



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:34 PM UTC

PDB ID : 3EO1 / pdb_00003eo1
Title : Structure of the Fab Fragment of GC-1008 in Complex with Transforming Growth Factor-Beta 3
Authors : Gruetter, C.; Gruetter, M.G.
Deposited on : 2008-09-26
Resolution : 3.10 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

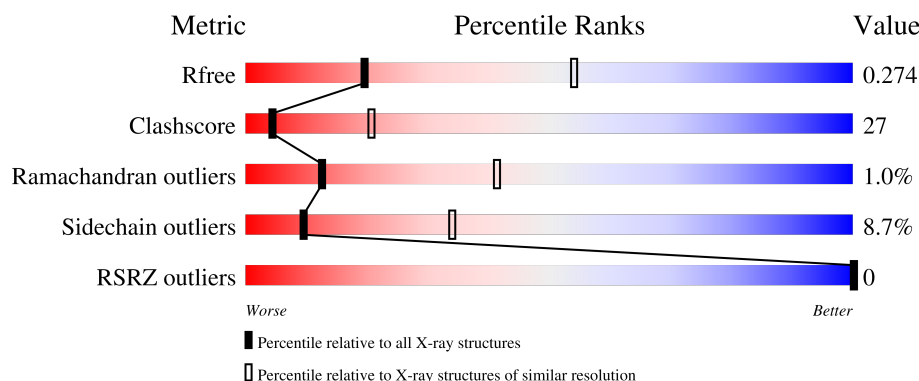
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	215	
1	D	215	
1	G	215	
1	J	215	
2	B	225	

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Mol	Chain	Length	Quality of chain
2	E	225	
2	H	225	
2	K	225	
3	C	112	
3	F	112	
3	I	112	
3	L	112	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16556 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 GC-1008 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1647	1028	280	334	5			
1	D	215	Total	C	N	O	S	0	0	0
			1647	1028	280	334	5			
1	G	215	Total	C	N	O	S	0	0	0
			1647	1028	280	334	5			
1	J	215	Total	C	N	O	S	0	0	0
			1647	1028	280	334	5			

- Molecule 2 is a protein called GC-1008 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1603	1009	263	323	8			
2	E	216	Total	C	N	O	S	0	0	0
			1603	1009	263	323	8			
2	H	216	Total	C	N	O	S	0	0	0
			1603	1009	263	323	8			
2	K	216	Total	C	N	O	S	0	0	0
			1603	1009	263	323	8			

- Molecule 3 is a protein called Transforming growth factor beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	112	Total	C	N	O	S	0	0	0
			889	564	148	167	10			
3	F	112	Total	C	N	O	S	0	0	0
			889	564	148	167	10			
3	I	112	Total	C	N	O	S	0	0	0
			889	564	148	167	10			
3	L	112	Total	C	N	O	S	0	0	0
			889	564	148	167	10			

