Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:25 AM UTC

PDB ID	:	1FJ1 / pdb_00001fj1
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:

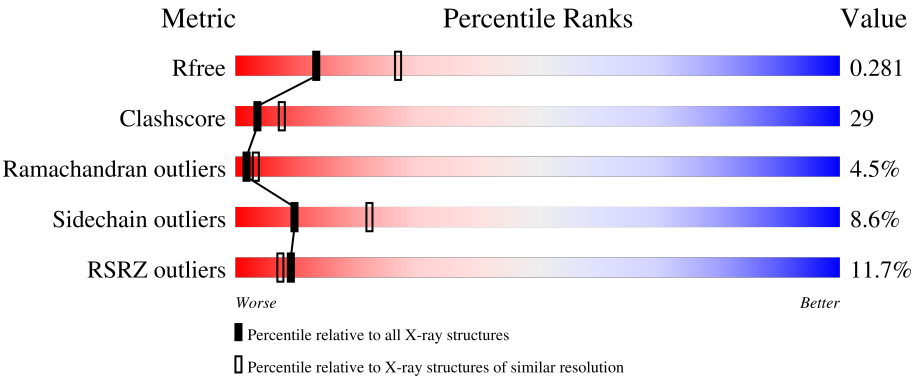
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.68 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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (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	68% 28% .
1	C	213	% 69% 27% .
2	B	213	4% 62% 28% 10%
2	D	213	7% 58% 28% 14%
3	E	257	27% 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.

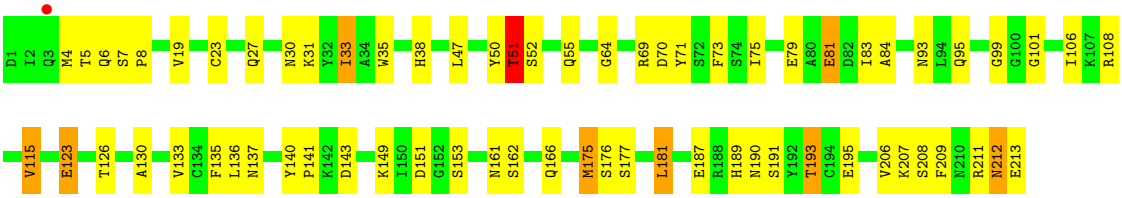
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	64	Total O 64 64	0	0
4	B	52	Total O 52 52	0	0
4	C	67	Total O 67 67	0	0
4	D	22	Total O 22 22	0	0
4	E	37	Total O 37 37	0	0
4	F	16	Total O 16 16	0	0

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.

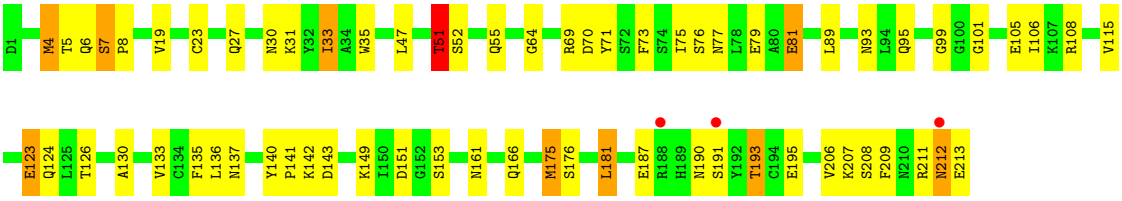
• Molecule 1: HYBRIDOMA ANTIBODY LA2 (LIGHT CHAIN)

Chain A:



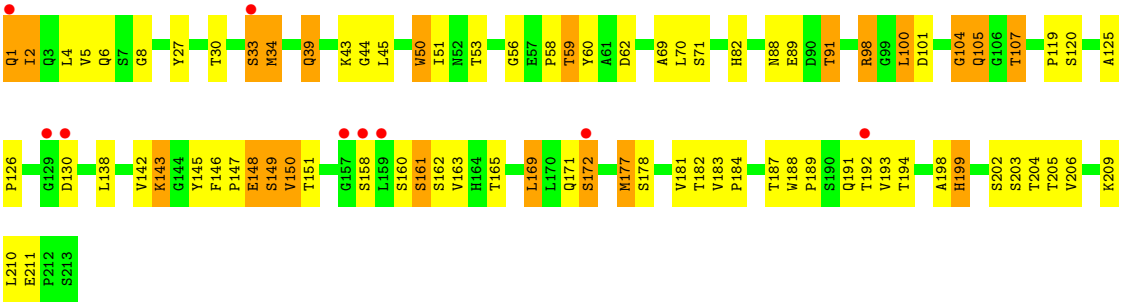
• Molecule 1: HYBRIDOMA ANTIBODY LA2 (LIGHT CHAIN)

