Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2023 – 05:28 AM EDT

PDB ID	:	1FJ1
Title	:	LYME DISEASE ANTIGEN OSPA IN COMPLEX WITH NEUTRALIZING ANTIBODY FAB LA-2
Authors	:	Ding, W.; Lawson, C.L.
Deposited on	:	2000-08-07
Resolution	:	2.68 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

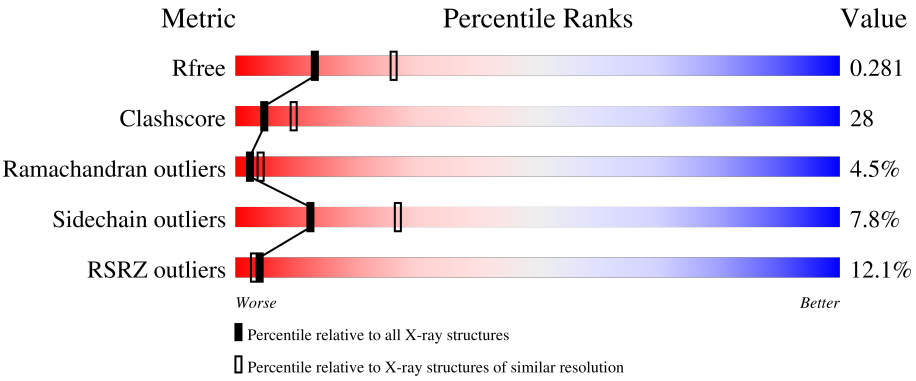
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.68 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	213	70% 27% .
1	C	213	% 72% 24% .
2	B	213	4% 66% 27% 8%
2	D	213	6% 60% 28% 12%
3	E	257	30% 46% 42% 9% ..

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Mol	Chain	Length	Quality of chain
3	F	257	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10542 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 HYBRIDOMA ANTIBODY LA2 (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1660	1033	284	337	6			
1	C	213	Total	C	N	O	S	0	0	0
			1660	1033	284	337	6			

- Molecule 2 is a protein called HYBRIDOMA ANTIBODY LA2 (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1589	1001	257	323	8			
2	D	213	Total	C	N	O	S	0	0	0
			1589	1001	257	323	8			

- Molecule 3 is a protein called OUTER SURFACE PROTEIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	251	Total	C	N	O	S	0	0	0
			1893	1170	313	408	2			
3	F	251	Total	C	N	O	S	0	0	0
			1893	1170	313	408	2			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	17	ALA	CYS	SEE REMARK 999	UNP P14013
E	39	LYS	ASN	variant	UNP P14013
E	84	CYS	SER	engineered mutation	UNP P14013
E	149	GLY	GLU	variant	UNP P14013
E	164	GLY	SER	variant	UNP P14013
F	17	ALA	CYS	SEE REMARK 999	UNP P14013
F	39	LYS	ASN	variant	UNP P14013
F	84	CYS	SER	engineered mutation	UNP P14013

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Chain	Residue	Modelled	Actual	Comment	Reference
F	149	GLY	GLU	variant	UNP P14013
F	164	GLY	SER	variant	UNP P14013

- Molecule 4 is water.

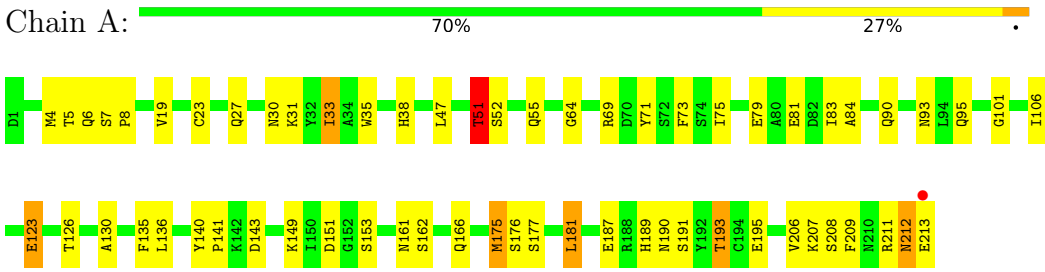
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	64	Total O 64 64	0	0
4	B	52	Total O 52 52	0	0
4	C	67	Total O 67 67	0	0
4	D	22	Total O 22 22	0	0
4	E	37	Total O 37 37	0	0
4	F	16	Total O 16 16	0	0

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.

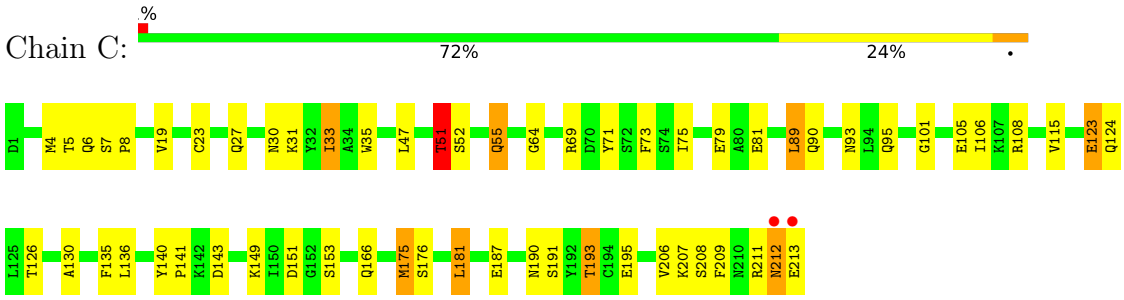
• Molecule 1: HYBRIDOMA ANTIBODY LA2 (LIGHT CHAIN)

Chain A:



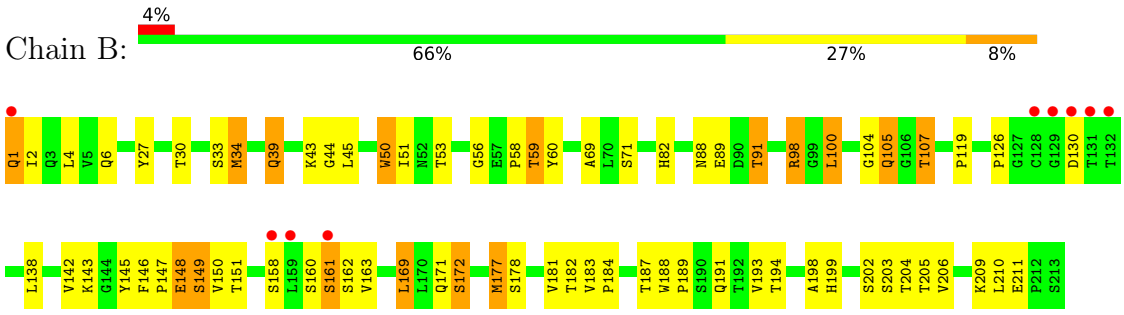
• Molecule 1: HYBRIDOMA ANTIBODY LA2 (LIGHT CHAIN)

Chain C:



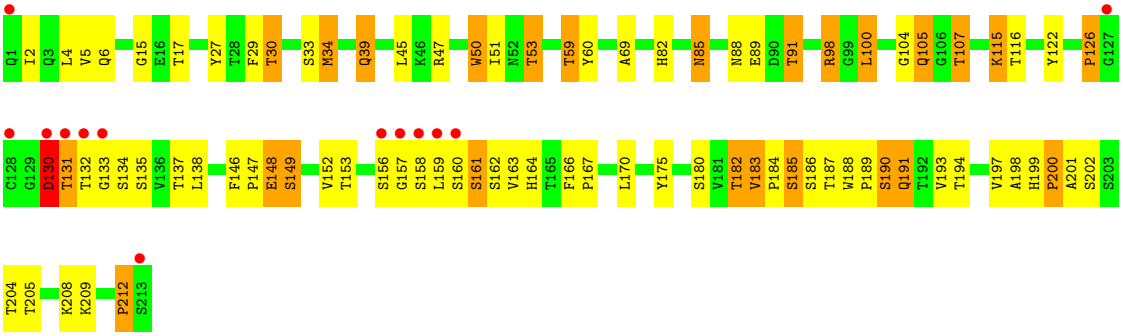
• Molecule 2: HYBRIDOMA ANTIBODY LA2 (HEAVY CHAIN)

Chain B:

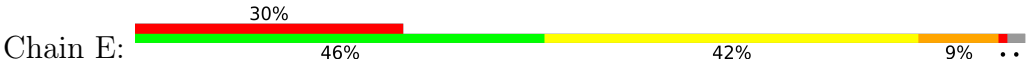


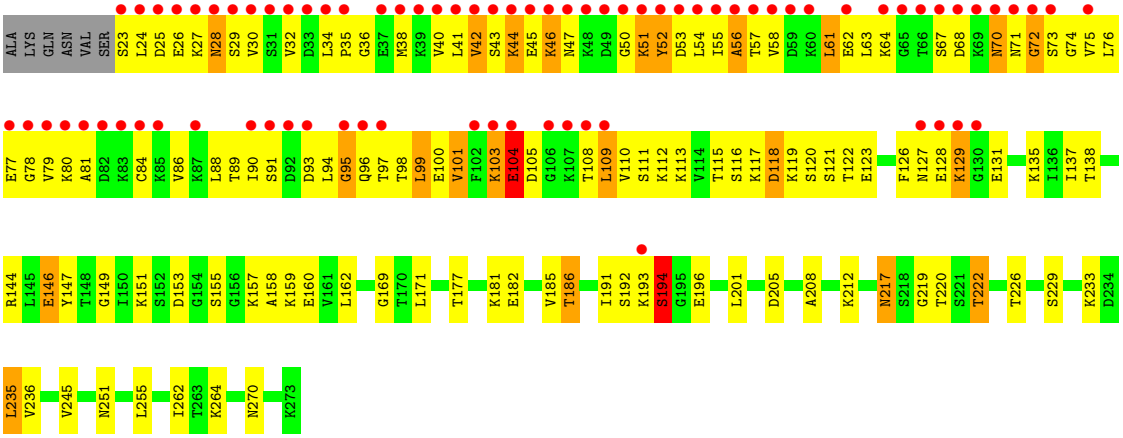
• Molecule 2: HYBRIDOMA ANTIBODY LA2 (HEAVY CHAIN)

Chain D:

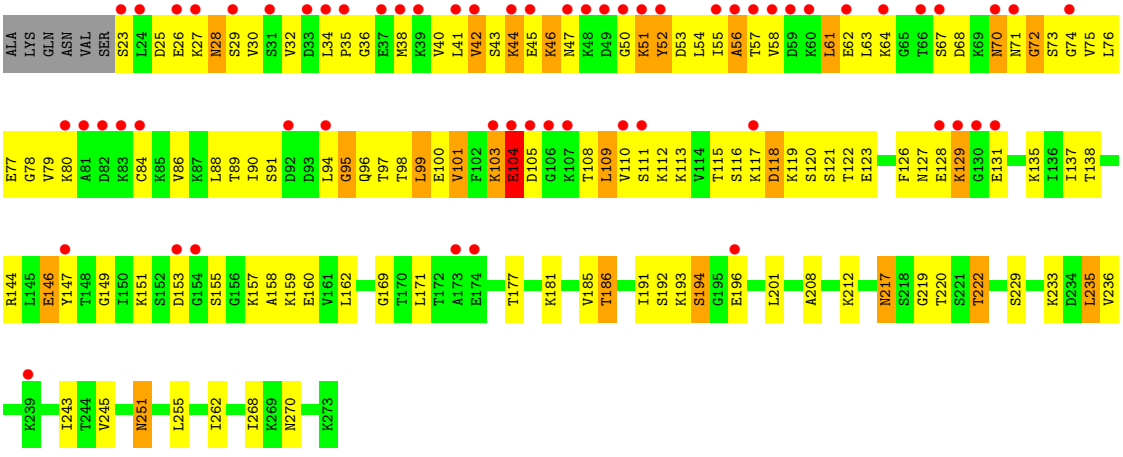


• Molecule 3: OUTER SURFACE PROTEIN A





• Molecule 3: OUTER SURFACE PROTEIN A



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	100.08Å 129.46Å 143.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.83 – 2.68 19.82 – 2.68	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.83-2.68) 96.7 (19.82-2.68)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.54 (at 2.67Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.226 , 0.281 0.226 , 0.281	Depositor DCC
R_{free} test set	5201 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.9	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	0.91	EDS
Total number of atoms	10542	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 3.65% 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	0.54	0/1697	0.77	0/2299
1	C	0.51	0/1697	0.76	1/2299 (0.0%)
2	B	0.56	0/1630	0.79	0/2225
2	D	0.47	0/1630	0.73	0/2225
3	E	0.42	0/1902	0.67	1/2550 (0.0%)
3	F	0.38	0/1902	0.65	0/2550
All	All	0.48	0/10458	0.73	2/14148 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	205	ASP	CB-CG-OD1	5.59	123.33	118.30
1	C	89	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1660	0	1597	61	0
1	C	1660	0	1597	59	0
2	B	1589	0	1548	80	0
2	D	1589	0	1548	81	0
3	E	1893	0	1965	153	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1893	0	1965	150	0
4	A	64	0	0	3	0
4	B	52	0	0	5	0
4	C	67	0	0	2	0
4	D	22	0	0	2	0
4	E	37	0	0	3	0
4	F	16	0	0	0	0
All	All	10542	0	10220	572	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 28.