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: GC-1008 Fab Light Chain

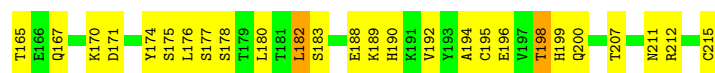


• Molecule 1: GC-1008 Fab Light Chain

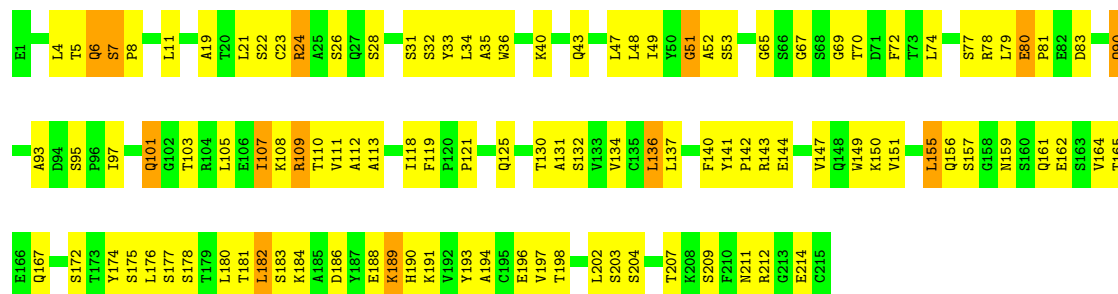


• Molecule 1: GC-1008 Fab Light Chain





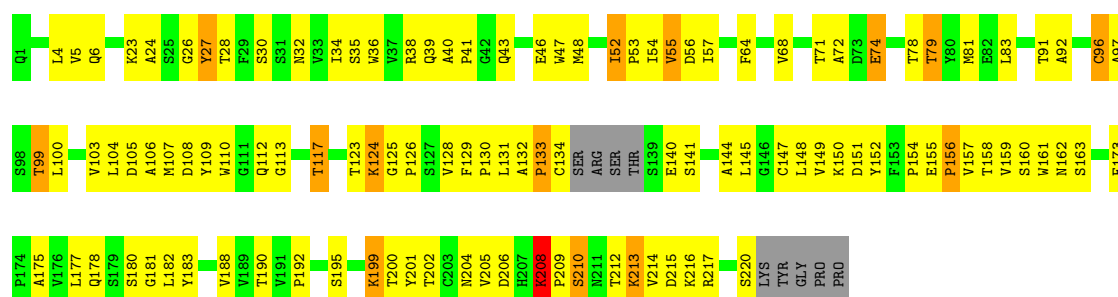
• Molecule 1: GC-1008 Fab Light Chain



• Molecule 2: GC-1008 Fab Heavy Chain

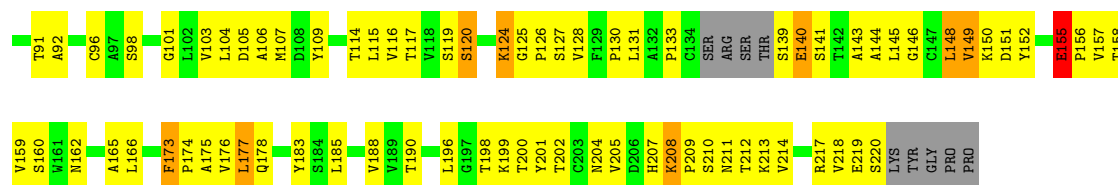


• Molecule 2: GC-1008 Fab Heavy Chain

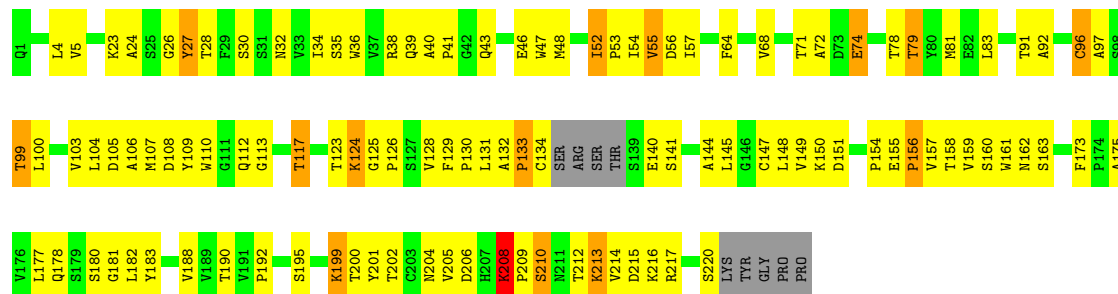


• Molecule 2: GC-1008 Fab Heavy Chain

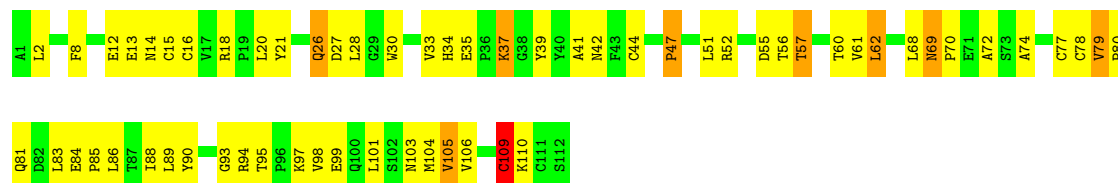




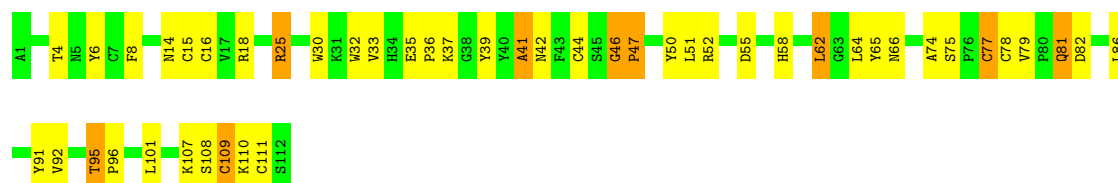
• Molecule 2: GC-1008 Fab Heavy Chain



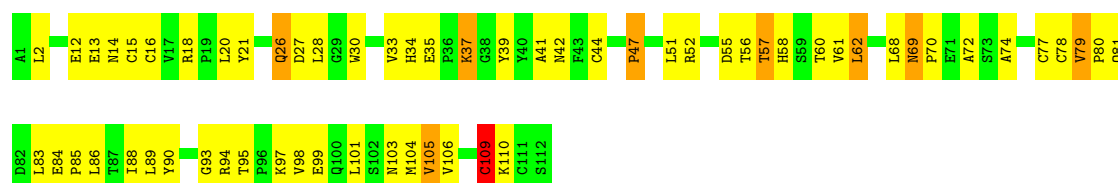
• Molecule 3: Transforming growth factor beta-3



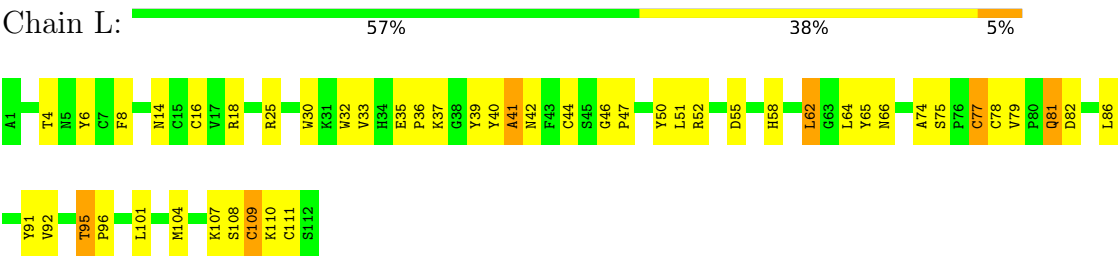
• Molecule 3: Transforming growth factor beta-3



• Molecule 3: Transforming growth factor beta-3



● Molecule 3: Transforming growth factor beta-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.04Å 149.13Å 149.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 3.10 35.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.00-3.10) 97.5 (35.00-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.255 , 0.279 0.247 , 0.274	Depositor DCC
R_{free} test set	724 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 111.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.027 for -h,l,k 0.388 for -l,-k,-h 0.027 for k,h,-l 0.019 for k,l,h 0.019 for l,h,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16556	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/1683	0.99	8/2286 (0.3%)
1	D	0.39	0/1683	0.98	6/2286 (0.3%)
1	G	0.43	0/1683	0.99	8/2286 (0.3%)
1	J	0.40	0/1683	0.98	6/2286 (0.3%)
2	B	0.43	0/1636	1.05	14/2231 (0.6%)
2	E	0.39	0/1636	1.06	11/2231 (0.5%)
2	H	0.43	0/1636	1.05	14/2231 (0.6%)
2	K	0.40	0/1636	1.06	11/2231 (0.5%)
3	C	0.56	0/914	1.09	10/1248 (0.8%)
3	F	0.52	0/914	1.03	4/1248 (0.3%)
3	I	0.56	0/914	1.09	10/1248 (0.8%)
3	L	0.52	0/914	1.03	4/1248 (0.3%)
All	All	0.44	0/16932	1.03	106/23060 (0.5%)

There are no bond length outliers.