Chain C:



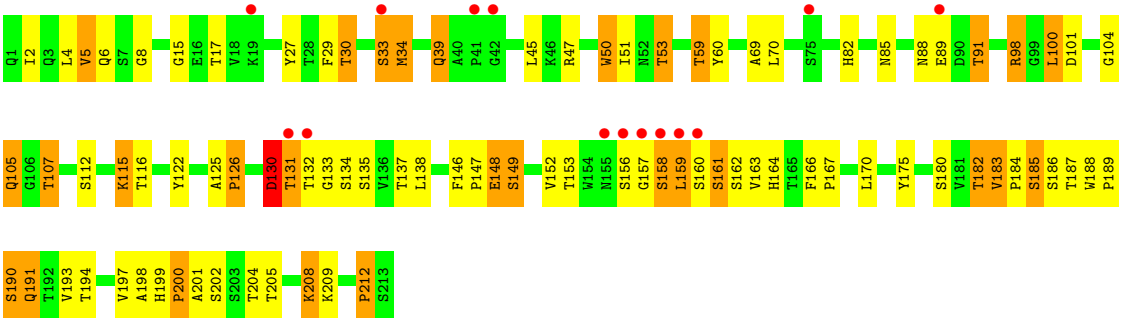
• Molecule 2: HYBRIDOMA ANTIBODY LA2 (HEAVY CHAIN)

Chain B:

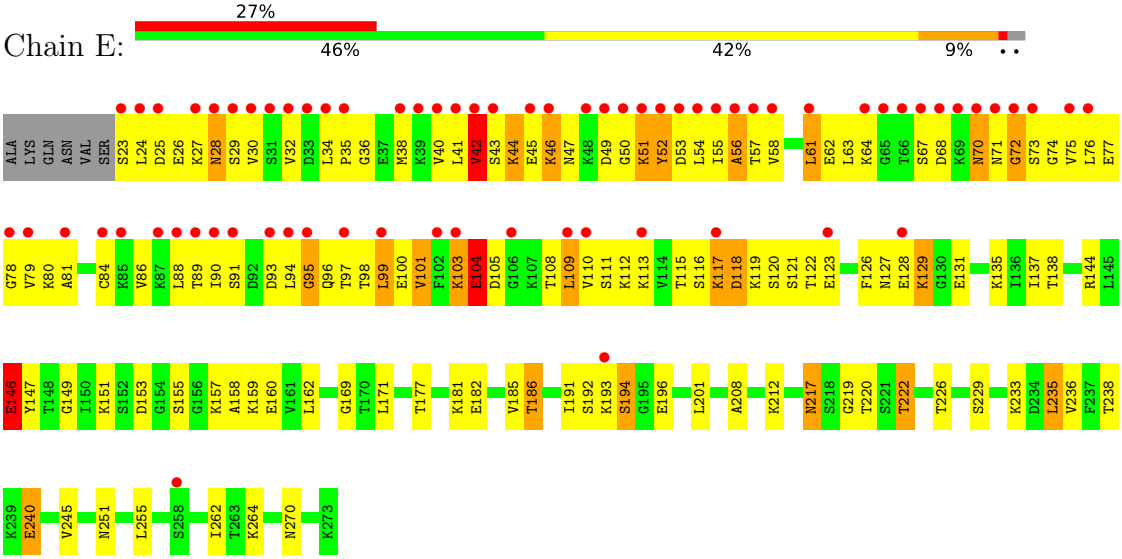


• Molecule 2: HYBRIDOMA ANTIBODY LA2 (HEAVY CHAIN)

