



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:00 AM UTC

PDB ID : 1PKQ / pdb_00001pkq
Title : Myelin Oligodendrocyte Glycoprotein-(8-18C5) Fab-complex
Authors : Breithaupt, C.; Schubart, A.; Zander, H.; Skerra, A.; Huber, R.; Linington, C.; Jacob, U.
Deposited on : 2003-06-06
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 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

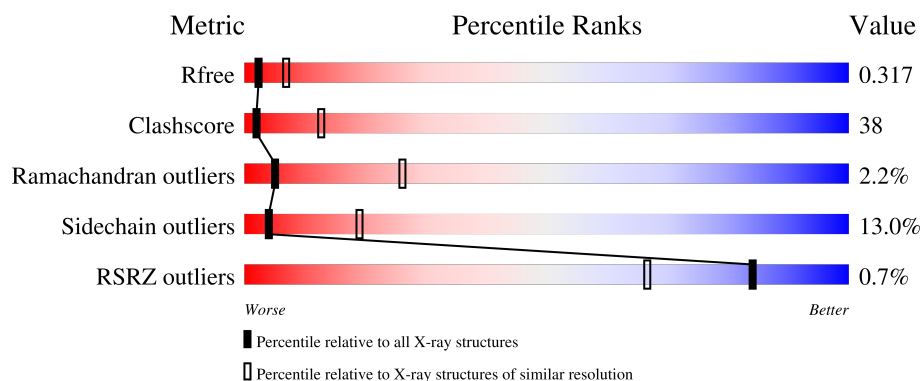
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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 $\leq 5\%$. 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	241	
1	F	241	
2	B	252	
2	G	252	
3	E	139	

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Mol	Chain	Length	Quality of chain
3	J	139	% 34% 40% 11% 15%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8517 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 (8-18C5) chimeric Fab, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	20	0	0
			1673	1045	279	344	5			
1	F	216	Total	C	N	O	S	23	0	0
			1649	1032	273	339	5			

- Molecule 2 is a protein called (8-18C5) chimeric Fab, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	23	0	0
			1633	1032	270	324	7			
2	G	214	Total	C	N	O	S	20	0	0
			1590	1007	262	314	7			

- Molecule 3 is a protein called Myelin Oligodendrocyte Glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	19	0	0
			951	592	174	182	3			
3	J	118	Total	C	N	O	S	34	0	0
			936	584	171	178	3			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	MET	-	cloning artifact	UNP Q63345
E	0	ARG	-	cloning artifact	UNP Q63345
E	1A	GLY	-	cloning artifact	UNP Q63345
E	1B	SER	-	cloning artifact	UNP Q63345
E	126	ARG	-	expression tag	UNP Q63345
E	127	SER	-	expression tag	UNP Q63345
E	128	ARG	-	expression tag	UNP Q63345
E	129	SER	-	expression tag	UNP Q63345

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Chain	Residue	Modelled	Actual	Comment	Reference
E	130	HIS	-	expression tag	UNP Q63345
E	131	HIS	-	expression tag	UNP Q63345
E	132	HIS	-	expression tag	UNP Q63345
E	133	HIS	-	expression tag	UNP Q63345
E	134	HIS	-	expression tag	UNP Q63345
E	135	HIS	-	expression tag	UNP Q63345
J	-3	MET	-	cloning artifact	UNP Q63345
J	-2	ARG	-	cloning artifact	UNP Q63345
J	-1	GLY	-	cloning artifact	UNP Q63345
J	0	SER	-	cloning artifact	UNP Q63345
J	126	ARG	-	expression tag	UNP Q63345
J	127	SER	-	expression tag	UNP Q63345
J	128	ARG	-	expression tag	UNP Q63345
J	129	SER	-	expression tag	UNP Q63345
J	130	HIS	-	expression tag	UNP Q63345
J	131	HIS	-	expression tag	UNP Q63345
J	132	HIS	-	expression tag	UNP Q63345
J	133	HIS	-	expression tag	UNP Q63345
J	134	HIS	-	expression tag	UNP Q63345
J	135	HIS	-	expression tag	UNP Q63345

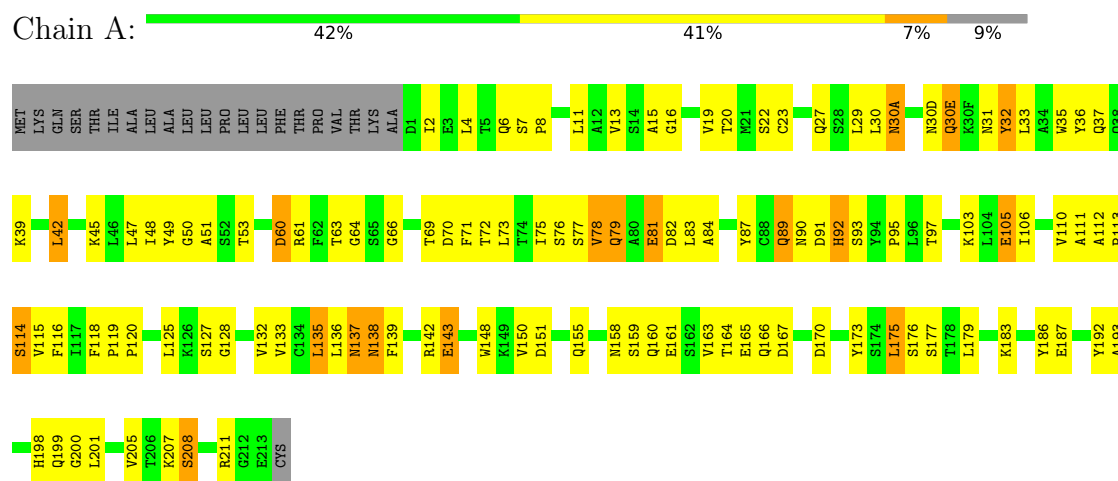
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	16	Total O 16 16	0	0
4	B	18	Total O 18 18	0	0
4	E	8	Total O 8 8	0	0
4	F	25	Total O 25 25	0	0
4	G	9	Total O 9 9	0	0
4	J	9	Total O 9 9	0	0

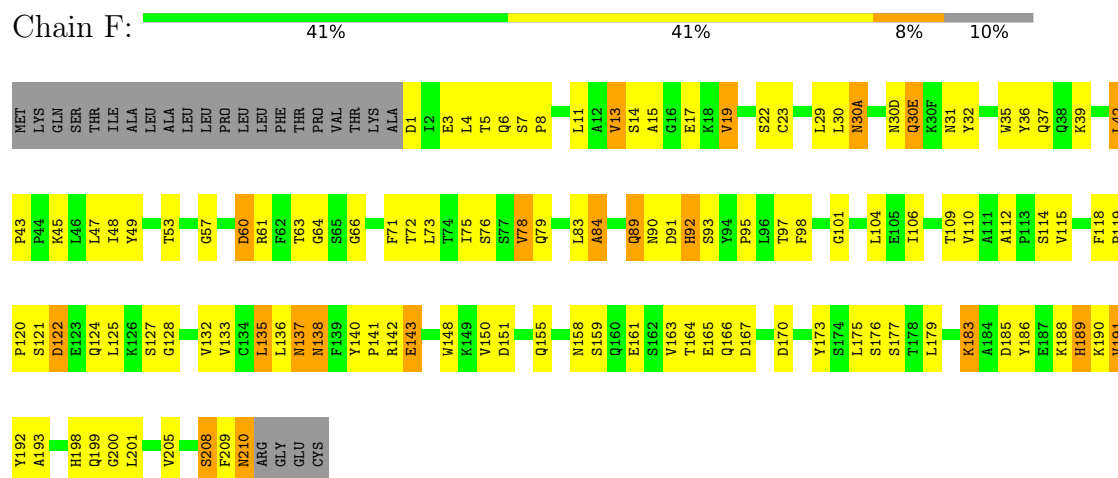
3 Residue-property plots

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.

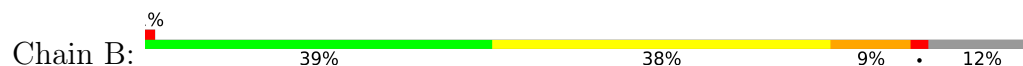
- Molecule 1: (8-18C5) chimeric Fab, light chain