All (572) 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:F:23:SER:HA	3:F:41:LEU:HD22	1.43	0.98
3:E:23:SER:HA	3:E:41:LEU:HD22	1.43	0.97
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.48	0.96
1:A:93:ASN:HD22	1:A:95:GLN:H	1.04	0.94
2:D:194:THR:HG22	2:D:209:LYS:HA	1.49	0.93
1:C:93:ASN:HD22	1:C:95:GLN:H	1.02	0.93
3:E:63:LEU:HD13	3:E:78:GLY:HA3	1.51	0.92
1:C:93:ASN:ND2	1:C:95:GLN:H	1.67	0.92
3:F:63:LEU:HD13	3:F:78:GLY:HA3	1.53	0.91
1:A:93:ASN:ND2	1:A:95:GLN:H	1.67	0.90
2:D:105:GLN:H	2:D:105:GLN:HE21	0.91	0.89
2:D:105:GLN:H	2:D:105:GLN:NE2	1.71	0.88
2:B:105:GLN:HE21	2:B:105:GLN:N	1.72	0.88
2:B:105:GLN:H	2:B:105:GLN:NE2	1.72	0.88
2:D:2:ILE:HD11	4:D:1225:HOH:O	1.73	0.87
2:B:105:GLN:HE21	2:B:105:GLN:H	0.88	0.87
1:C:106:ILE:H	1:C:166:GLN:HE22	1.23	0.85
2:D:105:GLN:HE21	2:D:105:GLN:N	1.74	0.85
2:D:30:THR:HA	2:D:53:THR:CG2	2.07	0.84
2:B:43:LYS:HB3	4:B:1332:HOH:O	1.75	0.84
3:E:28:ASN:HA	3:E:44:LYS:HD3	1.61	0.83
3:F:71:ASN:HB2	3:F:94:LEU:HD21	1.59	0.83
3:E:115:THR:HG22	3:E:116:SER:H	1.45	0.82
3:E:226:THR:HG22	4:E:1347:HOH:O	1.78	0.82
3:E:71:ASN:HB2	3:E:94:LEU:HD21	1.60	0.81
3:F:28:ASN:HA	3:F:44:LYS:HD3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:115:THR:HG22	3:F:116:SER:H	1.46	0.80
3:F:127:ASN:HD21	3:F:131:GLU:HB2	1.45	0.80
2:D:30:THR:HA	2:D:53:THR:HG23	1.62	0.80
3:F:55:ILE:HG22	3:F:56:ALA:H	1.47	0.80
1:A:93:ASN:HD22	1:A:95:GLN:N	1.79	0.79
1:A:130:ALA:O	1:A:181:LEU:HD12	1.83	0.79
3:E:127:ASN:HD21	3:E:131:GLU:HB2	1.46	0.79
1:C:93:ASN:HD22	1:C:95:GLN:N	1.79	0.78
3:E:101:VAL:HB	3:E:111:SER:HB3	1.65	0.78
3:F:235:LEU:CD1	3:F:245:VAL:HG22	2.14	0.78
2:B:142:VAL:HB	2:B:177:MET:HE2	1.66	0.78
3:E:55:ILE:HG22	3:E:56:ALA:H	1.46	0.77
1:C:130:ALA:O	1:C:181:LEU:HD12	1.84	0.77
2:B:6:GLN:H	2:B:105:GLN:HE22	1.33	0.77
1:A:38:HIS:HD2	4:A:1283:HOH:O	1.68	0.76
3:E:67:SER:HB3	3:E:74:GLY:HA3	1.67	0.76
3:E:116:SER:HB3	3:E:120:SER:HB3	1.67	0.76
1:A:33:ILE:CD1	1:A:51:THR:HB	2.16	0.76
3:F:46:LYS:HG2	3:F:47:ASN:H	1.49	0.76
3:F:101:VAL:HB	3:F:111:SER:HB3	1.67	0.76
2:D:88:ASN:O	2:D:91:THR:HG23	1.86	0.75
3:E:235:LEU:CD1	3:E:245:VAL:HG22	2.16	0.75
3:F:217:ASN:C	3:F:217:ASN:HD22	1.90	0.75
1:C:31:LYS:O	1:C:51:THR:HG22	1.87	0.74
1:C:33:ILE:CD1	1:C:51:THR:HB	2.18	0.74
2:B:184:PRO:HG2	2:B:187:THR:HG23	1.67	0.74
1:C:195:GLU:HG2	1:C:206:VAL:HG22	1.70	0.74
3:E:103:LYS:HD2	3:E:108:THR:HG21	1.68	0.74
3:F:67:SER:HB3	3:F:74:GLY:HA3	1.67	0.74
1:C:55:GLN:HE22	3:E:208:ALA:H	1.36	0.74
3:F:117:LYS:NZ	3:F:117:LYS:HB3	2.02	0.74
2:B:44:GLY:N	4:B:1332:HOH:O	2.20	0.73
3:E:46:LYS:HG2	3:E:47:ASN:H	1.53	0.73
2:B:27:TYR:CZ	2:B:98:ARG:HD3	2.23	0.73
2:B:160:SER:O	2:B:162:SER:N	2.19	0.73
3:E:217:ASN:HD22	3:E:217:ASN:C	1.90	0.73
2:B:194:THR:HG22	2:B:209:LYS:HA	1.69	0.73
2:D:183:VAL:HG22	2:D:184:PRO:HD2	1.69	0.73
3:F:35:PRO:HB3	3:F:117:LYS:HA	1.70	0.73
1:A:106:ILE:H	1:A:166:GLN:HE22	1.36	0.73
3:F:103:LYS:HD2	3:F:108:THR:HG21	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:35:PRO:HB3	3:E:117:LYS:HA	1.70	0.73
1:A:33:ILE:HD12	1:A:33:ILE:H	1.54	0.72
3:F:116:SER:HB3	3:F:120:SER:HB3	1.69	0.72
1:C:95:GLN:HE21	2:D:47:ARG:NH2	1.86	0.72
2:D:27:TYR:CZ	2:D:98:ARG:HD3	2.24	0.72
2:D:6:GLN:H	2:D:105:GLN:HE22	1.37	0.72
3:E:117:LYS:NZ	3:E:117:LYS:HB3	2.03	0.72
2:B:88:ASN:O	2:B:91:THR:HG23	1.88	0.72
1:C:33:ILE:HD12	1:C:33:ILE:H	1.55	0.71
3:F:70:ASN:H	3:F:70:ASN:ND2	1.87	0.70
2:D:59:THR:HG22	4:D:1362:HOH:O	1.91	0.70
3:E:70:ASN:H	3:E:70:ASN:ND2	1.90	0.70
3:F:71:ASN:CB	3:F:94:LEU:HD21	2.22	0.70
3:E:147:TYR:CD2	3:E:171:LEU:HD22	2.27	0.69
3:E:34:LEU:HD11	3:E:40:VAL:HB	1.74	0.69
3:F:46:LYS:HE2	3:F:50:GLY:O	1.92	0.69
1:A:31:LYS:O	1:A:51:THR:HG22	1.92	0.69
3:F:235:LEU:HD12	3:F:245:VAL:HG22	1.73	0.69
3:E:46:LYS:HE2	3:E:50:GLY:O	1.92	0.69
3:E:51:LYS:HG2	3:E:68:ASP:OD1	1.93	0.69
3:E:235:LEU:HD12	3:E:245:VAL:HG22	1.74	0.69
1:A:33:ILE:HD13	1:A:51:THR:HB	1.74	0.68
1:A:195:GLU:HG2	1:A:206:VAL:HG22	1.75	0.68
1:C:33:ILE:HD13	1:C:51:THR:HB	1.75	0.68
3:F:147:TYR:CD2	3:F:171:LEU:HD22	2.28	0.68
3:E:113:LYS:HA	3:E:123:GLU:HA	1.76	0.68
3:E:71:ASN:CB	3:E:94:LEU:HD21	2.23	0.67
3:F:113:LYS:HA	3:F:123:GLU:HA	1.75	0.67
2:D:160:SER:O	2:D:162:SER:N	2.28	0.67
1:A:6:GLN:NE2	1:A:101:GLY:H	1.92	0.67
2:B:6:GLN:HE21	2:B:107:THR:CG2	2.07	0.67
3:F:34:LEU:HD11	3:F:40:VAL:HB	1.75	0.67
3:E:63:LEU:CD1	3:E:86:VAL:HB	2.25	0.67
3:F:51:LYS:HG2	3:F:68:ASP:OD1	1.95	0.66
2:B:143:LYS:HE2	4:B:1358:HOH:O	1.95	0.66
3:E:25:ASP:HB3	3:E:28:ASN:OD1	1.96	0.66
3:E:67:SER:CB	3:E:74:GLY:HA3	2.26	0.66
1:C:105:GLU:HG2	4:C:1205:HOH:O	1.95	0.66
2:D:183:VAL:HG22	2:D:184:PRO:CD	2.25	0.66
3:E:115:THR:HG22	3:E:116:SER:N	2.10	0.66
1:C:4:MET:HE1	1:C:90:GLN:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:67:SER:CB	3:F:74:GLY:HA3	2.26	0.65
2:D:157:GLY:O	2:D:187:THR:HG21	1.96	0.65
3:E:185:VAL:HG21	3:E:212:LYS:HD2	1.79	0.65
3:F:25:ASP:HB3	3:F:28:ASN:OD1	1.97	0.65
3:E:127:ASN:ND2	3:E:131:GLU:HB2	2.12	0.65
3:F:157:LYS:HD3	3:F:158:ALA:N	2.12	0.64
1:C:6:GLN:NE2	1:C:101:GLY:H	1.95	0.64
3:E:157:LYS:HD3	3:E:158:ALA:N	2.12	0.64
3:F:127:ASN:ND2	3:F:131:GLU:HB2	2.10	0.64
3:E:23:SER:N	3:E:41:LEU:HB2	2.12	0.64
3:F:63:LEU:CD1	3:F:86:VAL:HB	2.26	0.64
3:E:51:LYS:HB3	3:E:68:ASP:HA	1.79	0.64
3:F:115:THR:HG22	3:F:116:SER:N	2.11	0.64
3:E:118:ASP:O	3:E:119:LYS:HB2	1.98	0.63
4:A:1017:HOH:O	1:C:69:ARG:HD2	1.97	0.63
3:F:80:LYS:HB3	3:F:84:CYS:H	1.63	0.63
2:B:6:GLN:NE2	2:B:107:THR:HG23	2.13	0.63
3:F:51:LYS:HB3	3:F:68:ASP:HA	1.80	0.63
2:B:160:SER:C	2:B:162:SER:H	2.01	0.63
1:C:106:ILE:H	1:C:166:GLN:NE2	1.95	0.63
2:D:6:GLN:HE21	2:D:107:THR:CG2	2.12	0.63
3:E:80:LYS:HB3	3:E:84:CYS:H	1.63	0.63
1:A:151:ASP:HA	1:A:191:SER:HB3	1.81	0.62
2:B:33:SER:O	2:B:53:THR:HG23	1.99	0.62
2:D:160:SER:C	2:D:162:SER:H	2.02	0.62
1:A:55:GLN:HA	1:A:55:GLN:HE21	1.63	0.62
2:B:142:VAL:HB	2:B:177:MET:CE	2.28	0.62
3:F:23:SER:N	3:F:41:LEU:HB2	2.14	0.62
1:A:4:MET:HE2	1:A:90:GLN:HB3	1.80	0.62
3:F:118:ASP:O	3:F:119:LYS:HB2	1.98	0.62
1:C:151:ASP:HA	1:C:191:SER:HB3	1.82	0.61
2:B:6:GLN:HE21	2:B:107:THR:HG23	1.63	0.61
2:D:15:GLY:HA2	2:D:85:ASN:HD22	1.65	0.61
3:E:220:THR:OG1	3:E:222:THR:HG23	2.00	0.61
2:D:133:GLY:O	2:D:134:SER:HB3	2.01	0.61
3:F:235:LEU:HD11	3:F:245:VAL:HG22	1.81	0.61
1:C:55:GLN:HE21	1:C:55:GLN:HA	1.65	0.61
2:D:6:GLN:NE2	2:D:107:THR:HG23	2.16	0.61
2:B:119:PRO:CB	2:B:145:TYR:HB3	2.27	0.61
2:D:100:LEU:HD13	3:E:229:SER:HB3	1.83	0.61
3:E:192:SER:OG	3:E:196:GLU:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLN:HE22	3:F:208:ALA:H	1.47	0.60
3:F:185:VAL:HG21	3:F:212:LYS:HD2	1.82	0.60
1:C:193:THR:HB	1:C:208:SER:CB	2.32	0.60
3:E:144:ARG:NH1	3:E:146:GLU:OE2	2.34	0.60
3:E:27:LYS:HD2	3:E:27:LYS:N	2.17	0.60
1:A:190:ASN:HD21	1:A:212:ASN:H	1.46	0.60
3:F:63:LEU:HB3	3:F:77:GLU:O	2.02	0.59
1:A:95:GLN:OE1	2:B:50:TRP:HZ3	1.85	0.59
1:A:193:THR:HB	1:A:208:SER:OG	2.03	0.59
3:E:155:SER:HA	3:E:171:LEU:O	2.02	0.59
2:B:209:LYS:HD2	2:B:211:GLU:OE1	2.01	0.59
3:E:121:SER:OG	3:E:138:THR:HB	2.02	0.59
3:F:70:ASN:H	3:F:70:ASN:HD22	1.49	0.59
1:A:193:THR:HB	1:A:208:SER:CB	2.31	0.59
3:F:25:ASP:OD2	3:F:26:GLU:N	2.36	0.59
2:B:202:SER:C	2:B:204:THR:H	2.05	0.59
3:E:201:LEU:C	3:E:201:LEU:HD23	2.23	0.59
1:C:30:ASN:HA	4:C:1051:HOH:O	2.03	0.59
3:E:235:LEU:HD11	3:E:245:VAL:HG22	1.83	0.59
3:E:117:LYS:HB3	3:E:117:LYS:HZ3	1.67	0.59
1:C:193:THR:HB	1:C:208:SER:HB2	1.85	0.58
3:E:63:LEU:HB3	3:E:77:GLU:O	2.03	0.58
3:F:201:LEU:HD23	3:F:201:LEU:C	2.24	0.58
1:A:136:LEU:HD12	1:A:136:LEU:N	2.19	0.58
2:B:71:SER:OG	2:B:82:HIS:HE1	1.86	0.58
3:E:42:VAL:HG12	3:E:43:SER:H	1.68	0.58
3:F:144:ARG:NH1	3:F:146:GLU:OE2	2.36	0.58
3:F:220:THR:OG1	3:F:222:THR:HG23	2.02	0.58
2:D:148:GLU:O	2:D:149:SER:CB	2.51	0.58
3:F:27:LYS:N	3:F:27:LYS:HD2	2.18	0.58
1:A:33:ILE:HD12	1:A:33:ILE:N	2.18	0.58
2:B:69:ALA:HB3	2:B:82:HIS:HB2	1.84	0.58
3:E:63:LEU:HD12	3:E:86:VAL:HB	1.85	0.58
2:D:191:GLN:HE21	2:D:191:GLN:HA	1.68	0.58
3:F:192:SER:OG	3:F:196:GLU:HB2	2.04	0.58
2:B:142:VAL:CG2	2:B:177:MET:HE1	2.34	0.58
3:F:46:LYS:CG	3:F:47:ASN:H	2.17	0.58
2:D:6:GLN:HE21	2:D:107:THR:HG23	1.69	0.57
1:C:33:ILE:HD11	1:C:71:TYR:CE1	2.38	0.57
2:D:187:THR:O	2:D:187:THR:HG22	2.04	0.57
3:E:70:ASN:H	3:E:70:ASN:HD22	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:25:ASP:OD2	3:E:26:GLU:N	2.37	0.57