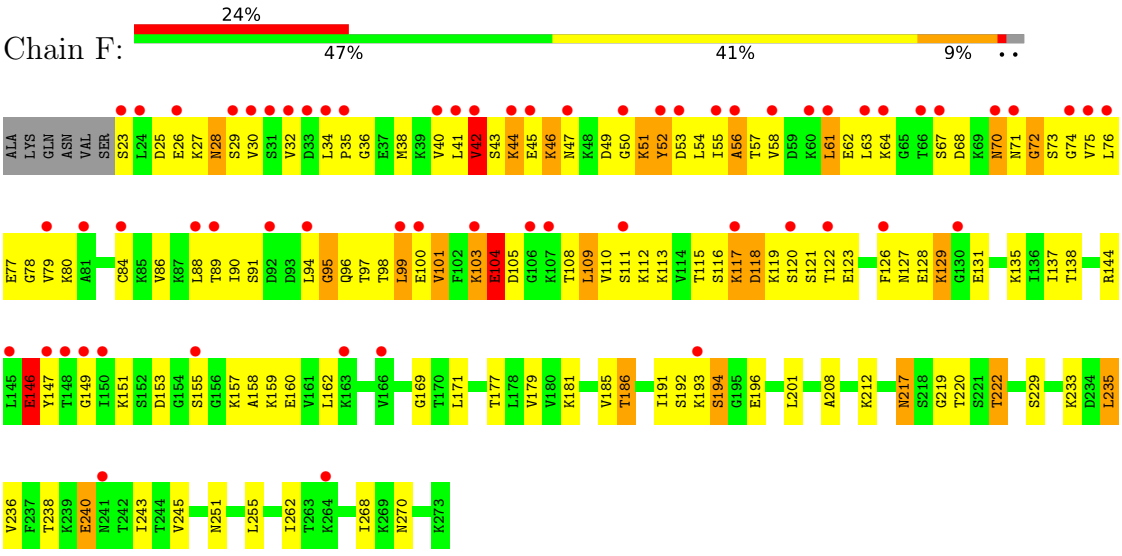
Chain D:



• 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 19.83 – 2.68	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.83-2.68) 96.4 (19.83-2.68)	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)	0.33 , 61.1	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	0.65	0/1697	1.09	5/2299 (0.2%)
1	C	0.62	0/1697	1.07	7/2299 (0.3%)
2	B	0.67	0/1630	1.12	13/2225 (0.6%)
2	D	0.55	0/1630	1.03	6/2225 (0.3%)
3	E	0.51	0/1902	0.93	3/2550 (0.1%)
3	F	0.45	0/1902	0.92	4/2550 (0.2%)
All	All	0.58	0/10458	1.03	38/14148 (0.3%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	137	ASN	N-CA-C	8.13	123.26	110.17
1	C	137	ASN	N-CA-C	8.07	123.17	110.17
2	D	33	SER	N-CA-C	7.45	120.11	111.02
2	B	33	SER	N-CA-C	7.29	119.92	111.02
2	B	143	LYS	N-CA-C	7.27	121.87	110.17
1	C	70	ASP	N-CA-C	6.96	119.86	108.52
2	B	125	ALA	CA-C-N	6.90	128.47	119.84
2	B	125	ALA	C-N-CA	6.90	128.47	119.84
1	A	70	ASP	N-CA-C	6.84	119.66	108.52
2	B	8	GLY	N-CA-C	6.44	120.02	112.23
3	F	238	THR	N-CA-C	6.39	118.57	110.33
2	D	101	ASP	N-CA-C	6.26	120.22	112.59
2	D	8	GLY	N-CA-C	6.25	119.50	112.00
3	E	49	ASP	N-CA-C	6.22	117.31	108.54
3	F	49	ASP	N-CA-C	6.20	117.28	108.54
3	E	238	THR	N-CA-C	6.14	118.25	110.33
2	B	199	HIS	CA-C-N	6.07	127.43	119.84
2	B	199	HIS	C-N-CA	6.07	127.43	119.84
3	F	146	GLU	N-CA-C	5.86	118.07	108.52
2	B	62	ASP	N-CA-C	5.83	118.39	111.33
1	A	133	VAL	N-CA-C	5.82	116.86	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	146	GLU	N-CA-C	5.80	117.97	108.52
1	A	99	GLY	N-CA-C	-5.67	103.72	112.85
2	B	150	VAL	N-CA-C	-5.53	99.86	108.81
2	B	101	ASP	N-CA-C	5.50	119.56	112.41
2	B	192	THR	N-CA-C	5.37	118.68	110.20
1	C	133	VAL	N-CA-C	5.31	116.13	108.48
3	F	179	VAL	N-CA-C	5.21	115.99	108.48
2	D	125	ALA	CA-C-N	5.18	126.32	119.84
2	D	125	ALA	C-N-CA	5.18	126.32	119.84
2	D	112	SER	N-CA-C	5.16	116.36	108.42
1	C	4	MET	CA-C-N	-5.12	116.18	122.84
1	C	4	MET	C-N-CA	-5.12	116.18	122.84
1	C	7	SER	N-CA-C	5.10	114.69	108.11
1	C	99	GLY	N-CA-C	-5.09	104.65	112.85
2	B	104	GLY	N-CA-C	-5.09	103.75	112.30
2	B	120	SER	N-CA-C	-5.04	101.50	109.96
1	A	115	VAL	N-CA-C	5.01	115.19	108.17

