O	2.32	0.47
1:A:50:TYR:CD2	2:B:102:TYR:HE2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:79:GLU:O	1:L:80:GLN:C	2.54	0.47
2:H:91:SER:O	2:H:92:ALA:HB2	2.15	0.47
1:L:186:TYR:CE2	1:L:211:ARG:HD2	2.50	0.47
1:L:183:LYS:O	1:L:187:GLU:HG3	2.14	0.47
1:L:24:ARG:HG3	1:L:70:ASP:OD2	2.16	0.46
1:L:153:SER:CB	1:L:154:GLU:HG2	2.44	0.46
2:B:148:CYS:HB2	2:B:162:TRP:HH2	1.79	0.46
2:H:51:ILE:O	2:H:51:ILE:HG23	2.14	0.46
1:A:4:MET:SD	1:A:90:GLN:HG2	2.55	0.46
1:A:83:ILE:HD11	1:A:106:ILE:HD11	1.97	0.46
2:H:134:PRO:HD3	2:H:146:LEU:HD23	1.97	0.46
1:L:52:SER:HB3	1:L:64:GLY:CA	2.45	0.46
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.98	0.46
1:A:29:ILE:O	1:A:29:ILE:CG2	2.64	0.46
2:H:12:VAL:HG21	2:H:86:LEU:HD13	1.98	0.46
2:H:202:THR:HG23	2:H:216:LYS:C	2.36	0.46
1:L:77:ASN:OD1	1:L:77:ASN:C	2.53	0.46
1:A:11:LEU:HD12	1:A:12:SER:N	2.31	0.46
1:A:115:VAL:HA	1:A:135:PHE:O	2.15	0.46
2:B:7:SER:OG	2:B:21:SER:HB2	2.16	0.46
2:B:87:THR:HG22	2:B:88:SER:H	1.79	0.46
2:H:52:ASN:CB	3:P:8:ASN:ND2	2.77	0.46
2:H:106:TYR:OH	3:P:8:ASN:O	2.34	0.46
2:B:160:VAL:HG22	2:B:205:VAL:HG22	1.98	0.46
1:L:150:ILE:HD12	1:L:155:ARG:HD3	1.97	0.46
1:A:136:LEU:CD2	1:A:196:ALA:HB2	2.46	0.46
1:A:144:ILE:HG12	1:A:145:ASN:N	2.30	0.46
1:A:1:ASP:HB3	1:A:95:PRO:HD2	1.98	0.46
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.97	0.46
2:H:11:LEU:HD21	2:H:154:PHE:CE2	2.51	0.46
2:H:153:TYR:OH	2:H:185:LEU:HD23	2.16	0.46
2:B:194:SER:N	2:B:195:PRO:CD	2.79	0.46
1:L:212:ASN:OD1	1:L:213:GLU:N	2.49	0.46
1:L:108:ARG:O	1:L:140:TYR:CE2	2.69	0.45
1:L:15:LEU:HD21	1:L:106:ILE:HD11	1.98	0.45
1:L:160:LEU:HD12	2:H:179:GLN:HG2	1.98	0.45
1:L:193:THR:HA	1:L:208:SER:HB3	1.99	0.45
1:A:110:ASP:HA	1:A:140:TYR:O	2.17	0.45
2:B:3:GLN:HB2	2:B:25:SER:OG	2.16	0.45
1:L:200:THR:O	1:L:201:SER:HB3	2.17	0.45
1:A:6:GLN:HE21	1:A:99:GLY:C	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:7:THR:O	1:L:8:THR:OG1	2.30	0.45
1:L:195:GLU:HG2	1:L:206:VAL:HG22	1.98	0.45
1:A:162:SER:OG	2:B:175:PRO:HD2	2.16	0.45
2:H:192:PRO:CD	2:H:195:PRO:HG2	2.26	0.45
2:B:171:VAL:HG12	2:B:172:HIS:N	2.31	0.45
1:L:158:GLY:O	1:L:179:LEU:HA	2.16	0.45
1:A:31:ASN:ND2	1:A:51:THR:CG2	2.76	0.45
2:B:100:VAL:HG21	2:B:109:ASP:OD2	2.17	0.45
2:H:120:SER:OG	2:H:121:SER:N	2.50	0.45
2:H:36:TRP:HB2	2:H:48:ILE:HB	1.98	0.45
1:L:144:ILE:HG23	1:L:145:ASN:N	2.32	0.45