3:E:157:LYS:NZ	3:E:159:LYS:HE2	2.19	0.57
1:A:33:ILE:HD11	1:A:71:TYR:CE1	2.39	0.57
2:D:29:PHE:O	2:D:53:THR:HG21	2.05	0.57
1:A:93:ASN:HD21	1:A:95:GLN:HG2	1.68	0.56
1:C:33:ILE:CD1	1:C:51:THR:CB	2.82	0.56
3:F:121:SER:OG	3:F:138:THR:HB	2.05	0.56
3:E:23:SER:N	3:E:55:ILE:HB	2.20	0.56
3:F:42:VAL:HG12	3:F:43:SER:H	1.68	0.56
2:B:6:GLN:NE2	2:B:107:THR:CG2	2.68	0.56
2:D:126:PRO:HD3	2:D:138:LEU:HD23	1.87	0.56
3:E:57:THR:HA	3:E:62:GLU:HA	1.87	0.56
3:F:109:LEU:N	3:F:109:LEU:HD12	2.20	0.56
2:B:138:LEU:CD1	2:B:193:VAL:HG21	2.36	0.56
2:D:161:SER:C	2:D:163:VAL:H	2.09	0.56
1:C:27:GLN:C	1:C:69:ARG:HG2	2.27	0.55
3:F:57:THR:HA	3:F:62:GLU:HA	1.87	0.55
3:F:63:LEU:HD12	3:F:86:VAL:HB	1.87	0.55
1:A:193:THR:HB	1:A:208:SER:HB2	1.88	0.55
1:C:33:ILE:HD12	1:C:33:ILE:N	2.20	0.55
3:F:28:ASN:HB2	3:F:44:LYS:HB2	1.88	0.55
1:A:33:ILE:CD1	1:A:51:THR:CB	2.83	0.55
1:C:211:ARG:HG2	1:C:211:ARG:HH11	1.71	0.55
1:C:190:ASN:HD21	1:C:212:ASN:H	1.54	0.55
3:E:34:LEU:HB2	3:E:38:MET:O	2.06	0.55
3:F:34:LEU:HB2	3:F:38:MET:O	2.07	0.55
2:B:171:GLN:O	2:B:172:SER:C	2.45	0.55
3:F:23:SER:N	3:F:55:ILE:HB	2.21	0.55
1:A:115:VAL:O	1:A:207:LYS:HE3	2.06	0.55
2:B:119:PRO:HB3	2:B:145:TYR:CB	2.31	0.55
3:E:42:VAL:HG11	3:E:70:ASN:C	2.26	0.55
3:E:109:LEU:HD12	3:E:109:LEU:N	2.21	0.55
3:E:28:ASN:HB2	3:E:44:LYS:HB2	1.88	0.55
2:D:89:GLU:CD	2:D:89:GLU:H	2.11	0.55
3:F:192:SER:O	3:F:194:SER:N	2.38	0.55
3:E:42:VAL:HG11	3:E:70:ASN:HA	1.89	0.54
1:C:93:ASN:HD21	1:C:95:GLN:HG2	1.71	0.54
2:B:4:LEU:O	2:B:104:GLY:HA2	2.06	0.54
2:B:33:SER:O	2:B:51:ILE:O	2.25	0.54
1:C:193:THR:HB	1:C:208:SER:OG	2.07	0.54
3:F:117:LYS:HB3	3:F:117:LYS:HZ3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:181:LYS:HD3	3:F:186:THR:HB	1.89	0.54
3:E:118:ASP:O	3:E:119:LYS:CB	2.56	0.54
3:E:217:ASN:ND2	3:E:220:THR:H	2.05	0.54
2:D:170:LEU:HD13	2:D:175:TYR:CD2	2.43	0.54
3:F:42:VAL:HG11	3:F:70:ASN:C	2.28	0.54
3:F:118:ASP:O	3:F:119:LYS:CB	2.56	0.54
3:F:157:LYS:NZ	3:F:159:LYS:HE2	2.21	0.54
2:D:6:GLN:NE2	2:D:107:THR:CG2	2.70	0.54
2:B:148:GLU:O	2:B:149:SER:HB2	2.07	0.53
2:B:162:SER:OG	2:B:182:THR:HB	2.07	0.53
3:E:80:LYS:CB	3:E:84:CYS:HB2	2.38	0.53
1:A:27:GLN:C	1:A:69:ARG:HG2	2.29	0.53
2:D:187:THR:O	2:D:191:GLN:HB2	2.07	0.53
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.73	0.53
1:C:149:LYS:HA	1:C:153:SER:O	2.09	0.53
1:A:149:LYS:HA	1:A:153:SER:O	2.09	0.53
3:E:103:LYS:HD2	3:E:108:THR:CG2	2.38	0.53
1:A:190:ASN:HD21	1:A:212:ASN:N	2.07	0.52
1:C:136:LEU:HD12	1:C:136:LEU:N	2.24	0.52
3:E:62:GLU:O	3:E:63:LEU:HD23	2.09	0.52
1:C:81:GLU:CD	1:C:81:GLU:H	2.12	0.52
3:F:42:VAL:HG12	3:F:43:SER:N	2.25	0.52
3:F:62:GLU:O	3:F:63:LEU:HD23	2.09	0.52
3:F:80:LYS:CB	3:F:84:CYS:HB2	2.39	0.52
3:F:155:SER:HA	3:F:171:LEU:O	2.09	0.52
2:D:33:SER:HA	3:E:251:ASN:OD1	2.08	0.52
2:D:188:TRP:CG	2:D:189:PRO:HA	2.44	0.52
3:F:217:ASN:C	3:F:217:ASN:ND2	2.62	0.52
3:E:42:VAL:CG1	3:E:43:SER:H	2.21	0.52
3:F:28:ASN:O	3:F:29:SER:HB2	2.09	0.52
3:F:217:ASN:ND2	3:F:219:GLY:H	2.07	0.52
2:B:138:LEU:HD13	2:B:193:VAL:HG21	1.91	0.52
3:E:46:LYS:CG	3:E:47:ASN:H	2.20	0.52
3:E:52:TYR:CE2	3:E:70:ASN:HB3	2.45	0.52
2:B:189:PRO:C	2:B:191:GLN:H	2.13	0.52
2:B:193:VAL:CG2	2:B:210:LEU:HB2	2.40	0.52
3:F:157:LYS:HZ2	3:F:159:LYS:HE2	1.75	0.52
2:B:148:GLU:HB2	4:B:1141:HOH:O	2.10	0.52
3:E:192:SER:O	3:E:194:SER:N	2.41	0.52
3:F:55:ILE:HG23	3:F:64:LYS:HA	1.92	0.52
1:A:33:ILE:HD11	1:A:51:THR:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:VAL:O	1:C:207:LYS:HE3	2.11	0.51
2:B:100:LEU:HD13	3:F:229:SER:HB3	1.90	0.51
3:E:75:VAL:C	3:E:76:LEU:HD22	2.31	0.51
2:D:148:GLU:O	2:D:149:SER:HB3	2.10	0.51
3:E:28:ASN:O	3:E:29:SER:HB2	2.10	0.51
3:F:42:VAL:HG11	3:F:70:ASN:HA	1.92	0.51
2:D:4:LEU:O	2:D:104:GLY:HA2	2.11	0.51
3:F:79:VAL:HG22	3:F:80:LYS:N	2.26	0.51
2:D:33:SER:O	2:D:51:ILE:O	2.29	0.51
3:F:52:TYR:CE2	3:F:70:ASN:HB3	2.46	0.51
2:B:163:VAL:HG22	2:B:181:VAL:HG23	1.92	0.50
3:F:217:ASN:ND2	3:F:219:GLY:N	2.59	0.50
1:A:33:ILE:HD13	1:A:51:THR:CB	2.42	0.50
3:E:42:VAL:HG12	3:E:43:SER:N	2.26	0.50
3:F:42:VAL:HA	3:F:54:LEU:HB3	1.93	0.50
1:C:33:ILE:HD11	1:C:51:THR:HB	1.94	0.50
3:E:32:VAL:HG11	3:E:71:ASN:O	2.11	0.50
2:B:89:GLU:CD	2:B:89:GLU:H	2.15	0.50
3:F:217:ASN:HD22	3:F:219:GLY:H	1.60	0.50
3:F:217:ASN:ND2	3:F:220:THR:H	2.10	0.50
2:B:6:GLN:H	2:B:105:GLN:NE2	2.05	0.50
2:D:137:THR:HG23	2:D:182:THR:HG22	1.92	0.50
3:F:91:SER:HB3	3:F:96:GLN:HB3	1.94	0.50
2:D:146:PHE:CD1	2:D:147:PRO:HA	2.47	0.49
2:D:189:PRO:C	2:D:191:GLN:H	2.15	0.49
3:E:55:ILE:HG23	3:E:64:LYS:HA	1.94	0.49
3:F:103:LYS:HD2	3:F:108:THR:CG2	2.41	0.49
3:E:42:VAL:HA	3:E:54:LEU:HB3	1.94	0.49
3:F:32:VAL:HG11	3:F:71:ASN:O	2.12	0.49
2:D:33:SER:O	2:D:34:MET:CB	2.60	0.49
3:E:181:LYS:HD3	3:E:186:THR:HB	1.93	0.49
3:E:70:ASN:ND2	3:E:70:ASN:N	2.56	0.49
3:E:79:VAL:HG22	3:E:80:LYS:N	2.28	0.49
3:F:75:VAL:C	3:F:76:LEU:HD22	2.32	0.49
2:B:163:VAL:CG2	2:B:181:VAL:HG23	2.42	0.49
1:A:55:GLN:HA	1:A:55:GLN:NE2	2.28	0.49
1:A:81:GLU:CD	1:A:81:GLU:H	2.14	0.49
2:B:39:GLN:HG2	2:B:45:LEU:HD23	1.94	0.49
3:E:127:ASN:HD21	3:E:131:GLU:CB	2.23	0.49
3:F:57:THR:OG1	3:F:62:GLU:HB2	2.13	0.49
2:B:2:ILE:N	2:B:2:ILE:CD1	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:TYR:OH	2:B:69:ALA:HA	2.13	0.49
2:D:60:TYR:OH	2:D:69:ALA:HA	2.13	0.49
3:E:57:THR:OG1	3:E:62:GLU:HB2	2.13	0.49
3:F:126:PHE:N	3:F:126:PHE:CD1	2.80	0.49
1:A:93:ASN:ND2	1:A:95:GLN:HG2	2.28	0.48
2:D:115:LYS:HD2	2:D:115:LYS:O	2.13	0.48
3:F:55:ILE:HG23	3:F:64:LYS:HB3	1.95	0.48
1:C:190:ASN:HD21	1:C:212:ASN:N	2.10	0.48
3:E:98:THR:HG22	3:E:98:THR:O	2.14	0.48
3:F:63:LEU:HD13	3:F:78:GLY:CA	2.35	0.48
2:D:6:GLN:H	2:D:105:GLN:NE2	2.07	0.48
2:D:88:ASN:O	2:D:91:THR:CG2	2.60	0.48
2:D:187:THR:CG2	2:D:191:GLN:HG3	2.44	0.48
3:E:91:SER:HB3	3:E:96:GLN:HB3	1.93	0.48
3:E:157:LYS:HZ2	3:E:159:LYS:HE2	1.76	0.48
2:D:130:ASP:O	2:D:131:THR:HB	2.14	0.48
3:E:126:PHE:N	3:E:126:PHE:CD1	2.82	0.48
3:E:27:LYS:HD2	3:E:27:LYS:H	1.78	0.48
1:A:106:ILE:H	1:A:166:GLN:NE2	2.09	0.48
2:D:170:LEU:HD13	2:D:175:TYR:CE2	2.49	0.48
2:D:187:THR:HG23	2:D:191:GLN:HG3	1.95	0.48
3:F:117:LYS:HB3	3:F:117:LYS:HZ2	1.79	0.48
2:B:33:SER:HB3	2:B:50:TRP:CD1	2.49	0.47
2:B:193:VAL:HG23	2:B:210:LEU:HB2	1.96	0.47
2:D:146:PHE:CG	2:D:147:PRO:HA	2.48	0.47
3:F:42:VAL:CG1	3:F:43:SER:H	2.21	0.47
3:F:75:VAL:HG12	3:F:89:THR:HG23	1.96	0.47
3:E:217:ASN:ND2	3:E:219:GLY:N	2.61	0.47
2:B:2:ILE:N	2:B:2:ILE:HD12	2.29	0.47
2:D:126:PRO:HD3	2:D:138:LEU:CD2	2.44	0.47
1:A:189:HIS:HE1	3:E:196:GLU:OE1	1.98	0.47
2:D:39:GLN:HG2	2:D:45:LEU:HD23	1.94	0.47
1:A:31:LYS:HB3	1:A:51:THR:CG2	2.44	0.47
2:D:33:SER:HB3	2:D:50:TRP:CD1	2.50	0.47
3:E:217:ASN:HD22	3:E:219:GLY:N	2.12	0.47
3:E:217:ASN:ND2	3:E:219:GLY:H	2.12	0.47
3:F:129:LYS:HD2	3:F:131:GLU:CD	2.35	0.47
1:A:38:HIS:CD2	4:A:1283:HOH:O	2.55	0.47
1:A:79:GLU:HB3	1:A:81:GLU:OE1	2.15	0.47
2:B:107:THR:HA	4:B:1170:HOH:O	2.15	0.47
3:E:43:SER:HB2	3:E:53:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:55:ILE:HG23	3:E:64:LYS:HB3	1.95	0.47
3:E:88:LEU:HG	3:E:90:ILE:HG13	1.97	0.47
3:E:91:SER:CB	3:E:96:GLN:HB3	2.45	0.47
1:C:175:MET:HE2	1:C:176:SER:C	2.35	0.47
2:D:133:GLY:C	2:D:135:SER:H	2.19	0.47
3:F:43:SER:HB2	3:F:53:ASP:OD2	2.15	0.47
3:E:38:MET:HE1	3:E:58:VAL:HG13	1.97	0.46
1:C:106:ILE:N	1:C:166:GLN:HE22	2.01	0.46
1:C:52:SER:HB2	1:C:64:GLY:O	2.15	0.46
1:C:124:GLN:HA	2:D:122:TYR:CE2	2.50	0.46
3:F:91:SER:CB	3:F:96:GLN:HB3	2.45	0.46
3:F:115:THR:CG2	3:F:116:SER:H	2.22	0.46
2:B:1:GLN:NE2	2:B:2:ILE:HD13	2.31	0.46
1:C:33:ILE:HD13	1:C:51:THR:CB	2.43	0.46
3:E:129:LYS:HD2	3:E:131:GLU:CD	2.35	0.46
3:F:217:ASN:HD22	3:F:219:GLY:N	2.12	0.46
2:B:202:SER:O	2:B:204:THR:HG23	2.15	0.46
2:D:194:THR:CG2	2:D:209:LYS:HA	2.34	0.46
3:F:27:LYS:HD2	3:F:27:LYS:H	1.78	0.46
2:B:27:TYR:CZ	2:B:98:ARG:CD	2.98	0.46
2:B:50:TRP:CH2	2:B:59:THR:HG21	2.51	0.46
2:B:50:TRP:CD1	2:B:51:ILE:N	2.83	0.46
1:C:33:ILE:HD11	1:C:71:TYR:CD1	2.51	0.46
3:E:217:ASN:HD22	3:E:219:GLY:H	1.64	0.46
1:C:33:ILE:CD1	1:C:51:THR:HG22	2.46	0.46
2:D:2:ILE:O	2:D:2:ILE:HG13	2.16	0.46
3:F:127:ASN:HD21	3:F:131:GLU:CB	2.21	0.46
1:A:175:MET:HE2	1:A:176:SER:O	2.14	0.46
1:A:209:PHE:CD1	1:A:209:PHE:C	2.88	0.46
3:E:75:VAL:HG12	3:E:89:THR:HG23	1.96	0.46
1:C:79:GLU:HB3	1:C:81:GLU:OE1	2.15	0.46
3:F:222:THR:HB	3:F:236:VAL:HG22	1.98	0.46
2:B:33:SER:O	2:B:34:MET:CB	2.63	0.45