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	27	TYR	N-CA-C	16.37	129.12	111.28
2	K	27	TYR	N-CA-C	16.36	129.11	111.28
1	A	171	ASP	N-CA-C	-8.38	97.16	110.14
1	G	171	ASP	N-CA-C	-8.37	97.17	110.14
3	F	41	ALA	N-CA-C	-8.09	96.38	109.96
3	L	41	ALA	N-CA-C	-8.08	96.38	109.96
2	H	120	SER	N-CA-C	-7.90	100.69	110.65
2	B	120	SER	N-CA-C	-7.90	100.70	110.65
2	B	106	ALA	N-CA-C	-7.19	100.17	110.59
2	H	106	ALA	N-CA-C	-7.18	100.17	110.59
1	D	77	SER	N-CA-C	7.13	118.94	111.03
1	J	77	SER	N-CA-C	7.12	118.94	111.03
2	B	148	LEU	N-CA-C	7.11	121.63	107.62
2	E	26	GLY	CA-C-N	7.11	129.81	120.28
2	E	26	GLY	C-N-CA	7.11	129.81	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	26	GLY	CA-C-N	7.11	129.80	120.28
2	K	26	GLY	C-N-CA	7.11	129.80	120.28
2	H	148	LEU	N-CA-C	7.10	121.60	107.62
2	B	157	VAL	N-CA-C	6.94	118.11	108.12
2	H	157	VAL	N-CA-C	6.91	118.08	108.12
2	H	207	HIS	N-CA-C	-6.81	98.14	108.96
2	B	207	HIS	N-CA-C	-6.78	98.18	108.96
1	A	51	GLY	N-CA-C	-6.78	97.12	113.18
1	G	51	GLY	N-CA-C	-6.76	97.15	113.18
3	C	93	GLY	N-CA-C	-6.60	105.60	111.67
3	I	93	GLY	N-CA-C	-6.59	105.61	111.67
3	C	79	VAL	N-CA-C	6.40	114.44	109.19
3	I	79	VAL	N-CA-C	6.38	114.42	109.19
2	B	26	GLY	N-CA-C	6.26	128.01	113.18
2	H	26	GLY	N-CA-C	6.25	128.00	113.18
3	I	72	ALA	N-CA-C	-6.23	105.62	113.72
2	K	141	SER	N-CA-C	6.22	118.32	110.24
3	C	72	ALA	N-CA-C	-6.21	105.65	113.72
2	K	173	PHE	N-CA-C	6.20	117.26	110.13
2	E	141	SER	N-CA-C	6.20	118.30	110.24
2	E	173	PHE	N-CA-C	6.16	117.22	110.13
2	E	52	ILE	CA-C-N	6.13	126.10	120.03
2	E	52	ILE	C-N-CA	6.13	126.10	120.03
2	H	149	VAL	N-CA-C	-6.13	101.68	109.58
3	C	37	LYS	N-CA-C	-6.12	105.81	113.28
3	I	37	LYS	N-CA-C	-6.12	105.82	113.28
2	B	149	VAL	N-CA-C	-6.11	101.70	109.58
3	L	46	GLY	CA-C-N	6.09	127.45	119.84
3	L	46	GLY	C-N-CA	6.09	127.45	119.84
2	K	52	ILE	CA-C-N	6.08	126.05	120.03
2	K	52	ILE	C-N-CA	6.08	126.05	120.03
3	I	26	GLN	N-CA-C	6.07	118.69	111.71
3	C	26	GLN	N-CA-C	6.05	118.67	111.71
3	F	46	GLY	CA-C-N	6.04	127.39	119.84
3	F	46	GLY	C-N-CA	6.04	127.39	119.84
1	A	211	ASN	N-CA-C	-6.01	101.87	110.59
1	G	211	ASN	N-CA-C	-6.01	101.88	110.59
1	D	51	GLY	N-CA-C	-5.93	99.12	113.18
1	G	3	VAL	N-CA-C	5.93	116.84	108.36
1	J	51	GLY	N-CA-C	-5.92	99.14	113.18
2	B	210	SER	N-CA-C	-5.92	102.55	110.55
2	H	210	SER	N-CA-C	-5.91	102.57	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	VAL	N-CA-C	5.91	116.81	108.36
2	K	210	SER	N-CA-C	-5.86	100.16	109.76
2	E	210	SER	N-CA-C	-5.84	100.18	109.76
2	H	155	GLU	N-CA-C	5.81	122.65	109.81
2	B	155	GLU	N-CA-C	5.80	122.63	109.81
1	D	134	VAL	N-CA-C	5.69	116.05	107.80
1	J	136	LEU	N-CA-C	5.68	117.38	107.49
1	J	134	VAL	N-CA-C	5.67	116.03	107.80
1	D	136	LEU	N-CA-C	5.67	117.36	107.49
3	C	57	THR	N-CA-C	-5.66	105.11	111.28
3	I	57	THR	N-CA-C	-5.65	105.12	111.28
1	D	203	SER	N-CA-C	-5.61	106.28	113.01
1	J	203	SER	N-CA-C	-5.60	106.29	113.01
2	H	199	LYS	N-CA-C	5.55	119.87	113.38
2	B	199	LYS	N-CA-C	5.52	119.84	113.38
1	A	156	GLN	N-CA-C	5.52	118.69	110.52
1	G	156	GLN	N-CA-C	5.51	118.68	110.52
3	C	109	CYS	N-CA-C	5.50	117.55	109.24
3	I	109	CYS	N-CA-C	5.49	117.53	109.24
2	H	173	PHE	N-CA-C	5.49	118.77	109.87
2	B	173	PHE	N-CA-C	5.49	118.76	109.87
3	C	105	VAL	N-CA-C	5.39	115.89	108.12
3	F	37	LYS	N-CA-C	-5.39	106.70	113.28
3	I	105	VAL	N-CA-C	5.38	115.87	108.12
3	C	69	ASN	CA-C-N	5.38	125.71	119.47
3	C	69	ASN	C-N-CA	5.38	125.71	119.47
3	I	69	ASN	CA-C-N	5.37	125.70	119.47
3	I	69	ASN	C-N-CA	5.37	125.70	119.47
3	L	37	LYS	N-CA-C	-5.36	106.74	113.28
1	A	127	LYS	N-CA-C	-5.36	106.72	113.20
1	G	127	LYS	N-CA-C	-5.36	106.72	113.20
2	H	208	LYS	CA-C-N	5.22	126.36	119.84
2	H	208	LYS	C-N-CA	5.22	126.36	119.84
2	B	208	LYS	CA-C-N	5.21	126.36	119.84
2	B	208	LYS	C-N-CA	5.21	126.36	119.84
1	D	159	ASN	N-CA-C	-5.10	105.35	112.03
1	J	159	ASN	N-CA-C	-5.08	105.37	112.03
1	G	32	SER	N-CA-C	5.06	116.48	109.54
2	H	208	LYS	N-CA-C	5.05	119.12	112.35
2	B	208	LYS	N-CA-C	5.05	119.12	112.35
1	A	32	SER	N-CA-C	5.04	116.45	109.54
2	E	24	ALA	N-CA-C	-5.04	99.57	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	24	ALA	N-CA-C	-5.03	99.58	108.23
2	E	208	LYS	CA-C-N	5.03	126.12	119.84
2	E	208	LYS	C-N-CA	5.03	126.12	119.84
2	K	208	LYS	CA-C-N	5.02	126.12	119.84
2	K	208	LYS	C-N-CA	5.02	126.12	119.84
1	A	29	LEU	N-CA-C	-5.01	101.93	109.85
1	G	29	LEU	N-CA-C	-5.00	101.94	109.85