1:L:79:GLU:CG	4:L:229:HOH:O	2.65	0.45
2:H:73:ASP:C	2:H:75:SER:N	2.70	0.44
1:L:31:ASN:C	1:L:51:THR:HB	2.37	0.44
1:A:149:LYS:HD2	1:A:195:GLU:OE1	2.17	0.44
1:A:186:TYR:CZ	1:A:211:ARG:HD2	2.52	0.44
1:A:39:LYS:HG2	4:A:242:HOH:O	2.17	0.44
2:B:87:THR:CG2	2:B:88:SER:N	2.79	0.44
1:L:28:ASP:OD2	1:L:68:GLY:HA2	2.18	0.44
2:B:61:ASN:O	2:B:62:GLU:C	2.55	0.44
2:H:162:TRP:HA	2:H:202:THR:O	2.18	0.44
2:H:33:GLY:O	2:H:34:ILE:HD13	2.17	0.44
1:L:170:ASP:C	1:L:170:ASP:OD1	2.55	0.44
1:L:155:ARG:O	1:L:156:GLN:HG2	2.17	0.44
1:A:119:PRO:HG3	1:A:209:PHE:CE2	2.52	0.44
1:A:8:THR:HG21	1:A:11:LEU:HB2	1.99	0.44
2:B:100:VAL:HG12	2:B:101:TYR:N	2.32	0.44
2:B:2:VAL:HG11	2:B:110:TYR:CD1	2.53	0.44
1:L:53:ARG:HD3	1:L:53:ARG:O	2.17	0.44
1:A:11:LEU:HD12	1:A:12:SER:H	1.83	0.44
2:B:20:MET:HB2	4:B:235:HOH:O	2.17	0.44
2:H:125:THR:HG22	2:H:154:PHE:HB3	1.99	0.44
2:H:220:PRO:O	2:H:222:ASP:CA	2.64	0.44
2:H:50:TYR:CD2	2:H:59:LYS:HB3	2.53	0.44
1:A:140:TYR:HD2	1:A:173:TYR:CE1	2.36	0.44
2:H:100:VAL:O	2:H:106:TYR:HA	2.18	0.44
2:H:2:VAL:HG12	2:H:3:GLN:N	2.33	0.44
2:B:76:SER:O	2:B:77:SER:C	2.57	0.43
2:B:43:GLN:N	4:B:227:HOH:O	2.50	0.43
2:B:4:LEU:HD23	2:B:24:ALA:HA	2.01	0.43
2:H:179:GLN:HB3	2:H:180:SER:H	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD11	2:B:102:TYR:CE2	2.54	0.43
2:B:129:VAL:HG13	2:B:148:CYS:SG	2.59	0.43
2:B:178:LEU:HA	2:B:182:LEU:O	2.18	0.43
2:B:196:ARG:HB3	2:B:196:ARG:HE	1.29	0.43
2:H:72:VAL:CG2	2:H:73:ASP:N	2.81	0.43
3:P:9:HIS:O	3:P:10:ASN:CB	2.66	0.43
2:B:171:VAL:CG1	2:B:172:HIS:N	2.82	0.43
2:H:127:PRO:HB3	2:H:153:TYR:CB	2.38	0.43
2:H:154:PHE:HA	2:H:155:PRO:HA	1.83	0.43
1:A:34:ASN:OD1	1:A:49:TYR:HB2	2.18	0.43
1:A:90:GLN:HG3	1:A:97:THR:OG1	2.19	0.43
2:H:171:VAL:HA	2:H:188:SER:O	2.18	0.43
1:L:139:PHE:HE1	1:L:142:LYS:O	2.01	0.43
2:H:29:PHE:CB	2:H:77:SER:HB3	2.49	0.43
1:L:31:ASN:O	1:L:51:THR:N	2.52	0.43
1:L:133:VAL:HG12	1:L:134:CYS:N	2.34	0.43
1:L:161:ASN:N	1:L:161:ASN:ND2	2.67	0.43
1:A:27:GLN:C	1:A:69:THR:HG22	2.38	0.43
1:A:107:LYS:O	1:A:107:LYS:NZ	2.29	0.42
2:B:212:THR:HA	4:B:234:HOH:O	2.19	0.42
1:L:161:ASN:N	1:L:161:ASN:HD22	2.14	0.42
1:A:106:ILE:HG22	1:A:107:LYS:N	2.34	0.42
1:A:133:VAL:CG1	1:A:134:CYS:N	2.82	0.42
1:L:114:THR:O	1:L:136:LEU:HA	2.19	0.42
1:A:89:GLN:HG3	1:A:98:PHE:CE1	2.54	0.42
2:B:35:ASN:HD22	2:B:108:PHE:HZ	1.67	0.42
2:B:29:PHE:CD2	2:B:77:SER:HA	2.54	0.42