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	1660	0	1597	64	0
1	C	1660	0	1597	65	0
2	B	1589	0	1548	85	0
2	D	1589	0	1548	85	0
3	E	1893	0	1965	159	0
3	F	1893	0	1965	155	0
4	A	64	0	0	3	0
4	B	52	0	0	5	0
4	C	67	0	0	3	0
4	D	22	0	0	2	0
4	E	37	0	0	3	0
4	F	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10542	0	10220	601	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 29.

All (601) 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:142:VAL:HB	2:B:177:MET:HE2	1.46	0.96
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
2:B:142:VAL:CB	2:B:177:MET:HE2	2.07	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ALA:O	1:A:181:LEU:HD12	1.83	0.79
3:F:217:ASN:C	3:F:217:ASN:HD22	1.90	0.79
3:E:127:ASN:HD21	3:E:131:GLU:HB2	1.46	0.79
3:F:117:LYS:HB3	3:F:117:LYS:HZ2	1.48	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
3:E:117:LYS:HB3	3:E:117:LYS:HZ2	1.49	0.78
3:E:217:ASN:HD22	3:E:217:ASN:C	1.90	0.78
2:B:142:VAL:CG2	2:B:177:MET:HE2	2.14	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
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:HB3	3:F:117:LYS:NZ	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:88:ASN:O	2:B:91:THR:HG23	1.88	0.72
3:E:117:LYS:HB3	3:E:117:LYS:NZ	2.03	0.71
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: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:70:ASN:H	3:E:70:ASN:ND2	1.90	0.68
2:B:160:SER:C	2:B:162:SER:H	2.01	0.67
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
2:D:160:SER:C	2:D:162:SER:H	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:202:SER:C	2:B:204:THR:H	2.05	0.64
3:E:201:LEU:C	3:E:201:LEU:HD23	2.23	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:201:LEU:HD23	3:F:201:LEU:C	2.24	0.63
3:F:51:LYS:HB3	3:F:68:ASP:HA	1.80	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:177:MET:C	2:B:177:MET:HE3	2.24	0.62
2:B:33:SER:O	2:B:53:THR:HG23	1.99	0.62
1:A:55:GLN:HA	1:A:55:GLN:HE21	1.63	0.62
3:F:23:SER:N	3:F:41:LEU:HB2	2.14	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:SER:C	2:D:163:VAL:H	2.09	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
1:C:27:GLN:C	1:C:69:ARG:HG2	2.27	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
2:B:171:GLN:O	2:B:172:SER:C	2.45	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:42:VAL:HG11	3:E:70:ASN:C	2.26	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
2:D:89:GLU:CD	2:D:89:GLU:H	2.11	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
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:F:42:VAL:HG11	3:F:70:ASN:C	2.28	0.58
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
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
1:A:27:GLN:C	1:A:69:ARG:HG2	2.29	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
1:C:4:MET:HE3	1:C:23:CYS:SG	2.43	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
1:A:161:ASN:HB3	1:A:175:MET:HE1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:81:GLU:CD	1:C:81:GLU:H	2.12	0.57
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
2:B:189:PRO:C	2:B:191:GLN:H	2.13	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
1:C:161:ASN:HB3	1:C:175:MET:HE1	1.87	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
3:E:75:VAL:C	3:E:76:LEU:HD22	2.31	0.56
3:F:57:THR:HA	3:F:62:GLU:HA	1.87	0.55
3:F:217:ASN:C	3:F:217:ASN:ND2	2.62	0.55
2:B:89:GLU:CD	2:B:89:GLU:H	2.15	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