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	1647	0	1597	96	1
1	D	1647	0	1597	98	0
1	G	1647	0	1597	94	0
1	J	1647	0	1597	101	1
2	B	1603	0	1584	95	0
2	E	1603	0	1584	104	0
2	H	1603	0	1584	91	0
2	K	1603	0	1584	100	0
3	C	889	0	850	47	0
3	F	889	0	850	33	0
3	I	889	0	850	49	0
3	L	889	0	850	33	0
All	All	16556	0	16124	870	1

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 27.

All (870) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ASP:HA	1:A:192:VAL:HB	1.43	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:HG3	1:A:77:SER:HA	1.46	0.98
1:G:152:ASP:HA	1:G:192:VAL:HB	1.43	0.96
1:G:18:ARG:HG3	1:G:77:SER:HA	1.46	0.95
2:E:91:THR:HG23	2:E:117:THR:HA	1.50	0.92
2:K:91:THR:HG23	2:K:117:THR:HA	1.50	0.90
3:C:39:TYR:CE2	3:C:41:ALA:HB2	2.07	0.90
3:I:39:TYR:CE2	3:I:41:ALA:HB2	2.07	0.88
2:B:81:MET:HE1	2:B:83:LEU:HB2	1.54	0.88
3:I:101:LEU:HD23	3:I:104:MET:HE2	1.57	0.87
3:C:101:LEU:HD23	3:C:104:MET:HE2	1.57	0.86
2:H:81:MET:HE1	2:H:83:LEU:HB2	1.54	0.85
1:J:5:THR:HA	1:J:101:GLN:HE22	1.43	0.84
1:D:5:THR:HA	1:D:101:GLN:HE22	1.43	0.84
2:B:68:VAL:HG13	2:B:81:MET:HE3	1.61	0.82
2:H:68:VAL:HG13	2:H:81:MET:HE3	1.61	0.81
2:B:91:THR:HG23	2:B:117:THR:HA	1.63	0.80
2:H:91:THR:HG23	2:H:117:THR:HA	1.63	0.80
3:F:39:TYR:CE2	3:F:41:ALA:HB2	2.16	0.80
3:L:39:TYR:CE2	3:L:41:ALA:HB2	2.16	0.80
2:H:23:LYS:HA	2:H:78:THR:HG22	1.64	0.80
1:A:162:GLU:HB3	1:A:178:SER:HA	1.65	0.79
2:B:23:LYS:HA	2:B:78:THR:HG22	1.64	0.79
2:E:162:ASN:HD21	2:E:201:TYR:HA	1.49	0.78
2:E:132:ALA:HB1	2:E:220:SER:HB2	1.66	0.78
3:I:14:ASN:HB2	3:I:52:ARG:NH1	1.99	0.78
2:E:163:SER:H	2:E:204:ASN:ND2	1.83	0.77
1:G:162:GLU:HB3	1:G:178:SER:HA	1.65	0.77
2:K:132:ALA:HB1	2:K:220:SER:HB2	1.66	0.77
3:C:14:ASN:HB2	3:C:52:ARG:NH1	1.99	0.77
1:A:121:PRO:HG2	1:A:126:LEU:HD11	1.67	0.76
2:K:162:ASN:HD21	2:K:201:TYR:HA	1.49	0.76
2:K:163:SER:H	2:K:204:ASN:ND2	1.82	0.76
1:G:121:PRO:HG2	1:G:126:LEU:HD11	1.67	0.76
2:B:201:TYR:HB2	2:B:217:ARG:HG2	1.69	0.75
1:G:20:THR:HG23	1:G:75:THR:HG22	1.69	0.75
3:L:82:ASP:HB2	3:L:108:SER:OG	1.87	0.75
2:H:201:TYR:HB2	2:H:217:ARG:HG2	1.69	0.75
3:F:82:ASP:HB2	3:F:108:SER:OG	1.87	0.74
1:A:34:LEU:HD13	1:A:35:ALA:N	2.04	0.73
1:A:20:THR:HG23	1:A:75:THR:HG22	1.69	0.73
1:G:34:LEU:HD13	1:G:35:ALA:N	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:18:ARG:O	3:I:42:ASN:HB3	1.89	0.72
2:K:112:GLN:HG2	2:K:113:GLY:N	2.05	0.72
1:G:136:LEU:HD13	2:H:188:VAL:HG11	1.71	0.72
3:I:51:LEU:HD22	2:K:74:GLU:HB2	1.70	0.72
1:J:136:LEU:HD22	2:K:188:VAL:HG11	1.72	0.71
1:A:136:LEU:HD13	2:B:188:VAL:HG11	1.71	0.71
1:D:136:LEU:HD22	2:E:188:VAL:HG11	1.72	0.71
3:C:18:ARG:O	3:C:42:ASN:HB3	1.89	0.71
1:J:176:LEU:HD23	1:J:177:SER:N	2.06	0.71
3:C:51:LEU:HD22	2:E:74:GLU:HB2	1.70	0.71
1:D:176:LEU:HD23	1:D:177:SER:N	2.06	0.70
1:J:33:TYR:HB3	1:J:93:ALA:HB2	1.73	0.70
2:K:39:GLN:O	2:K:92:ALA:HB1	1.91	0.70
2:E:39:GLN:O	2:E:92:ALA:HB1	1.91	0.70
2:E:130:PRO:HD3	2:E:216:LYS:HE2	1.74	0.69
1:A:136:LEU:HD11	2:B:188:VAL:HG21	1.74	0.69
2:E:112:GLN:HG2	2:E:113:GLY:N	2.05	0.69
2:K:130:PRO:HD3	2:K:216:LYS:HE2	1.74	0.69