2:B:56:GLY:O	2:B:58:PRO:HD3	2.15	0.45
2:B:160:SER:OG	2:B:161:SER:N	2.48	0.45
1:C:93:ASN:ND2	1:C:95:GLN:HG2	2.31	0.45
2:D:17:THR:HG21	2:D:82:HIS:CE1	2.51	0.45
2:D:50:TRP:CH2	2:D:59:THR:HG21	2.51	0.45
2:D:115:LYS:O	2:D:116:THR:C	2.54	0.45
2:B:187:THR:O	2:B:191:GLN:HB3	2.16	0.45
3:E:233:LYS:HE2	3:E:233:LYS:HB3	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:88:LEU:HG	3:F:90:ILE:HG13	1.98	0.45
3:F:135:LYS:HE2	3:F:137:ILE:HD11	1.98	0.45
3:F:233:LYS:HE2	3:F:233:LYS:HB3	1.83	0.45
3:F:243:ILE:CG2	3:F:262:ILE:HD12	2.46	0.45
2:B:189:PRO:C	2:B:191:GLN:N	2.69	0.45
3:E:222:THR:HB	3:E:236:VAL:HG22	1.97	0.45
3:E:245:VAL:HG23	3:E:262:ILE:HD11	1.98	0.45
3:F:55:ILE:HG22	3:F:56:ALA:N	2.24	0.45
3:F:75:VAL:HG12	3:F:89:THR:HA	1.98	0.45
2:B:202:SER:C	2:B:204:THR:N	2.69	0.45
2:B:202:SER:O	2:B:204:THR:N	2.50	0.45
1:A:181:LEU:HD12	1:A:181:LEU:N	2.31	0.45
3:E:55:ILE:O	3:E:56:ALA:HB2	2.16	0.45
3:E:115:THR:CG2	3:E:116:SER:N	2.80	0.45
1:C:209:PHE:C	1:C:209:PHE:CD1	2.90	0.45
3:F:98:THR:O	3:F:98:THR:HG22	2.17	0.45
2:D:184:PRO:C	2:D:186:SER:H	2.20	0.45
3:E:40:VAL:HA	3:E:56:ALA:HB2	1.99	0.45
3:E:182:GLU:HG3	4:E:1067:HOH:O	2.17	0.45
3:F:55:ILE:HG23	3:F:64:LYS:CA	2.46	0.45
3:F:70:ASN:HD22	3:F:70:ASN:N	2.11	0.45
3:F:243:ILE:HG22	3:F:262:ILE:HD12	1.99	0.45
2:B:50:TRP:CZ2	2:B:59:THR:HG21	2.52	0.45
2:D:148:GLU:CD	2:D:149:SER:H	2.21	0.45
3:E:23:SER:OG	3:E:41:LEU:HD13	2.16	0.45
3:E:25:ASP:CB	3:E:28:ASN:OD1	2.63	0.45
3:E:55:ILE:HG23	3:E:64:LYS:CA	2.47	0.45
3:F:25:ASP:CB	3:F:28:ASN:OD1	2.64	0.45
3:E:129:LYS:HB2	3:E:129:LYS:NZ	2.31	0.44
3:F:38:MET:HE1	3:F:58:VAL:HG13	1.98	0.44
3:E:115:THR:CG2	3:E:116:SER:H	2.22	0.44
1:A:175:MET:HE2	1:A:176:SER:C	2.37	0.44
2:D:50:TRP:CD1	2:D:51:ILE:N	2.84	0.44
3:E:217:ASN:C	3:E:217:ASN:ND2	2.63	0.44
3:F:149:GLY:O	3:F:151:LYS:HD2	2.18	0.44
2:D:132:THR:HB	2:D:185:SER:HB2	1.98	0.44
3:E:25:ASP:HB3	3:E:28:ASN:O	2.18	0.44
3:E:104:GLU:OE2	3:E:105:ASP:N	2.51	0.44
2:D:156:SER:CB	2:D:193:VAL:HG12	2.48	0.44
2:B:142:VAL:HB	2:B:177:MET:HG3	2.00	0.44
2:D:6:GLN:N	2:D:105:GLN:HE22	2.11	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:TRP:CE2	1:C:73:PHE:HB2	2.53	0.44
3:F:57:THR:HA	3:F:62:GLU:CB	2.48	0.44
1:A:35:TRP:CE2	1:A:73:PHE:HB2	2.53	0.44
3:E:35:PRO:HG2	3:E:95:GLY:HA2	2.00	0.44
3:E:42:VAL:HG11	3:E:70:ASN:CA	2.47	0.44
2:B:199:HIS:ND1	2:B:202:SER:HB2	2.33	0.43
3:E:35:PRO:CG	3:E:95:GLY:HA2	2.47	0.43
3:E:54:LEU:HD12	3:E:76:LEU:HD11	2.00	0.43
3:F:23:SER:OG	3:F:41:LEU:HD13	2.18	0.43
3:F:25:ASP:HB3	3:F:28:ASN:O	2.18	0.43
3:F:40:VAL:HA	3:F:56:ALA:HB2	2.00	0.43
1:A:135:PHE:C	1:A:136:LEU:HD12	2.38	0.43
1:C:212:ASN:O	1:C:213:GLU:C	2.56	0.43
3:E:75:VAL:HG12	3:E:89:THR:HA	2.00	0.43
3:F:34:LEU:HD11	3:F:90:ILE:HD13	1.99	0.43
2:B:146:PHE:CG	2:B:147:PRO:HA	2.53	0.43
2:D:160:SER:C	2:D:162:SER:N	2.69	0.43
2:D:166:PHE:HA	2:D:167:PRO:HD3	1.85	0.43
3:F:191:ILE:HA	3:F:196:GLU:O	2.19	0.43
2:B:6:GLN:N	2:B:105:GLN:HE22	2.09	0.43
3:E:57:THR:HA	3:E:62:GLU:CB	2.49	0.43
3:F:45:GLU:O	3:F:46:LYS:HB2	2.17	0.43
3:F:169:GLY:HA3	3:F:177:THR:O	2.18	0.43
2:B:150:VAL:HA	2:B:198:ALA:O	2.18	0.43
1:C:33:ILE:HA	1:C:89:LEU:O	2.18	0.43
3:F:129:LYS:HB2	3:F:129:LYS:NZ	2.34	0.43
1:C:23:CYS:HB2	1:C:35:TRP:CH2	2.53	0.43
3:E:191:ILE:HA	3:E:196:GLU:O	2.19	0.43
2:B:183:VAL:HB	2:B:184:PRO:HD2	2.01	0.43
3:F:57:THR:HA	3:F:62:GLU:CA	2.49	0.43
3:F:104:GLU:OE2	3:F:105:ASP:N	2.51	0.43
2:B:146:PHE:CD2	2:B:147:PRO:HA	2.54	0.43
2:D:50:TRP:CZ2	2:D:59:THR:HG21	2.54	0.43
3:E:149:GLY:O	3:E:151:LYS:HD2	2.18	0.43
3:F:262:ILE:HD13	3:F:268:ILE:HG12	2.01	0.43
3:E:160:GLU:HG2	3:E:162:LEU:CD2	2.48	0.43
1:A:162:SER:HB2	2:B:169:LEU:HD22	2.00	0.43
2:D:199:HIS:O	2:D:201:ALA:N	2.52	0.43
2:D:202:SER:C	2:D:204:THR:H	2.22	0.43
3:E:117:LYS:C	3:E:119:LYS:H	2.22	0.43
3:F:35:PRO:CG	3:F:95:GLY:HA2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:35:PRO:O	3:F:97:THR:HG23	2.19	0.43
1:A:23:CYS:HB2	1:A:35:TRP:CH2	2.54	0.42
1:A:30:ASN:O	1:A:31:LYS:HB2	2.19	0.42
3:E:45:GLU:O	3:E:46:LYS:HB2	2.17	0.42
3:E:63:LEU:HB3	3:E:78:GLY:HA3	2.01	0.42
3:E:135:LYS:HE2	3:E:137:ILE:HD11	2.00	0.42
3:F:63:LEU:HB3	3:F:78:GLY:HA3	2.01	0.42
2:B:209:LYS:HD2	2:B:211:GLU:CD	2.39	0.42
3:E:61:LEU:O	3:E:63:LEU:HG	2.20	0.42
3:E:169:GLY:HA3	3:E:177:THR:O	2.18	0.42
1:A:212:ASN:O	1:A:213:GLU:C	2.56	0.42
2:B:187:THR:O	2:B:191:GLN:CB	2.67	0.42
3:E:57:THR:HA	3:E:62:GLU:CA	2.50	0.42
3:F:35:PRO:HG2	3:F:95:GLY:HA2	2.02	0.42
3:F:61:LEU:O	3:F:63:LEU:HG	2.20	0.42
3:F:193:LYS:HD2	3:F:193:LYS:HA	1.83	0.42
2:D:89:GLU:CD	2:D:89:GLU:N	2.72	0.42
3:E:35:PRO:O	3:E:97:THR:HG23	2.18	0.42
3:E:42:VAL:CG1	3:E:43:SER:N	2.83	0.42
3:F:23:SER:HB2	3:F:62:GLU:OE2	2.19	0.42
1:A:123:GLU:O	1:A:126:THR:HB	2.19	0.42
2:B:177:MET:HE3	2:B:178:SER:CA	2.50	0.42
1:C:31:LYS:HB3	1:C:51:THR:CG2	2.49	0.42
3:E:63:LEU:HD13	3:E:78:GLY:CA	2.34	0.42
1:A:83:ILE:O	1:A:84:ALA:HB2	2.20	0.42
1:C:30:ASN:O	1:C:31:LYS:HB2	2.18	0.42
1:C:123:GLU:O	1:C:126:THR:HB	2.19	0.42
2:D:198:ALA:O	2:D:200:PRO:HD3	2.20	0.42
3:E:100:GLU:O	3:E:101:VAL:HG23	2.20	0.42
3:F:117:LYS:C	3:F:119:LYS:H	2.23	0.42
1:A:33:ILE:HD13	1:A:51:THR:HA	2.01	0.42
3:E:147:TYR:CE2	3:E:171:LEU:HD13	2.54	0.42
3:F:160:GLU:HG2	3:F:162:LEU:CD2	2.49	0.42
1:A:52:SER:HB2	1:A:64:GLY:O	2.20	0.42
1:A:161:ASN:ND2	1:A:177:SER:OG	2.52	0.42
1:C:19:VAL:CG2	1:C:75:ILE:HB	2.50	0.42
2:D:152:VAL:HG22	2:D:197:VAL:HG22	2.01	0.42
2:D:186:SER:O	2:D:190:SER:HB3	2.20	0.42
2:D:199:HIS:NE2	2:D:201:ALA:HB3	2.35	0.42
3:E:34:LEU:HD11	3:E:90:ILE:HD13	2.01	0.42
3:E:40:VAL:HG11	3:E:72:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:101:VAL:HG12	3:E:101:VAL:O	2.20	0.42
3:F:70:ASN:ND2	3:F:70:ASN:N	2.53	0.42
1:A:19:VAL:CG2	1:A:75:ILE:HB	2.50	0.41
3:F:51:LYS:HB2	3:F:51:LYS:NZ	2.35	0.41
3:F:55:ILE:O	3:F:56:ALA:HB2	2.19	0.41
3:F:245:VAL:HG23	3:F:262:ILE:HD11	2.01	0.41
1:A:95:GLN:OE1	2:B:50:TRP:CZ3	2.70	0.41
3:E:38:MET:CE	3:E:58:VAL:HG13	2.50	0.41
3:E:76:LEU:HB2	3:E:88:LEU:HB3	2.02	0.41
3:F:54:LEU:HD12	3:F:76:LEU:HD11	2.02	0.41
1:A:7:SER:HA	1:A:8:PRO:C	2.40	0.41
1:A:175:MET:CE	1:A:176:SER:O	2.68	0.41
2:B:88:ASN:O	2:B:91:THR:CG2	2.64	0.41
3:F:99:LEU:HD23	3:F:99:LEU:O	2.21	0.41
1:C:7:SER:HA	1:C:8:PRO:C	2.40	0.41
2:D:188:TRP:HH2	2:D:212:PRO:HA	1.85	0.41
3:E:35:PRO:HB2	3:E:95:GLY:HA2	2.02	0.41
2:B:33:SER:HA	3:F:251:ASN:OD1	2.21	0.41
3:F:147:TYR:CE2	3:F:171:LEU:HD13	2.56	0.41
3:F:30:VAL:O	3:F:42:VAL:N	2.53	0.41
1:C:33:ILE:HD13	1:C:51:THR:HA	2.03	0.41
3:E:24:LEU:HB3	3:E:29:SER:OG	2.21	0.41
3:E:42:VAL:CG1	3:E:70:ASN:HA	2.51	0.41
3:E:264:LYS:HE2	4:E:1322:HOH:O	2.20	0.41
3:F:76:LEU:HB2	3:F:88:LEU:HB3	2.03	0.41
2:B:188:TRP:HD1	2:B:193:VAL:HG13	1.86	0.41
2:D:164:HIS:HB2	2:D:180:SER:HB3	2.02	0.41
3:E:30:VAL:O	3:E:42:VAL:N	2.52	0.41
3:E:157:LYS:HD3	3:E:158:ALA:H	1.85	0.41
3:E:245:VAL:CG2	3:E:262:ILE:HD11	2.51	0.41
3:F:34:LEU:HA	3:F:35:PRO:HD3	1.91	0.41
3:F:41:LEU:HD12	3:F:41:LEU:N	2.35	0.41
3:F:55:ILE:HG23	3:F:64:LYS:CB	2.51	0.41
2:B:89:GLU:CD	2:B:89:GLU:N	2.75	0.41
1:C:140:TYR:CG	1:C:141:PRO:HA	2.56	0.41
3:E:23:SER:HB2	3:E:62:GLU:OE2	2.21	0.41
3:E:41:LEU:N	3:E:41:LEU:HD12	2.36	0.41
3:E:51:LYS:HD3	3:E:51:LYS:N	2.36	0.41
3:E:93:ASP:O	3:E:94:LEU:HB2	2.21	0.40
3:E:193:LYS:HD2	3:E:193:LYS:HA	1.86	0.40
3:F:42:VAL:HG11	3:F:70:ASN:CA	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:129:LYS:HD2	3:F:131:GLU:OE2	2.21	0.40
3:E:80:LYS:HG3	3:E:81:ALA:N	2.37	0.40
3:F:34:LEU:HD11	3:F:90:ILE:CD1	2.52	0.40
3:F:40:VAL:HG11	3:F:72:GLY:HA3	2.03	0.40
3:F:57:THR:CB	3:F:62:GLU:HB2	2.52	0.40
3:F:162:LEU:N	3:F:162:LEU:HD22	2.36	0.40
1:C:115:VAL:HA	1:C:135:PHE:O	2.21	0.40
2:D:189:PRO:C	2:D:191:GLN:N	2.73	0.40
1:A:140:TYR:CG	1:A:141:PRO:HA	2.56	0.40
1:C:211:ARG:HG2	1:C:211:ARG:NH1	2.35	0.40
2:D:5:VAL:HA	2:D:105:GLN:HE22	1.87	0.40
3:E:99:LEU:HD23	3:E:99:LEU:O	2.21	0.40
3:F:100:GLU:O	3:F:101:VAL:HG23	2.21	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	211/213 (99%)	205 (97%)	4 (2%)	2 (1%)	17	37
1	C	211/213 (99%)	204 (97%)	5 (2%)	2 (1%)	17	37
2	B	211/213 (99%)	194 (92%)	10 (5%)	7 (3%)	4	7
2	D	211/213 (99%)	177 (84%)	22 (10%)	12 (6%)	1	2
3	E	249/257 (97%)	201 (81%)	29 (12%)	19 (8%)	1	1
3	F	249/257 (97%)	202 (81%)	28 (11%)	19 (8%)	1	1
All	All	1342/1366 (98%)	1183 (88%)	98 (7%)	61 (4%)	2	4