2:D:189:PRO:C	2:D:191:GLN:H	2.15	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:81:GLU:CD	1:A:81:GLU:H	2.14	0.54
2:D:170:LEU:HD13	2:D:175:TYR:CD2	2.43	0.54
3:F:75:VAL:C	3:F:76:LEU:HD22	2.32	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
1:A:175:MET:HE2	1:A:176:SER:C	2.34	0.53
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
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
2:B:142:VAL:HB	2:B:177:MET:CE	2.28	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
3:F:157:LYS:HZ2	3:F:159:LYS:HE2	1.74	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: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
1:A:4:MET:HE3	1:A:23:CYS:SG	2.49	0.52
3:F:129:LYS:HD2	3:F:131:GLU:CD	2.35	0.52
2:B:193:VAL:CG2	2:B:210:LEU:HB2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:GLU:HB2	4:B:1141:HOH:O	2.10	0.52
2:D:208:LYS:HZ3	2:D:208:LYS:HB2	1.75	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
1:C:115:VAL:O	1:C:207:LYS:HE3	2.11	0.51
2:D:133:GLY:C	2:D:135:SER:H	2.19	0.51
2:B:100:LEU:HD13	3:F:229:SER:HB3	1.90	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:B:189:PRO:C	2:B:191:GLN:N	2.69	0.51
3:E:129:LYS:HD2	3:E:131:GLU:CD	2.35	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
1:A:209:PHE:CD1	1:A:209:PHE:C	2.88	0.50
2:B:163:VAL:HG22	2:B:181:VAL:HG23	1.92	0.50
3:E:157:LYS:HZ2	3:E:159:LYS:HE2	1.74	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
2:D:115:LYS:O	2:D:116:THR:C	2.54	0.50
2:D:160:SER:C	2:D:162:SER:N	2.69	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:202:SER:C	2:B:204:THR:N	2.69	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
1:C:209:PHE:C	1:C:209:PHE:CD1	2.90	0.49
2:D:146:PHE:CD1	2:D:147:PRO:HA	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:184:PRO:C	2:D:186:SER:H	2.20	0.49
2:D:148:GLU:CD	2:D:149:SER:H	2.21	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
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
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
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:O	2:D:115:LYS:HD2	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:E:217:ASN:C	3:E:217:ASN:ND2	2.63	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
1:A:135:PHE:C	1:A:136:LEU:HD12	2.38	0.48
1:C:212:ASN:O	1:C:213:GLU:C	2.56	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
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
1:C:142:LYS:NZ	4:C:1046:HOH:O	2.41	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ILE:N	2:B:2:ILE:HD12	2.29	0.47
2:B:177:MET:HE3	2:B:178:SER:CA	2.44	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
2:D:202:SER:C	2:D:204:THR:H	2.22	0.47
1:A:212:ASN:O	1:A:213:GLU:C	2.56	0.47
2:B:177:MET:HE3	2:B:178:SER:N	2.29	0.47
2:B:209:LYS:HD2	2:B:211:GLU:CD	2.39	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
2:D:89:GLU:CD	2:D:89:GLU:N	2.72	0.47
3:E:117:LYS:C	3:E:119:LYS:H	2.22	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
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
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
3:F:43:SER:HB2	3:F:53:ASP:OD2	2.15	0.47
3:F:117:LYS:C	3:F:119:LYS:H	2.23	0.47
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: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
1:A:7:SER:HA	1:A:8:PRO:C	2.40	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
2:D:189:PRO:C	2:D:191:GLN:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:7:SER:HA	1:C:8:PRO:C	2.40	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