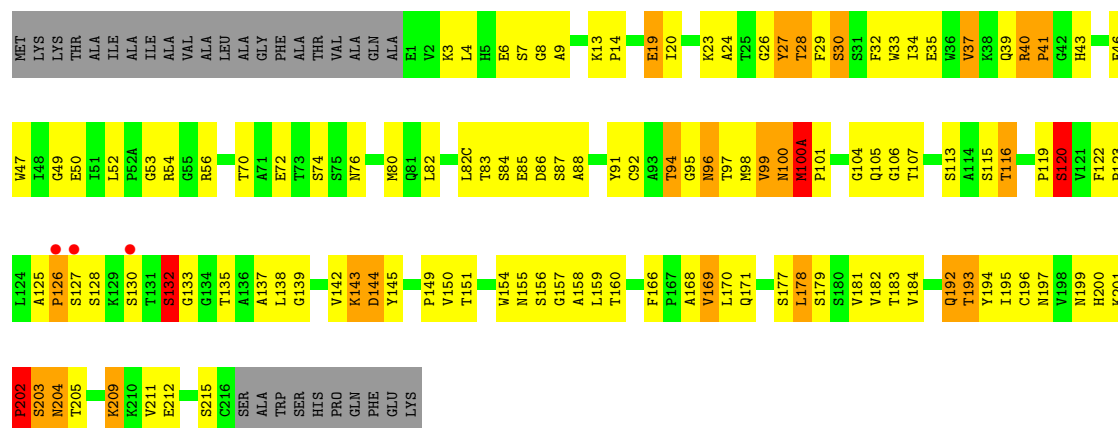


- Molecule 1: (8-18C5) chimeric Fab, light chain

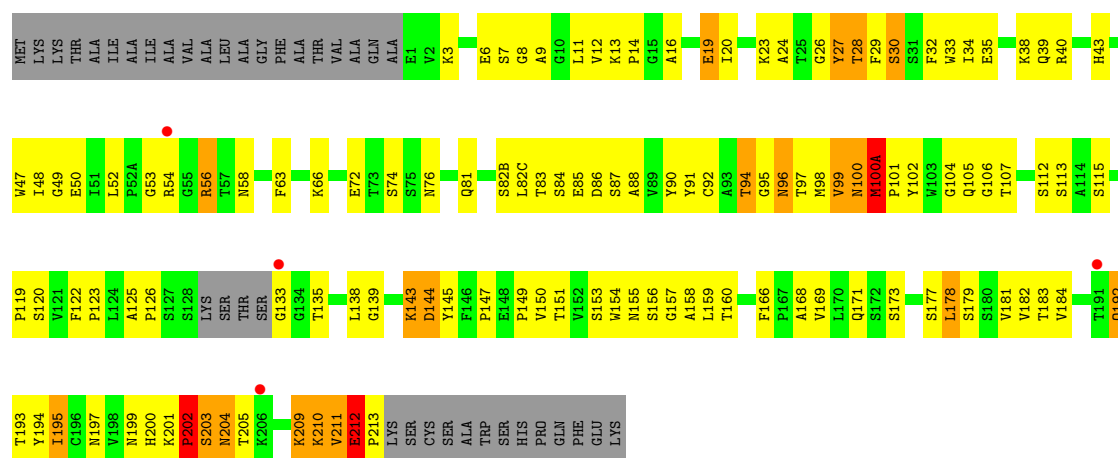


- Molecule 2: (8-18C5) chimeric Fab, heavy chain

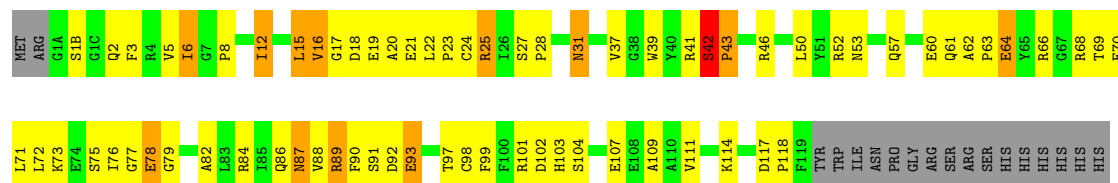




• Molecule 2: (8-18C5) chimeric Fab, heavy chain

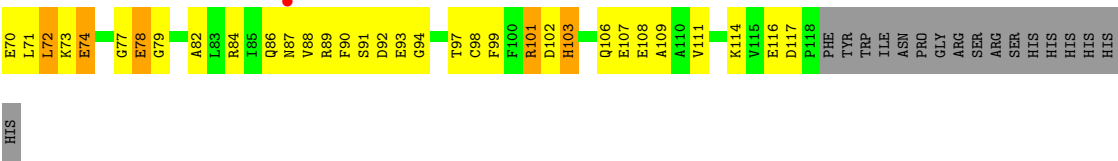


• Molecule 3: Myelin Oligodendrocyte Glycoprotein



• Molecule 3: Myelin Oligodendrocyte Glycoprotein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	124.48Å 40.00Å 134.20Å 90.00° 107.75° 90.00°	Depositor
Resolution (Å)	18.00 – 3.00 18.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	86.0 (18.00-3.00) 86.0 (18.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 3.02Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.319 0.252 , 0.317	Depositor DCC
R_{free} test set	1091 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8517	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0/1707	1.07	10/2317 (0.4%)
1	F	0.63	0/1683	1.08	12/2286 (0.5%)
2	B	0.71	0/1675	1.18	18/2286 (0.8%)
2	G	0.71	0/1631	1.13	12/2225 (0.5%)
3	E	0.71	0/972	1.09	3/1310 (0.2%)
3	J	0.70	0/957	1.02	3/1290 (0.2%)
All	All	0.68	0/8625	1.10	58/11714 (0.5%)

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	120	SER	N-CA-C	-9.41	94.06	109.40
1	F	183	LYS	N-CA-C	-7.85	102.72	111.28
1	F	30(E)	GLN	N-CA-C	-7.65	100.62	111.56
3	J	42	SER	N-CA-C	7.60	126.60	109.81
3	E	42	SER	N-CA-C	7.47	126.33	109.81
1	A	30(E)	GLN	N-CA-C	-7.40	101.16	111.52
2	B	40	ARG	CA-C-N	7.20	128.84	119.84
2	B	40	ARG	C-N-CA	7.20	128.84	119.84
2	B	30	SER	N-CA-C	6.80	121.43	113.20
1	F	89	GLN	N-CA-C	6.68	120.50	108.48
1	F	30(A)	ASN	N-CA-C	-6.62	98.48	109.46
1	A	89	GLN	N-CA-C	6.59	120.36	108.69
2	G	125	ALA	CA-C-N	6.54	126.52	119.78
2	G	125	ALA	C-N-CA	6.54	126.52	119.78
2	G	166	PHE	N-CA-C	6.49	119.04	110.08
1	F	112	ALA	CA-C-N	6.47	126.70	119.90
1	F	112	ALA	C-N-CA	6.47	126.70	119.90
2	B	37	VAL	N-CA-C	6.46	117.19	107.75
2	G	30	SER	N-CA-C	6.26	120.78	113.20
2	G	125	ALA	N-CA-C	6.26	118.70	109.50
2	B	115	SER	N-CA-C	6.25	120.23	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	LYS	N-CA-C	-6.13	104.60	111.28
2	B	125	ALA	N-CA-C	6.13	118.51	109.50
3	E	78	GLU	N-CA-C	-6.09	105.80	113.72
1	A	30(A)	ASN	N-CA-C	-6.04	99.43	109.46
1	F	128	GLY	N-CA-C	6.04	123.19	114.67
2	B	125	ALA	CA-C-N	6.03	125.99	119.78
2	B	125	ALA	C-N-CA	6.03	125.99	119.78
2	G	210	LYS	N-CA-C	-5.93	101.71	110.48
2	G	144	ASP	N-CA-C	5.87	119.34	111.24
2	B	192	GLN	N-CA-C	5.83	119.14	109.46
1	A	128	GLY	N-CA-C	5.81	122.86	114.67
2	G	143	LYS	N-CA-C	5.74	118.91	109.72
1	A	208	SER	N-CA-C	5.62	116.79	108.86
2	B	195	ILE	N-CA-C	5.60	115.95	108.11
1	A	165	GLU	N-CA-C	-5.59	103.16	110.53
1	F	165	GLU	N-CA-C	-5.55	103.20	110.53
2	G	27	TYR	N-CA-C	5.47	116.53	107.73
1	F	191	VAL	N-CA-C	5.44	115.68	107.80
2	B	27	TYR	N-CA-C	5.40	116.43	107.73
2	B	143	LYS	N-CA-C	5.32	118.23	109.72
3	E	6	ILE	N-CA-C	5.29	116.09	108.48
1	A	151	ASP	N-CA-C	-5.27	104.63	111.74
1	F	208	SER	N-CA-C	5.26	117.25	108.99
3	J	6	ILE	N-CA-C	5.19	115.95	108.48
1	A	32	TYR	N-CA-C	5.18	117.53	108.52
2	B	144	ASP	N-CA-C	5.17	118.37	111.24
1	F	151	ASP	N-CA-C	-5.16	104.77	111.74
1	A	137	ASN	N-CA-C	5.16	118.03	109.46
1	F	137	ASN	N-CA-C	5.15	118.01	109.46
2	G	195	ILE	N-CA-C	5.15	115.32	108.11
2	B	128	SER	N-CA-C	-5.14	105.75	112.23
2	G	192	GLN	N-CA-C	5.12	117.96	109.46
2	B	166	PHE	N-CA-C	5.11	117.70	110.24
2	B	215	SER	N-CA-C	-5.11	104.22	110.61
2	B	132	SER	N-CA-C	-5.05	99.76	108.69
2	G	115	SER	N-CA-C	5.03	117.60	110.50
3	J	78	GLU	N-CA-C	-5.02	106.58	113.30

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	1673	0	1629	115	0
1	F	1649	0	1607	130	0
2	B	1633	0	1580	132	0
2	G	1590	0	1543	137	0
3	E	951	0	910	74	0
3	J	936	0	900	63	0
4	A	16	0	0	0	0
4	B	18	0	0	4	0
4	E	8	0	0	1	0
4	F	25	0	0	2	0
4	G	9	0	0	1	0
4	J	9	0	0	1	0
All	All	8517	0	8169	620	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 38.