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	ASN
2	B	161	SER
1	C	212	ASN
2	D	149	SER
2	D	161	SER
3	E	42	VAL
3	E	52	TYR
3	F	42	VAL
3	F	52	TYR
1	A	51	THR
2	B	149	SER
2	B	172	SER
1	C	51	THR
2	D	131	THR
3	E	56	ALA
3	E	61	LEU
3	E	73	SER
3	E	99	LEU
3	E	101	VAL
3	E	128	GLU
3	E	194	SER
3	F	61	LEU
3	F	73	SER
3	F	99	LEU
3	F	101	VAL
3	F	128	GLU
3	F	194	SER
2	B	158	SER
2	D	185	SER
2	D	212	PRO
3	E	46	LYS
3	F	46	LYS
3	F	56	ALA
3	F	103	LYS
2	B	34	MET
2	D	34	MET
2	D	159	LEU
3	E	72	GLY
3	E	103	LYS
3	E	112	LYS
3	F	72	GLY
3	F	112	LYS
2	D	130	ASP

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Mol	Chain	Res	Type
3	E	36	GLY
3	E	44	LYS
3	E	104	GLU
3	E	118	ASP
3	F	36	GLY
3	F	44	LYS
3	F	104	GLU
3	F	118	ASP
2	B	126	PRO
2	B	203	SER
2	D	158	SER
2	D	190	SER
2	D	126	PRO
2	D	200	PRO
3	E	95	GLY
3	F	95	GLY
3	E	110	VAL
3	F	110	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	A	188/188 (100%)	177 (94%)	11 (6%)	19 40
1	C	188/188 (100%)	176 (94%)	12 (6%)	17 36
2	B	182/182 (100%)	165 (91%)	17 (9%)	9 19
2	D	182/182 (100%)	162 (89%)	20 (11%)	6 13
3	E	220/225 (98%)	204 (93%)	16 (7%)	14 30
3	F	220/225 (98%)	204 (93%)	16 (7%)	14 30
All	All	1180/1190 (99%)	1088 (92%)	92 (8%)	12 27