2:H:153:TYR:CD2	2:H:153:TYR:C	2.92	0.42
1:L:125:LEU:O	1:L:183:LYS:HD2	2.18	0.42
1:L:32:TYR:CD2	2:H:105:SER:OG	2.70	0.42
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.82	0.42
2:H:202:THR:HG22	2:H:203:CYS:N	2.34	0.42
1:L:153:SER:HB2	1:L:154:GLU:CG	2.48	0.42
2:H:59:LYS:HZ1	3:P:5:ASN:HD22	1.67	0.42
2:H:57:TYR:CE2	3:P:6:LEU:O	2.73	0.42
2:B:161:THR:HG1	2:B:204:ASN:HB2	1.82	0.42
2:B:36:TRP:HA	2:B:95:PHE:O	2.20	0.42
2:H:127:PRO:CB	2:H:153:TYR:HB3	2.40	0.42
2:H:28:THR:CG2	2:H:31:SER:OG	2.67	0.42
2:H:40:ARG:O	2:H:41:PRO:C	2.58	0.42
2:H:61:ASN:HD22	2:H:62:GLU:N	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:4:MET:HB2	1:L:98:PHE:O	2.19	0.42
2:B:16:SER:HB3	2:B:17:SER:H	1.41	0.42
2:B:158:VAL:CG2	2:B:207:HIS:HD2	2.33	0.42
2:B:35:ASN:OD1	2:B:50:TYR:CD1	2.71	0.42
1:L:55:HIS:NE2	1:L:62:PHE:O	2.52	0.42
1:L:77:ASN:OD1	1:L:77:ASN:O	2.37	0.42
1:A:116:SER:O	1:A:134:CYS:HA	2.20	0.42
1:A:50:TYR:CD2	2:B:102:TYR:CE2	3.08	0.42
2:B:107:TYR:CD1	2:B:107:TYR:C	2.92	0.42
3:P:3:GLY:C	3:P:4:ASP:O	2.54	0.42
2:H:163:ASN:O	2:H:165:GLY:N	2.53	0.42
2:H:181:ASP:O	2:H:182:LEU:HG	2.20	0.42
1:A:100:GLY:HA3	4:A:228:HOH:O	2.19	0.42
1:A:31:ASN:HB3	1:A:51:THR:HG1	1.85	0.42
2:H:39:GLN:O	2:H:92:ALA:HB1	2.19	0.42
1:L:54:LEU:HD11	2:H:102:TYR:OH	2.20	0.42
1:A:198:HIS:CE1	1:A:200:THR:HB	2.55	0.41
1:A:211:ARG:HB2	4:A:234:HOH:O	2.20	0.41
2:H:143:MET:HE2	2:H:190:THR:CG2	2.44	0.41
2:H:40:ARG:C	2:H:42:GLY:N	2.73	0.41
2:B:39:GLN:O	2:B:92:ALA:HB1	2.20	0.41
3:P:12:ARG:NH1	3:P:12:ARG:CG	2.47	0.41
1:A:58:VAL:HA	1:A:59:PRO:HD3	1.94	0.41
2:H:10:GLU:HA	2:H:10:GLU:OE1	2.20	0.41
2:H:135:GLY:HA2	2:H:221:ARG:HD3	2.01	0.41
2:H:35:ASN:ND2	2:H:108:PHE:CE1	2.89	0.41
2:H:61:ASN:HA	4:H:240:HOH:O	2.21	0.41
2:H:57:TYR:HE2	3:P:6:LEU:O	2.03	0.41
1:A:184:ASP:HA	4:A:215:HOH:O	2.21	0.41
2:B:104:GLY:O	2:B:105:SER:HB2	2.20	0.41
2:B:19:LYS:HA	2:B:81:MET:O	2.20	0.41
1:L:161:ASN:ND2	1:L:177:SER:OG	2.53	0.41
1:L:144:ILE:HG13	1:L:198:HIS:HD2	1.86	0.41
2:B:194:SER:O	2:B:198:SER:CB	2.69	0.41
2:B:15:GLY:C	2:B:85:SER:HA	2.41	0.41
1:L:116:SER:O	1:L:134:CYS:HA	2.20	0.41
2:B:144:VAL:O	2:B:144:VAL:HG13	2.21	0.41
2:H:182:LEU:HD23	2:H:182:LEU:HA	1.87	0.41
2:H:41:PRO:O	2:H:42:GLY:O	2.39	0.41
1:L:112:ALA:HA	1:L:200:THR:HG21	2.02	0.41
1:A:33:LEU:HD12	1:A:89:GLN:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:O	1:A:102:THR:HA	2.21	0.41