All (620) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:PRO:HG3	2:B:138:LEU:HB3	1.23	1.11
2:G:126:PRO:HG3	2:G:138:LEU:HB3	1.20	1.09
1:F:193:ALA:HB2	1:F:208:SER:HB3	1.26	1.08
3:E:1(B):SER:HB2	3:E:2:GLN:HG2	1.39	1.04
3:J:13:ARG:H	3:J:13:ARG:HD2	1.17	1.04
1:A:19:VAL:HG12	1:A:75:ILE:HB	1.39	1.01
2:G:54:ARG:HH21	3:J:107:GLU:HA	1.25	1.01
1:F:193:ALA:HB2	1:F:208:SER:CB	1.90	0.99
3:E:46:ARG:HD2	2:G:19:GLU:OE2	1.63	0.98
2:G:200:HIS:ND1	2:G:203:SER:HB3	1.80	0.96
1:A:6:GLN:HE22	1:A:87:TYR:HA	1.26	0.96
2:B:156:SER:H	2:B:197:ASN:HD21	1.01	0.95
2:G:156:SER:H	2:G:197:ASN:HD21	0.97	0.95
1:F:114:SER:HB2	1:F:137:ASN:HB3	1.48	0.93
2:B:200:HIS:ND1	2:B:203:SER:HB3	1.83	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:193:ALA:CB	1:F:208:SER:HB3	1.98	0.92
1:F:19:VAL:HG13	1:F:75:ILE:HB	1.48	0.92
2:G:123:PRO:HB3	2:G:211:VAL:HG13	1.53	0.91
3:E:15:LEU:HD22	3:E:15:LEU:H	1.37	0.90
3:E:5:VAL:HG12	3:E:109:ALA:HB2	1.54	0.89
3:E:62:ALA:HB1	3:E:64:GLU:OE2	1.72	0.89
2:G:94:THR:O	2:G:101:PRO:HD2	1.74	0.88
1:A:193:ALA:HB2	1:A:208:SER:HB3	1.54	0.87
2:B:204:ASN:HD22	2:B:205:THR:N	1.73	0.86
3:E:87:ASN:HD21	3:E:89:ARG:HH11	1.18	0.86
1:F:83:LEU:HB2	1:F:106:ILE:HD13	1.57	0.86
1:F:142:ARG:HG2	1:F:142:ARG:HH11	1.39	0.85
1:A:142:ARG:HG2	1:A:142:ARG:HH11	1.41	0.85
2:G:6:GLU:OE1	2:G:91:TYR:HA	1.75	0.85
2:G:204:ASN:HD22	2:G:205:THR:N	1.75	0.85
2:B:204:ASN:HD22	2:B:204:ASN:C	1.84	0.85
3:J:15:LEU:HD22	3:J:15:LEU:H	1.40	0.85
2:B:94:THR:O	2:B:101:PRO:HD2	1.77	0.84
3:E:25:ARG:HG3	3:E:25:ARG:HH11	1.41	0.84
3:J:5:VAL:HG12	3:J:109:ALA:HB2	1.59	0.84
2:B:96:ASN:HD21	2:B:99:VAL:HG23	1.43	0.84
3:J:25:ARG:HG3	3:J:25:ARG:HH11	1.43	0.83
2:G:204:ASN:HD22	2:G:204:ASN:C	1.85	0.83
2:B:6:GLU:OE1	2:B:91:TYR:HA	1.78	0.83
1:A:42:LEU:N	1:A:42:LEU:HD13	1.94	0.83
1:A:83:LEU:HD22	1:A:166:GLN:HB2	1.60	0.83
2:B:83:THR:HG22	2:B:85:GLU:H	1.44	0.82
2:G:156:SER:N	2:G:197:ASN:HD21	1.77	0.82
1:F:198:HIS:CD2	1:F:200:GLY:H	1.97	0.82
2:G:156:SER:H	2:G:197:ASN:ND2	1.78	0.82
2:B:97:THR:HG23	3:E:102:ASP:OD1	1.81	0.81
1:A:198:HIS:CD2	1:A:200:GLY:H	1.98	0.81
2:G:178:LEU:HD23	2:G:179:SER:N	1.96	0.81
1:A:83:LEU:HB2	1:A:106:ILE:HD13	1.62	0.81
1:F:4:LEU:N	1:F:4:LEU:HD12	1.96	0.80
2:B:6:GLU:H	2:B:105:GLN:HE22	1.29	0.80
1:A:11:LEU:HD11	1:A:19:VAL:CG2	2.12	0.80
2:G:7:SER:HA	2:G:107:THR:HG21	1.63	0.80
3:J:62:ALA:HB1	3:J:64:GLU:OE2	1.81	0.80
1:F:32:TYR:HB2	1:F:92:HIS:HB2	1.63	0.79
1:A:32:TYR:HB2	1:A:92:HIS:HB2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:CD2	1:A:166:GLN:HB2	2.12	0.79
1:F:42:LEU:N	1:F:42:LEU:HD13	1.97	0.79
2:B:156:SER:N	2:B:197:ASN:HD21	1.79	0.79
2:B:178:LEU:HD23	2:B:179:SER:N	1.96	0.79
2:G:83:THR:HG22	2:G:85:GLU:H	1.48	0.79
2:G:126:PRO:HG3	2:G:138:LEU:CB	2.08	0.79
1:A:198:HIS:HD2	1:A:200:GLY:H	1.30	0.79
2:G:96:ASN:HD21	2:G:99:VAL:HG23	1.47	0.79
1:A:11:LEU:HD11	1:A:19:VAL:HG23	1.65	0.78
3:E:72:LEU:HD22	3:E:82:ALA:HB3	1.64	0.78
1:F:155:GLN:HB3	1:F:158:ASN:HD21	1.47	0.78
2:G:6:GLU:H	2:G:105:GLN:HE22	1.29	0.78
2:G:54:ARG:NH2	3:J:107:GLU:HA	1.98	0.78
2:G:212:GLU:HB2	2:G:213:PRO:HD2	1.65	0.78
3:E:61:GLN:OE1	3:E:66:ARG:HA	1.84	0.78
2:B:156:SER:H	2:B:197:ASN:ND2	1.80	0.78
1:F:6:GLN:HG3	1:F:101:GLY:H	1.48	0.78
2:G:40:ARG:HG2	2:G:88:ALA:HB2	1.67	0.77
1:F:198:HIS:HD2	1:F:200:GLY:H	1.30	0.77
3:J:72:LEU:HD11	3:J:84:ARG:NH2	1.99	0.77
2:B:126:PRO:HG3	2:B:138:LEU:CB	2.12	0.76
3:E:68:ARG:HG2	3:E:68:ARG:HH11	1.50	0.76
2:B:119:PRO:HG3	2:B:145:TYR:HB3	1.68	0.76
2:B:7:SER:HA	2:B:107:THR:HG21	1.65	0.76
2:G:96:ASN:HD22	2:G:96:ASN:C	1.95	0.75
2:B:39:GLN:O	2:B:88:ALA:HB1	1.87	0.74
2:B:13:LYS:HD3	2:B:113:SER:HA	1.71	0.72
1:A:42:LEU:HD13	1:A:42:LEU:H	1.51	0.72
1:A:193:ALA:HB2	1:A:208:SER:CB	2.20	0.72
3:E:87:ASN:HD21	3:E:89:ARG:NH1	1.88	0.72
2:B:96:ASN:HD22	2:B:96:ASN:C	1.98	0.71
1:A:155:GLN:HB3	1:A:158:ASN:HD21	1.55	0.71
2:G:119:PRO:HG3	2:G:145:TYR:CB	2.21	0.71
2:B:54:ARG:HH21	3:E:107:GLU:HA	1.56	0.71
2:G:119:PRO:HG3	2:G:145:TYR:HB2	1.73	0.71
1:A:60:ASP:OD2	1:A:60:ASP:N	2.20	0.70
1:F:42:LEU:HD13	1:F:42:LEU:H	1.55	0.70
1:F:148:TRP:CE2	1:F:179:LEU:HB2	2.27	0.70
3:J:68:ARG:HG2	3:J:68:ARG:HH11	1.55	0.70
1:A:19:VAL:CG1	1:A:75:ILE:HB	2.18	0.70
2:G:96:ASN:ND2	2:G:99:VAL:H	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ASN:ND2	2:B:99:VAL:H	1.90	0.70
3:E:63:PRO:O	3:E:66:ARG:HG2	1.91	0.70
2:B:204:ASN:C	2:B:204:ASN:ND2	2.49	0.70
1:F:175:LEU:HD23	1:F:176:SER:N	2.06	0.70
2:G:201:LYS:C	2:G:203:SER:H	1.99	0.70
1:A:175:LEU:HD23	1:A:176:SER:N	2.07	0.70
2:G:155:ASN:CB	2:G:158:ALA:HB3	2.21	0.70
2:B:201:LYS:C	2:B:203:SER:H	1.99	0.69
1:F:110:VAL:HG22	1:F:141:PRO:HD3	1.74	0.68
2:B:119:PRO:HG3	2:B:145:TYR:CB	2.23	0.68
3:J:13:ARG:H	3:J:13:ARG:CD	1.93	0.68
1:A:35:TRP:CD1	1:A:48:ILE:HD11	2.29	0.67
2:B:155:ASN:CB	2:B:158:ALA:HB3	2.24	0.67
1:F:35:TRP:CD1	1:F:48:ILE:HD11	2.30	0.67
1:A:48:ILE:HD12	1:A:64:GLY:HA3	1.76	0.67
1:F:155:GLN:HB3	1:F:158:ASN:ND2	2.10	0.67
1:A:193:ALA:CB	1:A:208:SER:HB3	2.24	0.67
2:B:127:SER:H	2:B:130:SER:HB3	1.60	0.67
2:G:126:PRO:CG	2:G:138:LEU:HB3	2.11	0.67
2:B:13:LYS:CD	2:B:113:SER:HA	2.25	0.67
1:A:201:LEU:HD13	1:A:205:VAL:HG23	1.78	0.66
3:J:41:ARG:O	3:J:43:PRO:HD2	1.96	0.66
2:B:6:GLU:N	2:B:105:GLN:HE22	1.93	0.66
2:G:204:ASN:C	2:G:204:ASN:ND2	2.50	0.66
1:F:35:TRP:HB2	1:F:48:ILE:HG12	1.78	0.66
3:J:69:THR:O	3:J:70:GLU:HG3	1.96	0.66
1:A:148:TRP:CE2	1:A:179:LEU:HB2	2.31	0.65
3:J:15:LEU:HA	3:J:116:GLU:O	1.96	0.65
2:B:83:THR:HG22	2:B:84:SER:N	2.12	0.65
3:J:13:ARG:HD2	3:J:13:ARG:N	1.97	0.65
1:A:35:TRP:HB2	1:A:48:ILE:HG12	1.79	0.64
1:F:83:LEU:HB2	1:F:106:ILE:CD1	2.28	0.64
3:E:87:ASN:ND2	3:E:89:ARG:HH11	1.94	0.64
1:A:32:TYR:HB2	1:A:92:HIS:CB	2.26	0.64
2:G:212:GLU:HB2	2:G:213:PRO:CD	2.27	0.64
1:F:66:GLY:HA3	1:F:71:PHE:HA	1.80	0.64
1:A:30(A):ASN:CG	1:A:30(D):ASN:HD22	2.06	0.63
3:E:87:ASN:ND2	3:E:87:ASN:O	2.31	0.63
1:F:48:ILE:HD12	1:F:64:GLY:HA3	1.80	0.63
1:F:32:TYR:HB2	1:F:92:HIS:CB	2.27	0.63
2:G:6:GLU:N	2:G:105:GLN:HE22	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:203:SER:O	2:G:204:ASN:ND2	2.32	0.63
3:E:69:THR:O	3:E:70:GLU:HG3	1.99	0.63
1:F:30(A):ASN:CG	1:F:30(D):ASN:HD22	2.06	0.63
2:B:130:SER:OG	2:B:137:ALA:O	2.17	0.62
3:J:63:PRO:O	3:J:66:ARG:HG2	1.99	0.62
3:E:46:ARG:HH11	3:E:46:ARG:HG2	1.63	0.62
2:B:126:PRO:CG	2:B:138:LEU:HB3	2.15	0.62
2:G:159:LEU:HD21	2:G:182:VAL:HG21	1.80	0.62
1:F:201:LEU:HD13	1:F:205:VAL:HG23	1.81	0.62
2:G:24:ALA:HB1	2:G:27:TYR:HE1	1.64	0.62
2:B:143:LYS:HG2	2:B:144:ASP:CG	2.24	0.61
2:B:95:GLY:HA2	2:B:101:PRO:HD2	1.81	0.61
1:F:143:GLU:H	1:F:143:GLU:CD	2.07	0.61
1:A:4:LEU:HD23	1:A:23:CYS:SG	2.40	0.61
2:G:203:SER:OG	2:G:205:THR:OG1	2.18	0.61
2:G:83:THR:HG22	2:G:84:SER:N	2.15	0.61
3:J:73:LYS:O	3:J:74:GLU:C	2.42	0.61
2:B:6:GLU:H	2:B:105:GLN:NE2	1.98	0.61
2:G:155:ASN:HB3	2:G:158:ALA:HB3	1.81	0.61
2:G:171:GLN:CD	2:G:177:SER:HB2	2.26	0.61
3:E:90:PHE:C	3:E:92:ASP:H	2.09	0.61
1:F:19:VAL:HG11	1:F:78:VAL:HG23	1.82	0.61
1:F:191:VAL:HA	1:F:210:ASN:HA	1.83	0.61
2:B:200:HIS:CE1	2:B:203:SER:HB3	2.36	0.60
2:B:203:SER:O	2:B:204:ASN:CG	2.44	0.60
2:G:203:SER:O	2:G:204:ASN:CG	2.45	0.60
2:G:54:ARG:NH2	3:J:107:GLU:CD	2.59	0.60
2:G:95:GLY:HA2	2:G:101:PRO:HD2	1.83	0.60
2:G:143:LYS:HG2	2:G:144:ASP:CG	2.26	0.60
1:F:175:LEU:HD23	1:F:175:LEU:C	2.27	0.60
2:G:6:GLU:H	2:G:105:GLN:NE2	2.00	0.60
2:B:155:ASN:HB3	2:B:158:ALA:HB3	1.83	0.60
3:E:1(B):SER:C	3:E:2:GLN:H	2.09	0.60
3:J:25:ARG:HG3	3:J:25:ARG:NH1	2.14	0.60
2:B:159:LEU:HD21	2:B:182:VAL:HG21	1.84	0.60
3:E:52:ARG:NH2	3:E:60:GLU:OE2	2.34	0.60
3:E:87:ASN:O	3:E:87:ASN:CG	2.44	0.60
2:G:40:ARG:HG2	2:G:88:ALA:CB	2.31	0.60
1:A:143:GLU:H	1:A:143:GLU:CD	2.10	0.59
2:B:70:THR:HG22	3:J:44:PHE:CE2	2.37	0.59
2:B:157:GLY:C	2:B:159:LEU:H	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:90:PHE:HD2	3:E:90:PHE:O	1.85	0.59
3:J:8:PRO:HD2	3:J:111:VAL:HG22	1.83	0.59
2:G:143:LYS:HG2	2:G:144:ASP:OD2	2.02	0.59
2:B:24:ALA:HB1	2:B:27:TYR:HE1	1.68	0.59
2:G:178:LEU:HD23	2:G:178:LEU:C	2.27	0.59
1:A:7:SER:HA	1:A:8:PRO:C	2.26	0.59
1:A:32:TYR:CB	1:A:92:HIS:HB2	2.32	0.59
1:A:175:LEU:HD23	1:A:175:LEU:C	2.28	0.59
2:B:6:GLU:OE1	2:B:106:GLY:HA2	2.03	0.59
3:E:5:VAL:HG12	3:E:109:ALA:CB	2.29	0.59
2:B:32:PHE:HA	3:E:104:SER:O	2.03	0.58
2:B:83:THR:HG21	2:B:85:GLU:OE2	2.03	0.58
2:B:203:SER:O	2:B:204:ASN:ND2	2.36	0.58
1:A:19:VAL:HG11	1:A:75:ILE:HD12	1.84	0.58
1:A:30(A):ASN:CG	1:A:30(D):ASN:ND2	2.61	0.58
3:E:25:ARG:HG3	3:E:25:ARG:NH1	2.14	0.58
1:F:121:SER:O	1:F:122:ASP:C	2.46	0.58
2:B:201:LYS:O	2:B:203:SER:N	2.36	0.58
2:G:40:ARG:NH2	2:G:43:HIS:NE2	2.51	0.58
2:G:100:ASN:O	2:G:100(A):MET:HB2	2.02	0.58
2:G:201:LYS:C	2:G:203:SER:N	2.61	0.58
2:G:201:LYS:O	2:G:203:SER:N	2.36	0.58
1:F:30(A):ASN:CG	1:F:30(D):ASN:ND2	2.61	0.58
2:B:143:LYS:HG2	2:B:144:ASP:OD2	2.03	0.58
2:G:155:ASN:HB2	2:G:158:ALA:HB3	1.86	0.58
3:J:72:LEU:HD11	3:J:84:ARG:CZ	2.33	0.58
1:F:7:SER:HA	1:F:8:PRO:C	2.27	0.57
2:G:54:ARG:HH22	3:J:107:GLU:CD	2.13	0.57