2:H:54:ILE:HD13	2:H:74:GLU:HG2	1.74	0.69
2:B:126:PRO:HD2	2:B:212:THR:HG21	1.73	0.69
2:H:126:PRO:HD2	2:H:212:THR:HG21	1.73	0.69
2:B:54:ILE:HD13	2:B:74:GLU:HG2	1.74	0.69
3:C:12:GLU:HG2	3:C:52:ARG:HH22	1.58	0.69
1:J:109:ARG:HG2	1:J:172:SER:HB2	1.75	0.69
1:D:33:TYR:HB3	1:D:93:ALA:HB2	1.73	0.68
1:A:161:GLN:HE22	2:B:178:GLN:HA	1.58	0.68
1:D:109:ARG:HG2	1:D:172:SER:HB2	1.75	0.68
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.29	0.68
1:G:136:LEU:HD11	2:H:188:VAL:HG21	1.74	0.68
2:B:36:TRP:CE2	2:B:81:MET:HB2	2.29	0.67
1:A:151:VAL:HG12	1:A:156:GLN:HE22	1.59	0.67
1:G:161:GLN:HE22	2:H:178:GLN:HA	1.58	0.67
1:A:118:ILE:HD11	1:A:195:CYS:HB2	1.76	0.67
2:E:155:GLU:O	2:E:157:VAL:HG22	1.94	0.67
1:A:140:PHE:CE1	1:A:143:ARG:HA	2.30	0.67
1:G:118:ILE:HD11	1:G:195:CYS:HB2	1.76	0.67
1:G:151:VAL:HG12	1:G:156:GLN:HE22	1.59	0.67
3:I:12:GLU:HG2	3:I:52:ARG:HH22	1.58	0.67
1:G:140:PHE:CE1	1:G:143:ARG:HA	2.30	0.66
2:K:155:GLU:O	2:K:157:VAL:HG22	1.94	0.66
1:D:188:GLU:HA	1:D:212:ARG:HH12	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:188:GLU:HA	1:J:212:ARG:HH12	1.60	0.66
1:D:32:SER:HA	1:D:51:GLY:HA3	1.79	0.65
2:H:219:GLU:HG2	2:H:220:SER:H	1.61	0.65
2:K:72:ALA:HA	2:K:79:THR:HA	1.77	0.65
2:B:145:LEU:HB3	2:B:218:VAL:HG21	1.78	0.65
1:J:19:ALA:HB2	1:J:79:LEU:HD11	1.78	0.65
1:A:11:LEU:O	1:A:105:LEU:HD12	1.96	0.65
2:B:219:GLU:HG2	2:B:220:SER:H	1.61	0.65
3:C:80:PRO:HB2	3:C:83:LEU:HD11	1.78	0.65
1:D:186:ASP:HA	1:D:189:LYS:HD2	1.79	0.65
2:E:72:ALA:HA	2:E:79:THR:HA	1.77	0.65
3:I:83:LEU:HD23	3:I:103:ASN:HB3	1.78	0.65
1:D:19:ALA:HB2	1:D:79:LEU:HD11	1.78	0.65
2:B:162:ASN:HA	2:B:202:THR:HB	1.79	0.65
3:C:83:LEU:HD23	3:C:103:ASN:HB3	1.78	0.65
3:F:39:TYR:CZ	3:F:41:ALA:HB2	2.32	0.65
3:I:80:PRO:HB2	3:I:83:LEU:HD11	1.78	0.65
1:J:32:SER:HA	1:J:51:GLY:HA3	1.79	0.64
1:G:3:VAL:HG22	1:G:26:SER:HB3	1.79	0.64
1:G:11:LEU:O	1:G:105:LEU:HD12	1.97	0.64
2:H:52:ILE:HD12	2:H:57:ILE:HD11	1.80	0.64
2:B:52:ILE:HD12	2:B:57:ILE:HD11	1.80	0.64
2:H:145:LEU:HB3	2:H:218:VAL:HG21	1.78	0.64
2:K:124:LYS:HD3	2:K:125:GLY:N	2.13	0.64
2:H:162:ASN:HA	2:H:202:THR:HB	1.79	0.64
1:J:141:TYR:CD2	1:J:142:PRO:HA	2.33	0.64
1:J:189:LYS:HD3	1:J:190:HIS:ND1	2.13	0.64
3:L:39:TYR:CZ	3:L:41:ALA:HB2	2.32	0.64
1:D:141:TYR:CD2	1:D:142:PRO:HA	2.33	0.63
2:K:23:LYS:HA	2:K:78:THR:HG22	1.79	0.63
1:D:189:LYS:HD3	1:D:190:HIS:ND1	2.13	0.63
2:E:23:LYS:HA	2:E:78:THR:HG22	1.79	0.63
2:E:124:LYS:HD3	2:E:125:GLY:N	2.13	0.63
1:J:186:ASP:HA	1:J:189:LYS:HD2	1.79	0.63
1:A:115:SER:HB2	1:A:138:ASN:HB3	1.80	0.63
1:G:48:LEU:C	1:G:49:ILE:HD12	2.23	0.63
3:I:62:LEU:HD12	3:I:74:ALA:O	1.99	0.63
2:K:100:LEU:HG	2:K:106:ALA:O	1.99	0.63
1:D:24:ARG:HH11	1:D:24:ARG:HB3	1.64	0.63
2:E:133:PRO:HG2	2:E:134:CYS:H	1.63	0.63
2:E:100:LEU:HG	2:E:106:ALA:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:VAL:HG22	1:A:26:SER:HB3	1.80	0.63
2:E:99:THR:HA	2:E:107:MET:HA	1.79	0.63
3:F:81:GLN:HG2	3:F:110:LYS:HD3	1.81	0.63
2:K:99:THR:HA	2:K:107:MET:HA	1.79	0.63
2:B:219:GLU:HG2	2:B:220:SER:N	2.15	0.62
1:G:115:SER:HB2	1:G:138:ASN:HB3	1.81	0.62
1:G:188:GLU:HA	1:G:212:ARG:HH12	1.65	0.62