2:B:160:SER:C	2:B:162:SER:N	2.68	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: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
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
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: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
3:F:98:THR:O	3:F:98:THR:HG22	2.17	0.45
3:E:40:VAL:HA	3:E:56:ALA:HB2	1.99	0.45
2:B:89:GLU:CD	2:B:89:GLU:N	2.75	0.45
1:C:175:MET:HE2	1:C:176:SER:C	2.42	0.45
2:D:161:SER:C	2:D:163:VAL:N	2.75	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
1:C:135:PHE:C	1:C:136:LEU:HD12	2.42	0.45
3:E:23:SER:OG	3:E:41:LEU:HD13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:240:GLU:CD	3:E:240:GLU:H	2.25	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
1:A:161:ASN:CB	1:A:175:MET:HE1	2.47	0.44
3:E:115:THR:CG2	3:E:116:SER:H	2.22	0.44
2:D:50:TRP:CD1	2:D:51:ILE:N	2.84	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
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
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
3:F:38:MET:HE1	3:F:58:VAL:HG13	2.00	0.43
3:F:192:SER:C	3:F:194:SER:N	2.76	0.43
3:F:240:GLU:CD	3:F:240:GLU:H	2.25	0.43
1:A:175:MET:HE2	1:A:176:SER:O	2.18	0.43
2:B:146:PHE:CG	2:B:147:PRO:HA	2.53	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
1:C:81:GLU:CD	1:C:81:GLU:N	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ILE:HA	1:C:89:LEU:O	2.18	0.43
3:E:38:MET:HE1	3:E:58:VAL:HG13	2.00	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
3:F:127:ASN:C	3:F:129:LYS:H	2.27	0.43
1:A:162:SER:HB2	2:B:169:LEU:HD22	2.00	0.43
2:D:158:SER:O	2:D:159:LEU:C	2.61	0.43
2:D:199:HIS:O	2:D:201:ALA:N	2.52	0.43
3:F:35:PRO:CG	3:F:95:GLY:HA2	2.49	0.43
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:50:TYR:C	1:A:51:THR:HG23	2.44	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
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
3:E:192:SER:C	3:E:194:SER:N	2.77	0.42
2:B:187:THR:O	2:B:191:GLN:CB	2.67	0.42
1:C:161:ASN:CB	1:C:175:MET:HE1	2.47	0.42
3:E:38:MET:HE2	3:E:58:VAL:HG22	2.01	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
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:E:127:ASN:C	3:E:129:LYS:H	2.28	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
1:C:31:LYS:HB3	1:C:51:THR:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:A:30:ASN:O	1:A:31:LYS:HB2	2.19	0.41
3:F:51:LYS:HB2	3:F:51:LYS:NZ	2.35	0.41
3:E:61:LEU:O	3:E:62:GLU:C	2.63	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: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
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
3:E:72:GLY:C	3:E:74:GLY:H	2.28	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
2:D:198:ALA:C	2:D:200:PRO:HD3	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:F:72:GLY:C	3:F:74:GLY:H	2.29	0.40
3:F:129:LYS:HD2	3:F:131:GLU:OE2	2.21	0.40
1:C:76:SER:O	1:C:77:ASN:C	2.64	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
2:B:177:MET:HE3	2:B:177:MET:O	2.21	0.40
3:F:57:THR:CB	3:F:62:GLU:HB2	2.52	0.40
3:F:71:ASN:CG	3:F:94:LEU:HD11	2.46	0.40
3:F:162:LEU:N	3:F:162:LEU:HD22	2.36	0.40
3:F:245:VAL:C	4:F:1368:HOH:O	2.64	0.40
1:C:115:VAL:HA	1:C:135:PHE:O	2.21	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%)	14	31
1	C	211/213 (99%)	204 (97%)	5 (2%)	2 (1%)	14	31
2	B	211/213 (99%)	194 (92%)	10 (5%)	7 (3%)	3	6
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	3