1:A:155:GLN:HB3	1:A:158:ASN:ND2	2.18	0.57
2:B:83:THR:CG2	2:B:84:SER:N	2.67	0.57
1:F:36:TYR:OH	2:G:100(A):MET:HE3	2.05	0.57
2:B:96:ASN:HB2	4:B:229:HOH:O	2.04	0.57
1:A:11:LEU:N	1:A:11:LEU:HD23	2.19	0.57
1:A:142:ARG:HG2	1:A:142:ARG:NH1	2.18	0.57
2:B:171:GLN:CD	2:B:177:SER:HB2	2.30	0.57
3:J:5:VAL:HG12	3:J:109:ALA:CB	2.32	0.57
1:F:125:LEU:HB3	1:F:183:LYS:HE3	1.87	0.57
3:J:78:GLU:HG2	4:J:137:HOH:O	2.04	0.57
2:B:72:GLU:O	2:B:72:GLU:HG3	2.04	0.57
1:F:39:LYS:HB2	1:F:42:LEU:HD21	1.86	0.57
1:F:110:VAL:HG21	1:F:199:GLN:NE2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:184:VAL:HG21	2:G:194:TYR:CE2	2.40	0.56
1:A:30(A):ASN:ND2	3:E:53:ASN:ND2	2.53	0.56
1:A:33:LEU:HD22	1:A:71:PHE:CD2	2.40	0.56
2:B:100:ASN:O	2:B:100(A):MET:HB2	2.05	0.56
3:E:15:LEU:HD23	3:E:18:ASP:OD2	2.05	0.56
2:G:96:ASN:ND2	2:G:99:VAL:HG23	2.19	0.56
3:E:27:SER:HA	3:E:28:PRO:C	2.29	0.56
1:F:189:HIS:ND1	1:F:189:HIS:N	2.54	0.56
2:G:182:VAL:HG13	2:G:182:VAL:O	2.06	0.56
3:E:31:ASN:OD1	3:E:77:GLY:HA2	2.06	0.56
2:G:35:GLU:O	2:G:92:CYS:HA	2.06	0.56
1:A:30(A):ASN:ND2	3:E:53:ASN:HA	2.21	0.56
2:G:159:LEU:HD12	2:G:160:THR:H	1.71	0.56
2:G:96:ASN:ND2	2:G:98:MET:H	2.03	0.56
3:J:27:SER:HA	3:J:28:PRO:C	2.31	0.56
3:E:16:VAL:HG12	3:E:17:GLY:N	2.21	0.56
1:A:103:LYS:HE3	1:A:105:GLU:OE1	2.06	0.55
2:G:178:LEU:HD23	2:G:179:SER:C	2.31	0.55
2:G:200:HIS:CE1	2:G:203:SER:HB3	2.40	0.55
2:B:35:GLU:O	2:B:92:CYS:HA	2.06	0.55
3:J:15:LEU:HD23	3:J:18:ASP:OD2	2.06	0.55
2:B:178:LEU:HD23	2:B:179:SER:C	2.30	0.55
1:F:42:LEU:N	1:F:42:LEU:CD1	2.70	0.55
1:F:49:TYR:CD2	2:G:99:VAL:HG13	2.41	0.55
2:B:178:LEU:HD23	2:B:178:LEU:C	2.30	0.55
1:F:163:VAL:HG12	1:F:164:THR:N	2.22	0.55
1:A:42:LEU:N	1:A:42:LEU:CD1	2.67	0.55
1:F:136:LEU:N	1:F:136:LEU:HD12	2.22	0.55
1:F:60:ASP:OD2	1:F:60:ASP:N	2.26	0.55
2:B:201:LYS:C	2:B:203:SER:N	2.61	0.55
3:J:10:HIS:HE1	3:J:13:ARG:NH2	2.04	0.55
2:B:95:GLY:HA2	2:B:101:PRO:CD	2.37	0.55
2:B:96:ASN:ND2	2:B:99:VAL:HG23	2.17	0.55
3:J:13:ARG:CD	3:J:13:ARG:N	2.64	0.55
1:A:2:ILE:CD1	1:A:27:GLN:HB2	2.37	0.54
1:A:167:ASP:HB3	1:A:170:ASP:OD2	2.07	0.54
1:F:7:SER:O	1:F:22:SER:HB3	2.07	0.54
3:E:90:PHE:C	3:E:92:ASP:N	2.64	0.54
2:G:83:THR:CG2	2:G:84:SER:N	2.70	0.54
3:E:8:PRO:HD2	3:E:111:VAL:HG22	1.88	0.54
2:G:157:GLY:C	2:G:159:LEU:H	2.14	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:72:GLU:O	2:G:72:GLU:HG3	2.07	0.54
1:F:43:PRO:HG2	2:G:104:GLY:O	2.07	0.54
1:F:3:GLU:C	1:F:4:LEU:HD12	2.33	0.54
3:J:16:VAL:HG12	3:J:17:GLY:N	2.22	0.54
2:B:138:LEU:HD12	2:B:139:GLY:N	2.22	0.54
1:F:61:ARG:HB2	1:F:76:SER:OG	2.07	0.54
1:F:190:LYS:O	1:F:210:ASN:C	2.51	0.54
2:B:29:PHE:CD2	2:B:76:ASN:HA	2.43	0.54
3:E:18:ASP:O	3:E:88:VAL:HG23	2.07	0.54
1:F:125:LEU:C	1:F:127:SER:N	2.65	0.54
3:J:101:ARG:HD2	3:J:103:HIS:O	2.08	0.54
1:A:125:LEU:C	1:A:127:SER:N	2.65	0.53
1:F:106:ILE:HD12	1:F:106:ILE:N	2.23	0.53
2:G:123:PRO:HB3	2:G:211:VAL:CG1	2.34	0.53
1:A:39:LYS:HB2	1:A:42:LEU:HD21	1.90	0.53
2:B:139:GLY:HA2	2:B:154:TRP:CH2	2.43	0.53
3:E:46:ARG:HG2	3:E:46:ARG:NH1	2.22	0.53
1:F:155:GLN:CB	1:F:158:ASN:HD21	2.20	0.53
1:F:209:PHE:CG	1:F:209:PHE:O	2.61	0.53
2:B:83:THR:O	2:B:86:ASP:HB2	2.08	0.53
2:B:155:ASN:HB2	2:B:158:ALA:HB3	1.90	0.53
1:F:4:LEU:N	1:F:4:LEU:CD1	2.69	0.53
1:F:37:GLN:HB2	1:F:47:LEU:HD11	1.89	0.53
2:G:13:LYS:HD3	2:G:113:SER:HA	1.90	0.53
2:G:26:GLY:O	2:G:27:TYR:HB3	2.09	0.53
2:G:120:SER:HB3	2:G:122:PHE:CE2	2.43	0.53
1:A:125:LEU:C	1:A:127:SER:H	2.17	0.53
2:B:184:VAL:HG21	2:B:194:TYR:CE2	2.44	0.53
1:F:142:ARG:HG2	1:F:142:ARG:NH1	2.16	0.53
1:F:167:ASP:HB3	1:F:170:ASP:OD2	2.09	0.53
2:B:96:ASN:ND2	2:B:98:MET:H	2.07	0.53
1:F:71:PHE:O	1:F:72:THR:HG23	2.08	0.53
2:G:159:LEU:HD12	2:G:160:THR:N	2.23	0.53
1:F:57:GLY:N	4:F:215:HOH:O	2.38	0.52
1:F:125:LEU:C	1:F:127:SER:H	2.17	0.52
1:A:142:ARG:HH11	1:A:142:ARG:CG	2.16	0.52
2:G:95:GLY:HA2	2:G:101:PRO:CD	2.40	0.52
3:J:31:ASN:OD1	3:J:77:GLY:HA2	2.09	0.52
2:G:84:SER:O	2:G:87:SER:HB2	2.10	0.52
2:G:139:GLY:HA2	2:G:154:TRP:CH2	2.45	0.52
1:F:188:LYS:HB3	1:F:189:HIS:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:38:LYS:HB2	2:G:90:TYR:CE2	2.45	0.52
1:A:105:GLU:HG3	1:A:166:GLN:OE1	2.10	0.52
2:B:33:TRP:CD1	2:B:52:LEU:HD13	2.45	0.52
1:F:193:ALA:HB2	1:F:208:SER:HB2	1.85	0.52
1:F:189:HIS:N	1:F:189:HIS:HD1	2.07	0.52
2:G:6:GLU:OE1	2:G:106:GLY:HA2	2.09	0.52
1:F:142:ARG:HH11	1:F:142:ARG:CG	2.14	0.52
1:F:148:TRP:HZ2	1:F:177:SER:O	1.93	0.52
2:B:41:PRO:C	2:B:43:HIS:H	2.18	0.52
3:E:88:VAL:CG1	3:E:89:ARG:N	2.72	0.52
3:J:18:ASP:O	3:J:88:VAL:HG23	2.10	0.51
2:B:120:SER:HB3	2:B:122:PHE:CE2	2.45	0.51
1:F:11:LEU:N	1:F:11:LEU:HD23	2.25	0.51
1:A:155:GLN:HE21	1:A:158:ASN:ND2	2.09	0.51
2:B:82(C):LEU:HD13	2:B:86:ASP:HB3	1.93	0.51
1:F:121:SER:OG	2:G:122:PHE:HB3	2.10	0.51
1:F:192:TYR:O	1:F:208:SER:HB2	2.10	0.51
1:A:187:GLU:HA	1:A:211:ARG:NE	2.26	0.51
3:E:41:ARG:O	3:E:43:PRO:HD2	2.10	0.51
3:J:25:ARG:HA	3:J:79:GLY:O	2.11	0.51
2:G:178:LEU:C	2:G:178:LEU:CD2	2.84	0.51
2:B:29:PHE:CE2	2:B:76:ASN:HA	2.46	0.51
3:E:1(B):SER:C	3:E:2:GLN:N	2.66	0.51
2:G:30:SER:O	2:G:54:ARG:NH1	2.44	0.51
3:J:72:LEU:HD11	3:J:84:ARG:HH21	1.72	0.51
2:B:14:PRO:HD2	2:B:113:SER:OG	2.10	0.50
3:E:25:ARG:HA	3:E:79:GLY:O	2.11	0.50
1:F:32:TYR:CB	1:F:92:HIS:HB2	2.35	0.50
3:J:99:PHE:CD1	3:J:99:PHE:C	2.89	0.50
3:E:90:PHE:O	3:E:92:ASP:N	2.45	0.50
2:G:28:THR:HG23	2:G:32:PHE:HE1	1.77	0.50
1:A:7:SER:O	1:A:22:SER:HB3	2.12	0.50
2:B:182:VAL:HG13	2:B:182:VAL:O	2.12	0.50
1:F:4:LEU:HD23	1:F:23:CYS:SG	2.51	0.50
1:F:14:SER:N	1:F:17:GLU:OE1	2.36	0.50
1:A:163:VAL:HG12	1:A:164:THR:N	2.26	0.50
1:F:6:GLN:HG3	1:F:101:GLY:N	2.21	0.50
1:F:95:PRO:O	1:F:97:THR:HG23	2.12	0.50
1:F:138:ASN:HA	1:F:173:TYR:O	2.12	0.50
2:G:16:ALA:O	2:G:82(C):LEU:HD22	2.11	0.50
1:F:89:GLN:NE2	1:F:91:ASP:HA	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:VAL:HG13	1:F:140:TYR:O	2.12	0.50
2:G:83:THR:O	2:G:86:ASP:HB2	2.11	0.50
3:J:10:HIS:CE1	3:J:13:ARG:NH2	2.80	0.50
3:J:15:LEU:H	3:J:15:LEU:CD2	2.19	0.50
1:F:35:TRP:HB2	1:F:48:ILE:CG1	2.41	0.50
3:E:90:PHE:CD2	3:E:93:GLU:HB3	2.47	0.49
2:G:29:PHE:HB2	2:G:76:ASN:ND2	2.27	0.49
2:B:209:LYS:NZ	2:B:209:LYS:HA	2.27	0.49
2:B:200:HIS:CE1	2:B:202:PRO:HB2	2.48	0.49
3:E:117:ASP:OD1	3:E:118:PRO:HD2	2.12	0.49
1:F:176:SER:O	1:F:176:SER:OG	2.29	0.49
2:G:47:TRP:CH2	2:G:49:GLY:HA2	2.47	0.49
2:B:127:SER:N	2:B:130:SER:HB3	2.26	0.49
1:F:83:LEU:CD2	1:F:166:GLN:HB2	2.42	0.49
1:A:148:TRP:HZ2	1:A:177:SER:O	1.95	0.49
1:F:4:LEU:HB3	1:F:23:CYS:SG	2.51	0.49
2:G:34:ILE:O	2:G:50:GLU:HA	2.12	0.49
2:G:56:ARG:NH1	3:J:108:GLU:OE2	2.46	0.49
2:B:133:GLY:C	2:B:135:THR:H	2.21	0.49
2:B:171:GLN:NE2	2:B:177:SER:HB2	2.28	0.49
2:B:159:LEU:HD12	2:B:160:THR:H	1.78	0.49
3:E:21:GLU:C	3:E:22:LEU:HD23	2.38	0.49
1:A:79:GLN:CG	1:A:81:GLU:OE1	2.61	0.49
2:G:39:GLN:O	2:G:88:ALA:HB1	2.13	0.49
2:G:212:GLU:O	2:G:213:PRO:C	2.55	0.49
2:G:40:ARG:NH2	2:G:43:HIS:CD2	2.81	0.48
3:J:22:LEU:O	3:J:82:ALA:HA	2.13	0.48
1:A:95:PRO:O	1:A:97:THR:HG23	2.13	0.48
1:A:11:LEU:CD1	1:A:19:VAL:HG23	2.41	0.48
3:E:12:ILE:HD13	3:E:21:GLU:O	2.12	0.48
1:F:118:PHE:HB2	1:F:133:VAL:HB	1.94	0.48
1:A:116:PHE:CZ	2:B:132:SER:HB2	2.49	0.48
2:B:70:THR:HG22	3:J:44:PHE:CZ	2.48	0.48
2:B:100:ASN:OD1	2:B:100:ASN:N	2.46	0.48
2:G:29:PHE:CD2	2:G:76:ASN:HA	2.48	0.48
2:G:138:LEU:HD12	2:G:139:GLY:N	2.28	0.48
3:J:39:TRP:HA	3:J:97:THR:O	2.12	0.48
2:G:119:PRO:HG2	2:G:200:HIS:CB	2.44	0.48
2:G:171:GLN:NE2	2:G:177:SER:HB2	2.27	0.48
1:A:49:TYR:CD2	2:B:99:VAL:HG13	2.48	0.48
3:E:68:ARG:HG2	3:E:68:ARG:NH1	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:PRO:CG	2:G:104:GLY:O	2.62	0.48
1:A:30(A):ASN:HD22	3:E:53:ASN:ND2	2.10	0.48
1:F:185:ASP:O	1:F:189:HIS:ND1	2.47	0.48
2:G:133:GLY:C	2:G:135:THR:H	2.20	0.48
2:B:28:THR:HG23	2:B:32:PHE:HE1	1.79	0.48
2:G:29:PHE:CE2	2:G:76:ASN:HA	2.49	0.48
2:G:48:ILE:HG23	2:G:63:PHE:CG	2.49	0.48
3:J:6:ILE:HD11	3:J:27:SER:OG	2.14	0.48
2:G:97:THR:HG23	3:J:102:ASP:OD1	2.13	0.48
2:G:94:THR:HG23	2:G:95:GLY:N	2.29	0.47
2:B:26:GLY:O	2:B:27:TYR:HB3	2.13	0.47
2:B:178:LEU:C	2:B:178:LEU:CD2	2.88	0.47
2:B:150:VAL:HG22	2:B:200:HIS:HB2	1.95	0.47
3:E:99:PHE:CD1	3:E:99:PHE:C	2.93	0.47
1:A:11:LEU:HD23	1:A:11:LEU:H	1.78	0.47
1:A:29:LEU:O	1:A:31:ASN:HA	2.15	0.47
2:G:200:HIS:CE1	2:G:202:PRO:HB2	2.49	0.47
3:E:46:ARG:NH1	2:G:81:GLN:NE2	2.62	0.47
2:G:195:ILE:HG12	2:G:210:LYS:HA	1.97	0.47
1:A:136:LEU:HD12	1:A:136:LEU:N	2.29	0.47
2:B:34:ILE:O	2:B:50:GLU:HA	2.14	0.47
1:F:155:GLN:HE21	1:F:158:ASN:ND2	2.12	0.47
1:A:113:PRO:HG3	1:A:139:PHE:CB	2.44	0.47
1:A:15:ALA:HA	1:A:78:VAL:HG12	1.97	0.47
2:B:96:ASN:C	2:B:96:ASN:ND2	2.71	0.47
1:F:188:LYS:C	1:F:189:HIS:ND1	2.72	0.47
1:A:150:VAL:HG22	1:A:192:TYR:CD1	2.50	0.47
1:F:143:GLU:CD	1:F:143:GLU:N	2.72	0.47
2:B:54:ARG:NH2	3:E:107:GLU:HA	2.27	0.46
1:F:29:LEU:O	1:F:31:ASN:HA	2.14	0.46
2:G:153:SER:O	2:G:197:ASN:N	2.36	0.46
3:J:20:ALA:O	3:J:84:ARG:HA	2.15	0.46
1:A:132:VAL:HB	1:A:179:LEU:HB3	1.97	0.46
2:B:159:LEU:HD12	2:B:160:THR:N	2.30	0.46