2:B:104:GLY:O	2:B:105:SER:CB	2.69	0.41
2:B:117:LEU:HD12	2:B:118:THR:N	2.36	0.41
1:L:79:GLU:O	1:L:82:ASP:HB2	2.21	0.41
1:A:2:ILE:O	1:A:97:THR:HG21	2.20	0.40
2:B:174:PHE:HA	2:B:175:PRO:HD3	1.89	0.40
2:B:30:THR:HA	2:B:53:PRO:HB2	2.03	0.40
2:B:6:GLN:OE1	2:B:95:PHE:HA	2.21	0.40
2:H:61:ASN:C	2:H:63:LYS:H	2.24	0.40
1:L:122:SER:O	1:L:126:THR:HG22	2.21	0.40
1:L:4:MET:HE3	1:L:25:ALA:HA	2.03	0.40
1:A:133:VAL:HG22	1:A:178:THR:CG2	2.29	0.40
1:A:51:THR:C	1:A:52:SER:O	2.59	0.40
1:A:75:ILE:O	1:A:77:ASN:N	2.55	0.40
1:A:89:GLN:HG2	1:A:97:THR:O	2.20	0.40
2:H:53:PRO:O	2:H:74:LYS:HD3	2.21	0.40
2:H:76:SER:O	2:H:77:SER:C	2.59	0.40
1:L:149:LYS:HB2	1:L:193:THR:HB	2.04	0.40
1:A:11:LEU:O	1:A:104:LEU:HA	2.21	0.40
1:A:109:ALA:O	1:A:110:ASP:C	2.58	0.40
1:A:95:PRO:HB3	2:B:61:ASN:ND2	2.34	0.40
2:B:197:PRO:HB3	2:B:220:PRO:HG3	2.03	0.40
1:L:33:LEU:HD22	1:L:71:TYR:CB	2.51	0.40
1:A:100:GLY:C	4:A:228:HOH:O	2.60	0.40
2:H:30:THR:HA	2:H:53:PRO:HB2	2.03	0.40
1:A:140:TYR:CD2	1:A:141:PRO:HA	2.56	0.40
2:H:145:THR:HG22	2:H:146:LEU:N	2.37	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:GLU:OE2	1:L:188:ARG:NH1[1_465]	2.09	0.11
1:A:60:SER:OG	1:L:79:GLU:OE1[2_555]	2.17	0.03

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	212/214 (99%)	185 (87%)	18 (8%)	9 (4%)	3 16
1	L	212/214 (99%)	182 (86%)	22 (10%)	8 (4%)	3 18
2	B	214/222 (96%)	184 (86%)	19 (9%)	11 (5%)	2 12
2	H	212/222 (96%)	184 (87%)	16 (8%)	12 (6%)	1 10
3	P	8/12 (67%)	3 (38%)	3 (38%)	2 (25%)	0 0
All	All	858/884 (97%)	738 (86%)	78 (9%)	42 (5%)	2 13

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	GLU
2	B	43	GLN
2	B	89	GLU
2	B	105	SER
1	L	8	THR
1	L	76	SER
2	H	22	CYS
2	H	44	GLY
2	H	62	GLU
2	H	74	LYS
2	H	164	SER
2	H	221	ARG
3	P	5	ASN
3	P	10	ASN
1	A	8	THR
1	A	53	ARG
1	A	76	SER
2	B	16	SER
2	B	102	TYR
1	L	68	GLY
2	H	42	GLY

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Mol	Chain	Res	Type
2	H	43	GLN
1	A	57	GLY
2	B	62	GLU
2	B	104	GLY
1	L	50	TYR
1	L	53	ARG
1	L	112	ALA
1	A	50	TYR
1	A	112	ALA
1	A	155	ARG
2	B	92	ALA
2	B	179	GLN
1	L	57	GLY
2	H	92	ALA
2	H	122	ALA
1	L	154	GLU
2	H	41	PRO
2	H	127	PRO
2	B	18	VAL
2	B	48	ILE
1	A	68	GLY

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	187/192 (97%)	168 (90%)	19 (10%)	7 28
1	L	190/192 (99%)	165 (87%)	25 (13%)	4 18