1:A:48:LEU:C	1:A:49:ILE:HD12	2.23	0.62
1:G:176:LEU:HD23	1:G:177:SER:N	2.14	0.62
1:J:24:ARG:HH11	1:J:24:ARG:HB3	1.64	0.62
3:L:81:GLN:HG2	3:L:110:LYS:HD3	1.81	0.62
3:C:62:LEU:HD12	3:C:74:ALA:O	1.99	0.62
1:A:106:GLU:HG3	1:A:174:TYR:OH	2.00	0.62
2:K:133:PRO:HG2	2:K:134:CYS:H	1.63	0.61
1:A:137:LEU:HD12	1:A:176:LEU:HD22	1.82	0.61
1:A:176:LEU:HD23	1:A:177:SER:N	2.14	0.61
3:C:80:PRO:HB2	3:C:83:LEU:CD1	2.31	0.61
2:H:219:GLU:HG2	2:H:220:SER:N	2.15	0.61
1:A:188:GLU:HA	1:A:212:ARG:HH12	1.65	0.61
1:J:155:LEU:HD13	1:J:156:GLN:N	2.15	0.61
1:D:155:LEU:HD13	1:D:156:GLN:N	2.15	0.61
3:F:91:TYR:CE2	3:F:96:PRO:HG3	2.36	0.60
1:G:106:GLU:HG3	1:G:174:TYR:OH	2.00	0.60
1:G:109:ARG:HD3	1:G:110:THR:O	2.01	0.60
3:L:91:TYR:CE2	3:L:96:PRO:HG3	2.36	0.60
1:G:137:LEU:HD12	1:G:176:LEU:HD22	1.82	0.60
2:H:5:VAL:HB	2:H:23:LYS:HB3	1.84	0.60
3:I:14:ASN:HB2	3:I:52:ARG:HH11	1.65	0.60
1:G:143:ARG:HB3	1:G:174:TYR:CD2	2.37	0.60
2:B:155:GLU:HB2	2:B:183:TYR:CE2	2.37	0.60
3:I:80:PRO:HB2	3:I:83:LEU:CD1	2.31	0.60
1:J:188:GLU:C	1:J:212:ARG:HH22	2.09	0.60
1:A:109:ARG:HD3	1:A:110:THR:O	2.01	0.60
2:E:23:LYS:HD2	2:E:78:THR:CG2	2.32	0.59
3:C:14:ASN:HB2	3:C:52:ARG:HH11	1.64	0.59
1:D:8:PRO:HD2	1:D:11:LEU:HD12	1.84	0.59
1:D:188:GLU:C	1:D:212:ARG:HH22	2.09	0.59
1:G:119:PHE:HB2	1:G:134:VAL:HB	1.84	0.59
2:H:155:GLU:HB2	2:H:183:TYR:CE2	2.37	0.59
1:A:143:ARG:HB3	1:A:174:TYR:CD2	2.37	0.59
1:J:8:PRO:HD2	1:J:11:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:162:GLU:HB3	1:J:178:SER:HB2	1.85	0.59
2:E:30:SER:OG	2:E:54:ILE:HD11	2.03	0.59
3:I:68:LEU:C	3:I:70:PRO:HD3	2.28	0.59
1:A:159:ASN:O	1:A:180:LEU:HD12	2.03	0.58
2:B:5:VAL:HB	2:B:23:LYS:HB3	1.84	0.58
3:C:68:LEU:C	3:C:70:PRO:HD3	2.28	0.58
2:H:33:VAL:HG12	2:H:52:ILE:HG12	1.85	0.58
2:E:52:ILE:HD11	2:E:103:VAL:HG22	1.86	0.58
1:D:150:LYS:NZ	1:D:196:GLU:HG3	2.19	0.58
1:G:55:ARG:HG2	1:G:59:ILE:HB	1.86	0.58
1:J:150:LYS:NZ	1:J:196:GLU:HG3	2.19	0.58
2:K:23:LYS:HD2	2:K:78:THR:CG2	2.32	0.58
1:D:109:ARG:HD3	1:D:110:THR:O	2.03	0.58
2:E:133:PRO:HD3	2:E:145:LEU:HD22	1.86	0.58
1:J:109:ARG:HD3	1:J:110:THR:O	2.03	0.58
2:K:52:ILE:HD11	2:K:103:VAL:HG22	1.86	0.58
2:K:133:PRO:HD3	2:K:145:LEU:HD22	1.86	0.58
2:K:30:SER:OG	2:K:54:ILE:HD11	2.03	0.58
1:J:40:LYS:HB2	1:J:43:GLN:OE1	2.04	0.58
1:J:121:PRO:HB2	1:J:131:ALA:HB3	1.86	0.58
2:E:103:VAL:HG12	2:E:104:LEU:CD1	2.34	0.58
1:G:159:ASN:O	1:G:180:LEU:HD12	2.03	0.58
3:I:2:LEU:HD11	3:I:52:ARG:HE	1.69	0.58
2:K:202:THR:HA	2:K:216:LYS:O	2.04	0.58
1:A:119:PHE:HB2	1:A:134:VAL:HB	1.84	0.57
1:A:146:LYS:HG3	1:A:198:THR:HG23	1.86	0.57
1:J:97:ILE:HD11	2:K:104:LEU:HG	1.84	0.57
2:E:126:PRO:HD2	2:E:212:THR:HG21	1.86	0.57
2:B:33:VAL:HG12	2:B:52:ILE:HG12	1.85	0.57
3:C:27:ASP:O	3:C:28:LEU:HD23	2.04	0.57
1:D:40:LYS:HB2	1:D:43:GLN:OE1	2.04	0.57
1:D:97:ILE:HD11	2:E:104:LEU:HG	1.85	0.57
2:H:39:GLN:O	2:H:92:ALA:HB1	2.05	0.57
1:D:162:GLU:HB3	1:D:178:SER:HB2	1.85	0.57
3:L:79:VAL:C	3:L:109:CYS:SG	2.88	0.57
2:B:29:PHE:HZ	2:B:72:ALA:HB1	1.70	0.57
1:D:32:SER:HA	1:D:51:GLY:CA	2.35	0.57
1:D:150:LYS:HZ1	1:D:196:GLU:HG3	1.70	0.57