1:F:30:LEU:HD11	1:F:30(E):GLN:HA	1.97	0.46
1:F:132:VAL:HG12	1:F:148:TRP:CH2	2.50	0.46
3:E:88:VAL:HG12	3:E:89:ARG:N	2.29	0.46
1:F:30(D):ASN:O	1:F:30(E):GLN:HB2	2.15	0.46
3:E:20:ALA:O	3:E:84:ARG:HA	2.15	0.46
1:F:186:TYR:HA	1:F:192:TYR:OH	2.15	0.46
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HD21	1:A:166:GLN:HB2	1.95	0.46
1:A:116:PHE:CE1	2:B:132:SER:HB2	2.50	0.46
1:A:143:GLU:CD	1:A:143:GLU:N	2.74	0.46
3:E:1(B):SER:HB2	3:E:2:GLN:CG	2.28	0.46
1:F:15:ALA:HA	1:F:78:VAL:HG12	1.98	0.46
1:F:19:VAL:CG1	1:F:78:VAL:HG23	2.43	0.46
1:A:2:ILE:HG12	1:A:27:GLN:CG	2.46	0.46
1:F:135:LEU:HD22	2:G:181:VAL:HG21	1.98	0.46
1:A:30(D):ASN:O	1:A:30(E):GLN:HB2	2.15	0.46
3:E:15:LEU:O	3:E:18:ASP:HB2	2.16	0.46
3:E:25:ARG:HH11	3:E:25:ARG:CG	2.19	0.46
3:J:65:TYR:O	3:J:68:ARG:HB2	2.16	0.46
1:A:138:ASN:HA	1:A:173:TYR:O	2.16	0.46
2:B:29:PHE:HB2	2:B:76:ASN:ND2	2.30	0.46
3:J:73:LYS:O	3:J:74:GLU:O	2.34	0.45
1:F:190:LYS:O	1:F:210:ASN:HA	2.17	0.45
2:G:13:LYS:CD	2:G:113:SER:HA	2.46	0.45
2:G:144:ASP:HB2	4:G:230:HOH:O	2.16	0.45
3:J:90:PHE:C	3:J:92:ASP:H	2.25	0.45
2:B:30:SER:O	2:B:54:ARG:NH1	2.49	0.45
2:B:96:ASN:ND2	2:B:99:VAL:N	2.62	0.45
2:B:157:GLY:C	2:B:159:LEU:N	2.74	0.45
3:E:22:LEU:O	3:E:82:ALA:HA	2.17	0.45
2:G:211:VAL:HG12	2:G:211:VAL:O	2.16	0.45
3:J:88:VAL:CG1	3:J:89:ARG:N	2.80	0.45
1:A:118:PHE:HA	1:A:119:PRO:HD3	1.80	0.45
2:B:84:SER:O	2:B:87:SER:HB2	2.17	0.45
3:J:41:ARG:O	3:J:43:PRO:CD	2.63	0.45
1:A:35:TRP:HB2	1:A:48:ILE:CG1	2.44	0.45
3:E:52:ARG:O	3:E:57:GLN:NE2	2.49	0.45
1:A:89:GLN:NE2	1:A:91:ASP:HA	2.31	0.45
2:B:80:MET:HE3	2:B:82:LEU:HD11	1.99	0.45
3:E:71:LEU:O	3:E:73:LYS:HG3	2.15	0.45
1:F:121:SER:O	1:F:124:GLN:N	2.41	0.45
1:A:48:ILE:HA	1:A:53:THR:O	2.17	0.45
1:A:61:ARG:HB2	1:A:76:SER:OG	2.17	0.45
1:A:118:PHE:HB2	1:A:133:VAL:HB	1.99	0.45
2:B:6:GLU:OE2	2:B:104:GLY:HA3	2.17	0.45
2:G:33:TRP:CD1	2:G:52:LEU:HD13	2.51	0.45
3:J:21:GLU:C	3:J:22:LEU:HD23	2.42	0.45
2:B:83:THR:N	2:B:86:ASP:OD1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:VAL:CG2	1:F:78:VAL:HG11	2.47	0.45
1:F:71:PHE:O	1:F:72:THR:CG2	2.65	0.45
2:G:14:PRO:HD3	2:G:112:SER:C	2.41	0.45
2:B:132:SER:O	2:B:135:THR:O	2.35	0.45
2:B:203:SER:OG	2:B:205:THR:OG1	2.26	0.45
2:G:119:PRO:HG3	2:G:145:TYR:HB3	1.96	0.45
2:G:171:GLN:NE2	2:G:177:SER:CB	2.80	0.45
1:A:33:LEU:HD22	1:A:71:PHE:CG	2.52	0.45
2:B:53:GLY:O	2:B:54:ARG:C	2.60	0.45
1:F:71:PHE:C	1:F:72:THR:HG23	2.42	0.45
2:G:11:LEU:HD22	2:G:147:PRO:HD3	1.98	0.45
1:A:132:VAL:HG12	1:A:148:TRP:CH2	2.52	0.44
2:B:169:VAL:HG13	4:B:239:HOH:O	2.16	0.44
2:G:66:LYS:NZ	2:G:82(B):SER:O	2.51	0.44
2:G:123:PRO:CG	2:G:209:LYS:HG2	2.47	0.44
1:F:36:TYR:HA	1:F:45:LYS:O	2.17	0.44
1:F:83:LEU:O	1:F:84:ALA:HB2	2.17	0.44
2:B:6:GLU:CA	2:B:105:GLN:HE22	2.30	0.44
1:F:48:ILE:HA	1:F:53:THR:O	2.17	0.44
2:G:151:THR:OG1	2:G:199:ASN:HB3	2.17	0.44
3:J:15:LEU:O	3:J:18:ASP:HB2	2.16	0.44
1:A:27:GLN:O	1:A:69:THR:HG22	2.18	0.44
1:F:190:LYS:O	1:F:210:ASN:CA	2.66	0.44
2:G:54:ARG:NH2	3:J:106:GLN:O	2.50	0.44
1:A:112:ALA:HA	1:A:113:PRO:HD3	1.77	0.44
2:B:94:THR:HG23	2:B:95:GLY:N	2.31	0.44
3:E:15:LEU:H	3:E:15:LEU:CD2	2.16	0.44
1:F:115:VAL:N	4:F:221:HOH:O	2.50	0.44
1:F:132:VAL:HB	1:F:179:LEU:HB3	2.00	0.44
3:J:31:ASN:HA	3:J:77:GLY:HA2	1.99	0.44
2:B:96:ASN:HD21	2:B:99:VAL:CG2	2.24	0.44
1:F:11:LEU:HD23	1:F:11:LEU:H	1.82	0.44
2:G:6:GLU:OE2	2:G:104:GLY:HA3	2.17	0.44
3:J:52:ARG:O	3:J:57:GLN:NE2	2.51	0.44
3:E:39:TRP:HA	3:E:97:THR:O	2.18	0.44
3:E:31:ASN:HA	3:E:77:GLY:HA2	1.99	0.44
1:F:142:ARG:NH1	1:F:142:ARG:CG	2.76	0.44
1:F:186:TYR:CE2	1:F:192:TYR:CE2	3.06	0.44
1:A:16:GLY:HA2	1:A:77:SER:OG	2.18	0.43
1:A:159:SER:HB3	1:A:179:LEU:HD13	1.99	0.43
2:B:96:ASN:HD22	2:B:99:VAL:H	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:LEU:HB2	1:F:43:PRO:CD	2.48	0.43
1:F:119:PRO:HA	1:F:120:PRO:HD3	1.92	0.43
1:A:30:LEU:HD11	1:A:30(E):GLN:HA	1.99	0.43
2:B:8:GLY:O	2:B:9:ALA:C	2.60	0.43
3:E:6:ILE:HD11	3:E:27:SER:OG	2.18	0.43
1:F:159:SER:HB3	1:F:179:LEU:HD13	1.99	0.43
2:G:100:ASN:OD1	2:G:100:ASN:N	2.44	0.43
2:G:101:PRO:HG2	2:G:102:TYR:CD2	2.54	0.43
1:A:115:VAL:O	1:A:207:LYS:HE3	2.19	0.43
1:A:142:ARG:NH1	1:A:142:ARG:CG	2.77	0.43
2:B:123:PRO:HB3	2:B:211:VAL:HG22	1.99	0.43
3:E:90:PHE:C	3:E:90:PHE:CD2	2.97	0.43
3:J:41:ARG:HH12	3:J:94:GLY:HA3	1.83	0.43
1:A:61:ARG:HH21	1:A:82:ASP:CG	2.25	0.43
1:A:135:LEU:HD22	2:B:181:VAL:HG11	2.01	0.43
1:A:192:TYR:O	1:A:208:SER:HB2	2.19	0.43
2:B:37:VAL:HG13	2:B:46:GLU:O	2.18	0.43
2:G:8:GLY:O	2:G:9:ALA:C	2.62	0.43
3:E:16:VAL:CG1	3:E:17:GLY:N	2.80	0.43
1:F:150:VAL:HG11	1:F:189:HIS:CD2	2.54	0.43
2:G:100(A):MET:N	2:G:101:PRO:CD	2.81	0.43
2:B:47:TRP:CH2	2:B:49:GLY:HA2	2.53	0.43
2:B:100(A):MET:N	2:B:101:PRO:CD	2.81	0.43
3:E:68:ARG:HH11	3:E:68:ARG:CG	2.23	0.43
2:G:96:ASN:C	2:G:96:ASN:ND2	2.67	0.43
3:J:25:ARG:NH1	3:J:25:ARG:CG	2.80	0.43
3:J:71:LEU:O	3:J:73:LYS:HG3	2.19	0.43
3:E:3:PHE:CD1	3:E:3:PHE:C	2.97	0.43
2:G:53:GLY:O	2:G:54:ARG:C	2.61	0.43
1:A:36:TYR:HA	1:A:45:LYS:O	2.19	0.42
1:A:187:GLU:HA	1:A:211:ARG:CD	2.49	0.42
2:B:40:ARG:HB3	2:B:88:ALA:HB2	2.01	0.42
2:B:123:PRO:HG3	2:B:209:LYS:HG2	2.00	0.42
3:E:68:ARG:O	3:E:86:GLN:OE1	2.37	0.42
1:F:35:TRP:CD1	1:F:48:ILE:CD1	3.02	0.42
2:G:157:GLY:C	2:G:159:LEU:N	2.77	0.42
3:J:8:PRO:HG3	3:J:23:PRO:HD2	2.00	0.42
1:A:186:TYR:CE1	1:A:192:TYR:CE2	3.07	0.42
2:B:82(C):LEU:HA	2:B:86:ASP:OD1	2.19	0.42
3:E:46:ARG:HD3	4:E:143:HOH:O	2.18	0.42
1:F:118:PHE:HA	1:F:119:PRO:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:30:LYS:HE3	3:J:35:MET:CE	2.49	0.42
1:A:48:ILE:HD11	1:A:73:LEU:HD13	2.01	0.42
1:A:83:LEU:O	1:A:84:ALA:HB2	2.19	0.42
1:F:19:VAL:CG1	1:F:75:ILE:HB	2.35	0.42
1:F:48:ILE:HD11	1:F:73:LEU:HD13	2.01	0.42
1:F:185:ASP:O	1:F:189:HIS:CE1	2.72	0.42
1:A:201:LEU:HD13	1:A:205:VAL:CG2	2.49	0.42
1:F:148:TRP:CD2	1:F:179:LEU:HD22	2.55	0.42
1:A:50:GLY:O	1:A:51:ALA:HB3	2.19	0.42
1:F:198:HIS:CG	1:F:199:GLN:N	2.87	0.42
1:A:148:TRP:CD2	1:A:179:LEU:HD22	2.54	0.42
1:A:155:GLN:CB	1:A:158:ASN:HD21	2.29	0.42
1:F:5:THR:O	1:F:5:THR:HG22	2.19	0.42
2:G:16:ALA:C	2:G:82(C):LEU:HD23	2.44	0.42
2:G:154:TRP:HA	2:G:195:ILE:O	2.20	0.42
1:A:186:TYR:O	1:A:211:ARG:HD3	2.19	0.42
2:B:151:THR:OG1	2:B:199:ASN:HB3	2.19	0.42
3:E:8:PRO:HG3	3:E:23:PRO:HD2	2.02	0.42
2:G:16:ALA:O	2:G:82(C):LEU:CD2	2.67	0.42
3:J:16:VAL:CG1	3:J:17:GLY:N	2.83	0.42
1:A:125:LEU:O	1:A:127:SER:N	2.53	0.42
2:B:170:LEU:HD12	2:B:170:LEU:HA	1.92	0.42
3:E:1(B):SER:CB	3:E:2:GLN:HG2	2.28	0.42
1:A:114:SER:HB3	1:A:137:ASN:HB3	2.01	0.42
2:B:19:GLU:HB2	4:B:240:HOH:O	2.20	0.42
1:F:136:LEU:N	1:F:136:LEU:CD1	2.83	0.42
2:B:4:LEU:HD12	2:B:4:LEU:N	2.35	0.41
2:B:70:THR:CG2	3:J:44:PHE:CE2	3.03	0.41
1:F:175:LEU:C	1:F:175:LEU:CD2	2.93	0.41
1:F:201:LEU:HD13	1:F:205:VAL:CG2	2.50	0.41
2:G:24:ALA:HB1	2:G:27:TYR:CE1	2.49	0.41
2:G:96:ASN:HD21	2:G:99:VAL:N	2.18	0.41
2:G:98:MET:C	3:J:103:HIS:ND1	2.78	0.41
1:A:39:LYS:HG3	1:A:84:ALA:HB2	2.02	0.41
1:F:122:ASP:O	1:F:125:LEU:N	2.52	0.41
1:F:159:SER:HB3	1:F:179:LEU:CD1	2.50	0.41
1:F:163:VAL:CG1	1:F:164:THR:N	2.83	0.41
2:G:119:PRO:CA	2:G:145:TYR:HB3	2.50	0.41
2:B:123:PRO:CG	2:B:209:LYS:HG2	2.50	0.41
2:G:6:GLU:CA	2:G:105:GLN:HE22	2.32	0.41
1:A:35:TRP:CE2	1:A:73:LEU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:90:PHE:C	3:E:90:PHE:HD2	2.28	0.41
2:G:47:TRP:CZ2	2:G:49:GLY:HA2	2.55	0.41
2:G:150:VAL:HG22	2:G:200:HIS:HB2	2.03	0.41
2:B:83:THR:CG2	2:B:84:SER:H	2.34	0.41
2:B:116:THR:H	2:B:116:THR:HG22	1.58	0.41
1:A:2:ILE:HG12	1:A:27:GLN:HB2	2.02	0.41
1:A:69:THR:C	1:A:70:ASP:OD2	2.64	0.41
2:G:153:SER:OG	2:G:197:ASN:HB2	2.21	0.41
1:A:66:GLY:HA3	1:A:71:PHE:HA	2.02	0.41
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.85	0.41
3:E:25:ARG:NH1	3:E:25:ARG:CG	2.79	0.41
1:A:160:GLN:HE22	2:B:171:GLN:HG2	1.86	0.41
1:A:198:HIS:CG	1:A:199:GLN:N	2.89	0.41
2:B:96:ASN:HD21	2:B:99:VAL:N	2.17	0.41
2:B:142:VAL:N	2:B:178:LEU:O	2.54	0.41
3:J:50:LEU:HD22	3:J:50:LEU:HA	1.84	0.41
2:B:193:THR:N	4:B:233:HOH:O	2.53	0.41
1:A:159:SER:HB3	1:A:179:LEU:CD1	2.51	0.40
3:E:76:ILE:C	3:E:78:GLU:H	2.27	0.40
1:F:150:VAL:HG22	1:F:192:TYR:CD1	2.56	0.40
2:G:12:VAL:HG12	2:G:13:LYS:N	2.36	0.40
1:A:119:PRO:HA	1:A:120:PRO:HD3	1.92	0.40
1:F:83:LEU:HD12	1:F:104:LEU:O	2.21	0.40
2:G:171:GLN:C	2:G:173:SER:N	2.79	0.40
1:A:110:VAL:HG12	1:A:111:ALA:N	2.36	0.40
2:B:154:TRP:CZ3	2:B:196:CYS:HB3	2.57	0.40
2:B:6:GLU:OE2	2:B:106:GLY:N	2.41	0.40
2:B:95:GLY:CA	2:B:101:PRO:HD2	2.51	0.40
3:E:2:GLN:HG3	3:E:2:GLN:O	2.22	0.40
1:F:35:TRP:CE2	1:F:73:LEU:HB2	2.56	0.40
1:F:89:GLN:HB2	1:F:98:PHE:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/241 (90%)	199 (92%)	17 (8%)	1 (0%)	24	60
1	F	214/241 (89%)	191 (89%)	20 (9%)	3 (1%)	9	36
2	B	219/252 (87%)	190 (87%)	25 (11%)	4 (2%)	6	31
2	G	210/252 (83%)	181 (86%)	25 (12%)	4 (2%)	6	30
3	E	119/139 (86%)	102 (86%)	11 (9%)	6 (5%)	1	10
3	J	116/139 (84%)	100 (86%)	10 (9%)	6 (5%)	1	9
All	All	1095/1264 (87%)	963 (88%)	108 (10%)	24 (2%)	5	26