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

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Mol	Chain	Res	Type
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
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%)	176 (94%)	12 (6%)	16 35
1	C	188/188 (100%)	176 (94%)	12 (6%)	16 35
2	B	182/182 (100%)	161 (88%)	21 (12%)	5 12
2	D	182/182 (100%)	161 (88%)	21 (12%)	5 12
3	E	220/225 (98%)	202 (92%)	18 (8%)	10 24
3	F	220/225 (98%)	202 (92%)	18 (8%)	10 24
All	All	1180/1190 (99%)	1078 (91%)	102 (9%)	10 22

All (102) 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	81	GLU
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	2	ILE
2	B	5	VAL
2	B	30	THR
2	B	39	GLN
2	B	50	TRP
2	B	59	THR
2	B	70	LEU
2	B	91	THR
2	B	98	ARG

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Mol	Chain	Res	Type
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	165	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	81	GLU
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	5	VAL
2	D	30	THR
2	D	39	GLN
2	D	50	TRP
2	D	53	THR
2	D	59	THR
2	D	70	LEU
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

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Mol	Chain	Res	Type
2	D	205	THR
2	D	208	LYS
3	E	28	ASN
3	E	42	VAL
3	E	51	LYS
3	E	70	ASN
3	E	104	GLU
3	E	109	LEU
3	E	117	LYS
3	E	122	THR
3	E	129	LYS
3	E	146	GLU
3	E	153	ASP
3	E	186	THR
3	E	217	ASN
3	E	222	THR
3	E	235	LEU
3	E	240	GLU
3	E	255	LEU
3	E	270	ASN
3	F	28	ASN
3	F	42	VAL
3	F	51	LYS
3	F	70	ASN
3	F	104	GLU
3	F	109	LEU
3	F	117	LYS
3	F	122	THR
3	F	129	LYS
3	F	146	GLU
3	F	153	ASP
3	F	186	THR
3	F	217	ASN
3	F	222	THR
3	F	235	LEU
3	F	240	GLU
3	F	255	LEU
3	F	270	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) 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	156	GLN
1	A	161	ASN
1	A	166	GLN
1	A	189	HIS
1	A	190	ASN
1	A	210	ASN
2	B	3	GLN
2	B	82	HIS
2	B	105	GLN
2	B	155	ASN
1	C	3	GLN
1	C	6	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
1	C	210	ASN
2	D	3	GLN
2	D	85	ASN
2	D	105	GLN
2	D	191	GLN
3	E	70	ASN
3	E	96	GLN
3	E	190	ASN
3	E	217	ASN
3	E	270	ASN
3	F	70	ASN
3	F	96	GLN
3	F	190	ASN