1:J:150:LYS:HZ1	1:J:196:GLU:HG3	1.69	0.57
2:K:148:LEU:HD12	2:K:149:VAL:N	2.20	0.57
3:C:79:VAL:C	3:C:109:CYS:SG	2.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:PRO:HB2	1:D:131:ALA:HB3	1.86	0.57
1:D:130:THR:HB	1:D:183:SER:HA	1.86	0.57
3:I:79:VAL:C	3:I:109:CYS:SG	2.88	0.57
1:J:196:GLU:HA	1:J:207:THR:HG23	1.87	0.57
1:D:95:SER:HB2	2:E:104:LEU:HD21	1.87	0.57
1:G:146:LYS:HG3	1:G:198:THR:HG23	1.86	0.57
3:I:27:ASP:O	3:I:28:LEU:HD23	2.04	0.57
1:A:119:PHE:HE2	2:B:146:GLY:H	1.53	0.56
1:J:32:SER:HA	1:J:51:GLY:CA	2.35	0.56
1:A:55:ARG:HG2	1:A:59:ILE:HB	1.86	0.56
3:F:79:VAL:C	3:F:109:CYS:SG	2.88	0.56
2:B:39:GLN:O	2:B:92:ALA:HB1	2.05	0.56
1:D:151:VAL:HG13	1:D:193:TYR:HE2	1.70	0.56
1:G:38:GLN:HB2	1:G:87:TYR:CE2	2.40	0.56
2:K:126:PRO:HD2	2:K:212:THR:HG21	1.86	0.56
2:B:6:GLN:HA	2:B:21:SER:O	2.05	0.56
1:J:95:SER:HB2	2:K:104:LEU:HD21	1.87	0.56
1:J:130:THR:HB	1:J:183:SER:HA	1.86	0.56
1:D:34:LEU:HD22	1:D:90:GLN:O	2.06	0.56
1:D:196:GLU:HA	1:D:207:THR:HG23	1.87	0.56
2:E:148:LEU:HD12	2:E:149:VAL:N	2.20	0.56
2:E:202:THR:HA	2:E:216:LYS:O	2.04	0.56
2:H:29:PHE:HZ	2:H:72:ALA:HB1	1.70	0.56
3:I:60:THR:HG21	2:K:54:ILE:HD12	1.88	0.56
1:J:130:THR:HG21	1:J:184:LYS:N	2.21	0.56
2:K:103:VAL:HG12	2:K:104:LEU:CD1	2.34	0.56
1:J:4:LEU:HD23	1:J:23:CYS:SG	2.45	0.56
1:J:34:LEU:HD22	1:J:90:GLN:O	2.06	0.56
3:C:2:LEU:HD11	3:C:52:ARG:HE	1.69	0.56
1:G:36:TRP:CG	1:G:74:LEU:HD13	2.41	0.56
1:D:4:LEU:HD23	1:D:23:CYS:SG	2.45	0.55
1:D:130:THR:HG21	1:D:184:LYS:N	2.21	0.55
3:L:77:CYS:O	3:L:111:CYS:HA	2.07	0.55
1:G:50:TYR:O	1:G:54:SER:HB3	2.06	0.55
2:B:51:VAL:HG23	2:B:58:ALA:HB2	1.89	0.55
1:D:97:ILE:HB	2:E:47:TRP:CG	2.42	0.55
3:F:77:CYS:O	3:F:111:CYS:HA	2.06	0.55
2:H:6:GLN:HA	2:H:21:SER:O	2.05	0.55
1:G:165:THR:HG22	1:G:175:SER:H	1.70	0.55
2:K:36:TRP:CE2	2:K:81:MET:HB2	2.42	0.55
2:E:150:LYS:HG3	2:E:151:ASP:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:36:TRP:CZ3	2:E:96:CYS:HB2	2.42	0.55
2:H:51:VAL:HG23	2:H:58:ALA:HB2	1.89	0.55
2:H:126:PRO:HB2	2:H:149:VAL:HG13	1.88	0.55
1:J:151:VAL:HG13	1:J:193:TYR:HE2	1.70	0.55
2:K:150:LYS:HG3	2:K:151:ASP:N	2.21	0.55
1:A:36:TRP:CG	1:A:74:LEU:HD13	2.41	0.55
1:A:38:GLN:HB2	1:A:87:TYR:CE2	2.40	0.55
1:J:97:ILE:HB	2:K:47:TRP:CG	2.42	0.55
1:A:155:LEU:HD12	1:A:155:LEU:H	1.72	0.55
2:B:126:PRO:HB2	2:B:149:VAL:HG13	1.88	0.55
2:K:36:TRP:CZ3	2:K:96:CYS:HB2	2.42	0.55
2:K:41:PRO:O	2:K:43:GLN:HG2	2.06	0.55
2:B:39:GLN:C	2:B:92:ALA:HB1	2.32	0.55
1:A:165:THR:HG22	1:A:175:SER:H	1.70	0.54
2:B:33:VAL:CG1	2:B:52:ILE:HG12	2.37	0.54
2:B:128:VAL:HG21	2:B:214:VAL:HG11	1.89	0.54
2:H:57:ILE:O	2:H:57:ILE:HG13	2.07	0.54
2:K:154:PRO:HG2	2:K:156:PRO:HD2	1.89	0.54
2:E:154:PRO:HG2	2:E:156:PRO:HD2	1.89	0.54
1:G:119:PHE:HE2	2:H:146:GLY:H	1.53	0.54
2:B:162:ASN:OD1	2:B:200:THR:HG22	2.06	0.54
2:E:144:ALA:C	2:E:145:LEU:HD23	2.33	0.54
2:H:33:VAL:CG1	2:H:52:ILE:HG12	2.37	0.54
2:H:128:VAL:HG21	2:H:214:VAL:HG11	1.89	0.54
2:H:162:ASN:OD1	2:H:200:THR:HG22	2.06	0.54
1:J:140:PHE:CE1	1:J:143:ARG:HA	2.43	0.54
1:A:50:TYR:O	1:A:54:SER:HB3	2.06	0.54
3:C:60:THR:HG21	2:E:54:ILE:HD12	1.88	0.54