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	74	GLU
1	F	122	ASP
2	B	168	ALA
2	B	202	PRO
3	E	31	ASN
3	E	103	HIS
1	F	138	ASN
2	G	168	ALA
1	A	138	ASN
3	E	42	SER
3	E	43	PRO
3	E	91	SER
2	G	202	PRO
3	J	31	ASN
3	J	42	SER
3	J	43	PRO
2	B	100(A)	MET
2	G	100(A)	MET
3	J	103	HIS
1	F	84	ALA
2	B	41	PRO
2	G	212	GLU
3	J	16	VAL
3	E	16	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/210 (91%)	173 (91%)	18 (9%)	8	32
1	F	189/210 (90%)	172 (91%)	17 (9%)	9	34
2	B	181/207 (87%)	154 (85%)	27 (15%)	3	15
2	G	177/207 (86%)	152 (86%)	25 (14%)	3	16
3	E	98/116 (84%)	82 (84%)	16 (16%)	2	12
3	J	97/116 (84%)	79 (81%)	18 (19%)	1	9
All	All	933/1066 (88%)	812 (87%)	121 (13%)	4	19

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	20	THR
1	A	42	LEU
1	A	60	ASP
1	A	63	THR
1	A	72	THR
1	A	78	VAL
1	A	79	GLN
1	A	81	GLU
1	A	90	ASN
1	A	92	HIS
1	A	93	SER
1	A	105	GLU
1	A	114	SER
1	A	135	LEU
1	A	143	GLU
1	A	161	GLU
1	A	175	LEU
2	B	3	LYS
2	B	19	GLU
2	B	20	ILE
2	B	23	LYS