2	B	181/190 (95%)	165 (91%)	16 (9%)	10 36
2	H	184/190 (97%)	160 (87%)	24 (13%)	4 19
3	P	9/11 (82%)	6 (67%)	3 (33%)	0 1
All	All	751/775 (97%)	664 (88%)	87 (12%)	5 23

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	10	SER
1	A	14	SER
1	A	29	ILE
1	A	41	ASP
1	A	58	VAL
1	A	60	SER
1	A	63	SER
1	A	67	SER
1	A	96	ARG
1	A	105	GLU
1	A	107	LYS
1	A	136	LEU
1	A	142	LYS
1	A	145	ASN
1	A	157	ASN
1	A	178	THR
1	A	199	LYS
1	A	205	ILE
2	B	7	SER
2	B	55	ASN
2	B	106	TYR
2	B	113	GLN
2	B	118	THR
2	B	142	SER
2	B	159	THR
2	B	168	SER
2	B	186	SER
2	B	193	SER
2	B	194	SER
2	B	196	ARG
2	B	203	CYS
2	B	212	THR
2	B	216	LYS
2	B	219	VAL
1	L	7	THR
1	L	14	SER
1	L	53	ARG
1	L	58	VAL
1	L	61	ARG
1	L	63	SER
1	L	69	THR
1	L	77	ASN

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Mol	Chain	Res	Type
1	L	79	GLU
1	L	96	ARG
1	L	97	THR
1	L	105	GLU
1	L	108	ARG
1	L	123	GLU
1	L	126	THR
1	L	127	SER
1	L	145	ASN
1	L	154	GLU
1	L	165	ASP
1	L	176	SER
1	L	179	LEU
1	L	200	THR
1	L	201	SER
1	L	211	ARG
1	L	214	CYS
2	H	7	SER
2	H	11	LEU
2	H	20	MET
2	H	25	SER
2	H	40	ARG
2	H	50	TYR
2	H	52	ASN
2	H	55	ASN
2	H	61	ASN
2	H	69	THR
2	H	77	SER
2	H	87	THR
2	H	106	TYR
2	H	113	GLN
2	H	123	LYS
2	H	127	PRO
2	H	144	VAL
2	H	166	SER
2	H	179	GLN
2	H	196	ARG
2	H	204	ASN
2	H	216	LYS
2	H	221	ARG
2	H	222	ASP
3	P	9	HIS

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Mol	Chain	Res	Type
3	P	10	ASN
3	P	12	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	31	ASN
1	A	37	GLN
1	A	55	HIS
1	A	92	ASN
1	A	157	ASN
1	A	161	ASN
1	A	190	ASN
2	B	3	GLN
2	B	52	ASN
2	B	61	ASN
2	B	82	GLN
2	B	113	GLN
1	L	6	GLN
1	L	31	ASN
1	L	161	ASN
1	L	189	HIS
2	H	6	GLN
2	H	52	ASN
2	H	55	ASN
2	H	61	ASN
2	H	113	GLN
3	P	5	ASN
3	P	8	ASN
3	P	9	HIS
3	P	10	ASN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	214/214 (100%)	-0.16	0 100 100	12, 32, 56, 63	0
1	L	214/214 (100%)	-0.20	1 (0%) 91 75	10, 30, 48, 60	0
2	B	218/222 (98%)	-0.06	2 (0%) 84 63	8, 38, 58, 68	0
2	H	216/222 (97%)	-0.22	1 (0%) 91 75	1, 31, 54, 65	0
3	P	10/12 (83%)	1.92	5 (50%) 0 0	35, 44, 51, 58	0
All	All	872/884 (98%)	-0.14	9 (1%) 82 59	1, 33, 56, 68	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	5	ASN	3.4
2	H	222	ASP	3.1
3	P	10	ASN	3.1
1	L	7	THR	2.9
3	P	4	ASP	2.8
3	P	3	GLY	2.4
2	B	222	ASP	2.2
2	B	103	GLY	2.2
3	P	12	ARG	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.