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Mol	Chain	Res	Type
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 oligosaccharides 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%)	-0.27	1 (0%) 87 86	14, 29, 56, 100	0
1	C	213/213 (100%)	0.02	3 (1%) 73 71	14, 32, 85, 100	0
2	B	213/213 (100%)	0.02	9 (4%) 40 36	15, 33, 76, 100	0
2	D	213/213 (100%)	0.67	14 (6%) 24 21	17, 54, 97, 100	0
3	E	251/257 (97%)	1.17	70 (27%) 1 1	16, 66, 100, 100	0
3	F	251/257 (97%)	1.32	62 (24%) 2 1	20, 86, 100, 100	0
All	All	1354/1366 (99%)	0.53	159 (11%) 9 7	14, 46, 100, 100	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	158	SER	5.9
3	E	30	VAL	5.8
3	E	24	LEU	5.8
3	E	42	VAL	5.6
3	E	32	VAL	5.6
3	E	53	ASP	5.4
3	E	23	SER	5.4
3	F	23	SER	5.3
3	F	74	GLY	5.2
3	E	54	LEU	5.1
3	E	52	TYR	5.1
3	E	43	SER	5.0
2	D	156	SER	4.9
3	E	71	ASN	4.8
3	F	24	LEU	4.8
3	F	34	LEU	4.7
3	F	35	PRO	4.7
3	E	29	SER	4.6
3	E	40	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	42	GLY	4.5
3	E	41	LEU	4.5
3	E	81	ALA	4.4
3	E	110	VAL	4.3
3	E	79	VAL	4.3
3	E	34	LEU	4.2
2	D	158	SER	4.2
3	F	45	GLU	4.2
2	D	159	LEU	4.1
3	E	102	PHE	4.1
3	E	58	VAL	4.0
3	E	88	LEU	3.9
3	E	109	LEU	3.9
3	F	130	GLY	3.9
3	E	39	LYS	3.8
2	D	160	SER	3.8
3	F	56	ALA	3.8
3	E	50	GLY	3.7
3	F	75	VAL	3.7
3	F	150	ILE	3.6
3	F	71	ASN	3.5
3	F	67	SER	3.5
3	E	69	LYS	3.5
3	F	47	ASN	3.4
3	E	49	ASP	3.4
3	F	30	VAL	3.4
3	F	147	TYR	3.4
3	F	92	ASP	3.4
3	E	56	ALA	3.4
3	F	76	LEU	3.4
3	F	94	LEU	3.4
3	E	55	ILE	3.3
3	E	31	SER	3.3
3	E	76	LEU	3.2
3	E	57	THR	3.2
3	E	97	THR	3.2
3	E	28	ASN	3.2
2	D	132	THR	3.2
3	E	67	SER	3.1
2	D	19	LYS	3.1
3	E	75	VAL	3.1
3	E	94	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
3	E	84	CYS	3.0
3	F	106	GLY	3.0
3	E	193	LYS	3.0
3	E	72	GLY	3.0
3	F	31	SER	3.0
3	F	111	SER	3.0
3	E	103	LYS	3.0
3	E	66	THR	2.9
3	E	35	PRO	2.9
2	B	172	SER	2.9
2	B	159	LEU	2.9
3	E	87	LYS	2.9
3	E	91	SER	2.9
3	F	44	LYS	2.9
2	D	155	ASN	2.9
1	C	191	SER	2.8
3	F	163	LYS	2.8
3	E	70	ASN	2.8
3	E	65	GLY	2.8
2	B	1	GLN	2.8
3	F	64	LYS	2.8
3	F	52	TYR	2.8
3	F	55	ILE	2.7
3	F	29	SER	2.7
3	E	90	ILE	2.7
3	F	66	THR	2.7
3	F	79	VAL	2.7
3	E	51	LYS	2.7
3	E	89	THR	2.6
3	E	61	LEU	2.6
2	B	157	GLY	2.6
3	F	100	GLU	2.6
3	F	149	GLY	2.6
3	F	42	VAL	2.6
3	F	145	LEU	2.6
1	C	212	ASN	2.6
2	B	192	THR	2.6
3	F	84	CYS	2.6
2	B	129	GLY	2.5
1	A	3	GLN	2.5
2	D	75	SER	2.5
3	E	99	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	117	LYS	2.5
3	E	93	ASP	2.5
2	D	131	THR	2.5
3	E	85	LYS	2.4
3	F	107	LYS	2.4
3	F	264	LYS	2.4
3	E	73	SER	2.4
2	B	130	ASP	2.4
3	F	50	GLY	2.4
3	E	48	LYS	2.4
3	E	64	LYS	2.4
3	E	117	LYS	2.4
3	F	58	VAL	2.4
3	F	41	LEU	2.4
3	E	78	GLY	2.4
3	F	126	PHE	2.4
3	F	60	LYS	2.3
2	D	41	PRO	2.3
1	C	188	ARG	2.3
3	E	38	MET	2.3
3	F	81	ALA	2.3
3	E	25	ASP	2.3
3	F	155	SER	2.3
3	F	32	VAL	2.3
3	F	70	ASN	2.2
3	F	33	ASP	2.2
3	F	166	VAL	2.2
3	F	103	LYS	2.2
3	F	26	GLU	2.2
2	D	157	GLY	2.2
2	D	33	SER	2.2
3	F	61	LEU	2.2
3	F	88	LEU	2.2
3	E	46	LYS	2.2
3	E	113	LYS	2.2
3	E	95	GLY	2.2
3	E	123	GLU	2.1
3	E	27	LYS	2.1
3	F	193	LYS	2.1
3	F	241	ASN	2.1
3	E	106	GLY	2.1
3	E	258	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	148	THR	2.1
3	F	63	LEU	2.1
3	E	33	ASP	2.1
2	B	33	SER	2.1
3	F	122	THR	2.1
3	F	40	VAL	2.1
2	D	89	GLU	2.0
3	E	45	GLU	2.0
3	E	128	GLU	2.0
3	F	89	THR	2.0
3	E	68	ASP	2.0
3	F	53	ASP	2.0
3	F	120	SER	2.0
3	F	99	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides 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.