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Mol	Chain	Res	Type
2	B	28	THR
2	B	56	ARG
2	B	74	SER
2	B	94	THR
2	B	96	ASN
2	B	99	VAL
2	B	100	ASN
2	B	100(A)	MET
2	B	116	THR
2	B	120	SER
2	B	126	PRO
2	B	132	SER
2	B	149	PRO
2	B	169	VAL
2	B	178	LEU
2	B	183	THR
2	B	192	GLN
2	B	193	THR
2	B	202	PRO
2	B	203	SER
2	B	204	ASN
2	B	209	LYS
2	B	212	GLU
3	E	12	ILE
3	E	15	LEU
3	E	19	GLU
3	E	24	CYS
3	E	25	ARG
3	E	37	VAL
3	E	42	SER
3	E	50	LEU
3	E	64	GLU
3	E	75	SER
3	E	87	ASN
3	E	89	ARG
3	E	93	GLU
3	E	98	CYS
3	E	101	ARG
3	E	114	LYS
1	F	1	ASP
1	F	13	VAL
1	F	19	VAL

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Mol	Chain	Res	Type
1	F	42	LEU
1	F	60	ASP
1	F	63	THR
1	F	78	VAL
1	F	79	GLN
1	F	90	ASN
1	F	92	HIS
1	F	93	SER
1	F	109	THR
1	F	135	LEU
1	F	143	GLU
1	F	161	GLU
1	F	189	HIS
1	F	210	ASN
2	G	3	LYS
2	G	19	GLU
2	G	20	ILE
2	G	23	LYS
2	G	28	THR
2	G	56	ARG
2	G	58	ASN
2	G	74	SER
2	G	94	THR
2	G	96	ASN
2	G	99	VAL
2	G	100	ASN
2	G	100(A)	MET
2	G	149	PRO
2	G	169	VAL
2	G	178	LEU
2	G	183	THR
2	G	192	GLN
2	G	193	THR
2	G	202	PRO
2	G	203	SER
2	G	204	ASN
2	G	209	LYS
2	G	211	VAL
2	G	212	GLU
3	J	13	ARG
3	J	15	LEU
3	J	19	GLU