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	33	ILE
1	A	47	LEU
1	A	51	THR
1	A	108	ARG
1	A	123	GLU
1	A	143	ASP
1	A	175	MET
1	A	181	LEU
1	A	187	GLU
1	A	193	THR
2	B	1	GLN
2	B	30	THR
2	B	39	GLN
2	B	50	TRP
2	B	59	THR
2	B	91	THR
2	B	98	ARG
2	B	100	LEU
2	B	105	GLN
2	B	107	THR
2	B	130	ASP
2	B	148	GLU
2	B	151	THR
2	B	169	LEU
2	B	177	MET
2	B	205	THR
2	B	206	VAL
1	C	5	THR
1	C	33	ILE
1	C	47	LEU
1	C	51	THR
1	C	55	GLN
1	C	108	ARG
1	C	123	GLU
1	C	143	ASP
1	C	175	MET
1	C	181	LEU
1	C	187	GLU
1	C	193	THR
2	D	30	THR
2	D	39	GLN
2	D	50	TRP

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Mol	Chain	Res	Type
2	D	53	THR
2	D	59	THR
2	D	85	ASN
2	D	91	THR
2	D	98	ARG
2	D	100	LEU
2	D	105	GLN
2	D	107	THR
2	D	115	LYS
2	D	130	ASP
2	D	148	GLU
2	D	153	THR
2	D	182	THR
2	D	183	VAL
2	D	191	GLN
2	D	205	THR
2	D	208	LYS
3	E	28	ASN
3	E	51	LYS
3	E	70	ASN
3	E	104	GLU
3	E	109	LEU
3	E	122	THR
3	E	129	LYS
3	E	146	GLU
3	E	153	ASP
3	E	186	THR
3	E	194	SER
3	E	217	ASN
3	E	222	THR
3	E	235	LEU
3	E	255	LEU
3	E	270	ASN
3	F	28	ASN
3	F	51	LYS
3	F	70	ASN
3	F	104	GLU
3	F	109	LEU
3	F	122	THR
3	F	129	LYS
3	F	146	GLU
3	F	153	ASP