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Mol	Chain	Res	Type
3	J	24	CYS
3	J	25	ARG
3	J	37	VAL
3	J	50	LEU
3	J	60	GLU
3	J	64	GLU
3	J	72	LEU
3	J	86	GLN
3	J	87	ASN
3	J	91	SER
3	J	93	GLU
3	J	98	CYS
3	J	101	ARG
3	J	114	LYS
3	J	117	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	27	GLN
1	A	30(D)	ASN
1	A	31	ASN
1	A	79	GLN
1	A	137	ASN
1	A	155	GLN
1	A	160	GLN
1	A	198	HIS
2	B	5	HIS
2	B	43	HIS
2	B	58	ASN
2	B	81	GLN
2	B	96	ASN
2	B	164	HIS
2	B	171	GLN
2	B	197	ASN
2	B	204	ASN
3	E	2	GLN
3	E	53	ASN
3	E	87	ASN
1	F	6	GLN
1	F	27	GLN

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Mol	Chain	Res	Type
1	F	30(D)	ASN
1	F	31	ASN
1	F	79	GLN
1	F	89	GLN
1	F	137	ASN
1	F	155	GLN
1	F	199	GLN
1	F	210	ASN
2	G	5	HIS
2	G	58	ASN
2	G	81	GLN
2	G	96	ASN
2	G	164	HIS
2	G	171	GLN
2	G	192	GLN
2	G	197	ASN
2	G	204	ASN
3	J	10	HIS
3	J	53	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	219/241 (90%)	-0.07	0	100	100	14, 32, 44, 51	8 (3%)
1	F	216/241 (89%)	-0.03	0	100	100	16, 34, 51, 62	8 (3%)
2	B	221/252 (87%)	0.03	3 (1%)	73	51	11, 32, 59, 71	8 (3%)
2	G	214/252 (84%)	0.13	4 (1%)	66	43	12, 35, 55, 66	7 (3%)
3	E	121/139 (87%)	-0.04	0	100	100	8, 30, 50, 66	5 (4%)
3	J	118/139 (84%)	-0.10	1 (0%)	82	64	12, 28, 44, 59	9 (7%)
All	All	1109/1264 (87%)	-0.00	8 (0%)	84	66	8, 32, 52, 71	45 (4%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	87	ASN	3.8
2	G	191	THR	3.4
2	G	133	GLY	2.6
2	B	130	SER	2.6
2	B	126	PRO	2.3
2	G	206	LYS	2.2
2	B	127	SER	2.1
2	G	54	ARG	2.1

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.