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Mol	Chain	Res	Type
3	F	186	THR
3	F	217	ASN
3	F	222	THR
3	F	235	LEU
3	F	251	ASN
3	F	255	LEU
3	F	270	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	6	GLN
1	A	38	HIS
1	A	55	GLN
1	A	93	ASN
1	A	95	GLN
1	A	137	ASN
1	A	138	ASN
1	A	156	GLN
1	A	161	ASN
1	A	166	GLN
1	A	189	HIS
1	A	190	ASN
2	B	3	GLN
2	B	82	HIS
2	B	105	GLN
2	B	164	HIS
1	C	3	GLN
1	C	6	GLN
1	C	37	GLN
1	C	38	HIS
1	C	55	GLN
1	C	93	ASN
1	C	95	GLN
1	C	137	ASN
1	C	138	ASN
1	C	156	GLN
1	C	161	ASN
1	C	166	GLN
1	C	189	HIS
1	C	190	ASN

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Mol	Chain	Res	Type
2	D	3	GLN
2	D	85	ASN
2	D	105	GLN
2	D	191	GLN
3	E	70	ASN
3	E	190	ASN
3	E	217	ASN
3	E	270	ASN
3	F	70	ASN
3	F	190	ASN
3	F	217	ASN
3	F	270	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 monosaccharides 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	213/213 (100%)	-0.37	1 (0%) 91 92	14, 29, 56, 100	0
1	C	213/213 (100%)	-0.15	2 (0%) 84 85	14, 32, 85, 100	0
2	B	213/213 (100%)	-0.05	9 (4%) 36 34	15, 33, 76, 100	0
2	D	213/213 (100%)	0.33	13 (6%) 21 19	17, 54, 97, 100	0
3	E	251/257 (97%)	1.47	78 (31%) 0 0	16, 66, 100, 100	0
3	F	251/257 (97%)	1.27	61 (24%) 0 0	20, 86, 100, 100	0
All	All	1354/1366 (99%)	0.47	164 (12%) 4 3	14, 46, 100, 100	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	23	SER	16.1
3	E	23	SER	10.4
3	E	24	LEU	9.5
3	E	52	TYR	8.4
3	E	30	VAL	7.8
2	D	158	SER	7.5
3	E	29	SER	7.3
3	E	53	ASP	7.2
3	E	81	ALA	7.2
3	E	50	GLY	7.1
2	D	128	CYS	7.1
3	E	27	LYS	6.8
3	F	84	CYS	6.4
3	E	42	VAL	6.3
3	E	43	SER	6.2
3	E	49	ASP	6.0
3	E	48	LYS	6.0
3	E	51	LYS	6.0
3	E	32	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
2	D	159	LEU	5.8
3	E	58	VAL	5.8
3	E	69	LYS	5.7
3	E	68	ASP	5.7
3	F	60	LYS	5.6
3	E	40	VAL	5.6
3	F	24	LEU	5.6
3	E	28	ASN	5.6
3	E	44	LYS	5.6
3	E	84	CYS	5.5
3	F	35	PRO	5.5
3	E	47	ASN	5.4
3	E	33	ASP	5.4
3	E	45	GLU	5.4
3	F	94	LEU	5.4
3	E	92	ASP	5.3
3	E	35	PRO	5.3
3	E	41	LEU	5.3
3	E	66	THR	5.1
3	F	105	ASP	5.0
3	E	71	ASN	4.9
2	D	213	SER	4.9
2	D	160	SER	4.8
3	E	64	LYS	4.8
3	F	107	LYS	4.8
3	E	102	PHE	4.8
3	F	128	GLU	4.7
2	B	158	SER	4.7
3	F	49	ASP	4.7
3	E	70	ASN	4.6
3	F	58	VAL	4.6
3	E	87	LYS	4.6
3	F	45	GLU	4.6
3	E	46	LYS	4.6
3	F	39	LYS	4.6
3	E	67	SER	4.6
3	E	109	LEU	4.6
3	F	48	LYS	4.5
3	F	129	LYS	4.5
3	F	70	ASN	4.4
3	F	34	LEU	4.3
3	E	72	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
3	F	55	ILE	4.3
3	F	104	GLU	4.3
2	D	156	SER	4.3
3	F	26	GLU	4.3
3	E	90	ILE	4.3
3	F	83	LYS	4.2
2	D	1	GLN	4.2
3	E	37	GLU	4.2
2	B	129	GLY	4.1
3	E	59	ASP	4.1
3	E	26	GLU	4.1
2	B	128	CYS	4.0
3	E	91	SER	4.0
3	F	33	ASP	4.0
3	E	34	LEU	3.9
3	E	103	LYS	3.9
3	E	83	LYS	3.9
3	E	107	LYS	3.9
3	F	106	GLY	3.9
3	E	25	ASP	3.8
2	B	161	SER	3.8
3	E	55	ILE	3.8
3	E	128	GLU	3.8
3	E	60	LYS	3.8
3	E	56	ALA	3.7
3	F	47	ASN	3.7
3	E	39	LYS	3.7
3	F	51	LYS	3.6
3	F	153	ASP	3.6
3	F	64	LYS	3.6
3	F	50	GLY	3.6
3	E	93	ASP	3.5
3	E	54	LEU	3.5
3	F	71	ASN	3.5
3	E	75	VAL	3.5
3	E	95	GLY	3.5
2	B	130	ASP	3.5
3	F	59	ASP	3.5
3	E	31	SER	3.4
1	C	212	ASN	3.4
3	E	106	GLY	3.4
3	F	62	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
3	F	27	LYS	3.4
3	F	81	ALA	3.3
2	B	131	THR	3.3
3	E	82	ASP	3.3
3	F	130	GLY	3.3
3	E	108	THR	3.3
3	F	174	GLU	3.3
3	F	173	ALA	3.2
2	B	1	GLN	3.2
3	F	103	LYS	3.1
3	E	79	VAL	3.1
2	D	157	GLY	3.1
3	E	96	GLN	3.1
3	F	74	GLY	3.0
3	F	80	LYS	3.0
3	F	37	GLU	3.0
3	F	154	GLY	3.0
3	E	85	LYS	3.0
3	E	57	THR	2.9
3	E	80	LYS	2.9
3	F	56	ALA	2.9
3	F	41	LEU	2.9
3	E	97	THR	2.9
3	F	82	ASP	2.8
2	D	133	GLY	2.8
2	D	131	THR	2.8
3	F	57	THR	2.8
3	E	127	ASN	2.8
3	F	52	TYR	2.8
3	F	92	ASP	2.7
3	F	147	TYR	2.7
3	F	110	VAL	2.7
3	F	42	VAL	2.7
2	D	132	THR	2.7
2	D	127	GLY	2.6
3	E	104	GLU	2.6
3	F	44	LYS	2.6
3	E	62	GLU	2.6
2	D	130	ASP	2.5
3	E	77	GLU	2.5
3	E	65	GLY	2.5
3	E	193	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	73	SER	2.5
3	F	117	LYS	2.5
1	C	213	GLU	2.5
3	F	38	MET	2.5
3	E	130	GLY	2.4
1	A	213	GLU	2.4
3	F	66	THR	2.3
3	E	78	GLY	2.2
2	B	132	THR	2.2
3	F	31	SER	2.2
3	F	239	LYS	2.2
3	F	196	GLU	2.2
3	E	38	MET	2.2
3	F	111	SER	2.1
3	F	131	GLU	2.1
3	E	129	LYS	2.1
2	B	159	LEU	2.1
3	F	29	SER	2.1
3	F	67	SER	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.