1:G:155:LEU:H	1:G:155:LEU:HD12	1.72	0.54
2:K:144:ALA:C	2:K:145:LEU:HD23	2.33	0.54
3:I:89:LEU:HD13	3:I:98:VAL:HG22	1.89	0.54
2:B:33:VAL:HG12	2:B:52:ILE:HA	1.89	0.54
3:C:39:TYR:CZ	3:C:41:ALA:HB2	2.43	0.54
1:D:140:PHE:CE1	1:D:143:ARG:HA	2.43	0.54
2:E:41:PRO:O	2:E:43:GLN:HG2	2.06	0.54
2:E:36:TRP:CE2	2:E:81:MET:HB2	2.42	0.54
2:H:33:VAL:HA	2:H:53:PRO:HD3	1.90	0.54
3:I:39:TYR:CZ	3:I:41:ALA:HB2	2.43	0.54
1:J:6:GLN:HA	1:J:22:SER:O	2.08	0.53
2:B:162:ASN:HB2	2:B:165:ALA:HB3	1.90	0.53
2:H:39:GLN:C	2:H:92:ALA:HB1	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:GLU:OE2	3:C:37:LYS:HE2	2.08	0.53
2:B:175:ALA:HB2	2:B:185:LEU:HD23	1.90	0.53
3:C:89:LEU:HD13	3:C:98:VAL:HG22	1.89	0.53
1:D:6:GLN:HA	1:D:22:SER:O	2.08	0.53
1:J:181:THR:O	1:J:182:LEU:HD22	2.09	0.53
2:E:144:ALA:CB	2:E:190:THR:HA	2.39	0.53
1:J:118:ILE:HG22	1:J:119:PHE:N	2.24	0.53
2:K:144:ALA:CB	2:K:190:THR:HA	2.39	0.53
2:B:57:ILE:HG13	2:B:57:ILE:O	2.07	0.53
2:H:33:VAL:HG12	2:H:52:ILE:HA	1.89	0.53
2:H:162:ASN:HB2	2:H:165:ALA:HB3	1.90	0.53
3:I:55:ASP:HB2	3:I:110:LYS:HD2	1.90	0.53
1:D:7:SER:HA	1:D:8:PRO:C	2.34	0.53
1:D:118:ILE:HG22	1:D:119:PHE:N	2.23	0.53
2:H:159:VAL:HG22	2:H:205:VAL:HG13	1.91	0.53
3:C:55:ASP:HB2	3:C:110:LYS:HD2	1.89	0.52
1:G:151:VAL:HG13	1:G:154:ALA:HB3	1.91	0.52
2:K:36:TRP:CH2	2:K:96:CYS:HB2	2.45	0.52
1:A:149:TRP:HB2	1:A:156:GLN:HG3	1.92	0.52
3:I:35:GLU:OE2	3:I:37:LYS:HE2	2.08	0.52
2:E:36:TRP:CH2	2:E:96:CYS:HB2	2.45	0.52
1:J:7:SER:HA	1:J:8:PRO:C	2.34	0.52
1:J:49:ILE:HD12	1:J:74:LEU:HD13	1.92	0.52
3:F:55:ASP:HB2	3:F:110:LYS:HD2	1.92	0.52
2:H:17:SER:HB2	2:H:84:SER:HA	1.92	0.52
1:J:21:LEU:HD11	1:J:103:THR:HB	1.91	0.52
2:B:33:VAL:HA	2:B:53:PRO:HD3	1.90	0.52
2:B:155:GLU:OE1	2:B:175:ALA:HB3	2.10	0.52
1:D:147:VAL:HG13	1:D:197:VAL:HG12	1.92	0.52
3:L:55:ASP:HB2	3:L:110:LYS:HD2	1.92	0.52
2:H:155:GLU:OE1	2:H:175:ALA:HB3	2.10	0.52
1:D:181:THR:O	1:D:182:LEU:HD22	2.09	0.52
1:A:37:TYR:HH	2:B:107:MET:H	1.58	0.52
1:A:182:LEU:HD13	1:A:183:SER:N	2.24	0.52
1:G:182:LEU:HD13	1:G:183:SER:N	2.24	0.52
1:J:141:TYR:CD1	1:J:142:PRO:HG3	2.45	0.52
1:J:119:PHE:CD1	2:K:131:LEU:HB3	2.45	0.52
1:D:21:LEU:HD11	1:D:103:THR:HB	1.91	0.51
1:D:119:PHE:CD1	2:E:131:LEU:HB3	2.45	0.51
2:K:199:LYS:HZ3	2:K:200:THR:HG22	1.75	0.51
2:B:159:VAL:HG22	2:B:205:VAL:HG13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:TYR:CD1	1:D:142:PRO:HG3	2.45	0.51
2:E:144:ALA:HB2	2:E:190:THR:HA	1.92	0.51
2:E:158:THR:OG1	2:E:206:ASP:HB3	2.11	0.51
1:G:149:TRP:HB2	1:G:156:GLN:HG3	1.92	0.51
2:K:144:ALA:HB2	2:K:190:THR:HA	1.92	0.51
1:A:142:PRO:O	1:A:143:ARG:HG2	2.10	0.51
3:C:8:PHE:HE2	3:L:40:TYR:HE1	1.56	0.51
1:D:191:LYS:HE2	1:D:211:ASN:HB3	1.93	0.51
1:G:142:PRO:O	1:G:143:ARG:HG2	2.10	0.51
2:H:175:ALA:HB2	2:H:185:LEU:HD23	1.90	0.51
3:F:92:VAL:O	3:F:95:THR:HG23	2.11	0.51
2:K:40:ALA:HB3	2:K:43:GLN:HB2	1.92	0.51
1:G:12:SER:HB3	1:G:106:GLU:CD	2.36	0.51
1:G:141:TYR:CE1	1:G:142:PRO:HG3	2.46	0.51
3:I:57:THR:HG23	2:K:54:ILE:HG22	1.93	0.51
1:A:12:SER:HB3	1:A:106:GLU:CD	2.36	0.51
3:C:57:THR:HG23	2:E:54:ILE:HG22	1.93	0.51
2:E:5:VAL:HB	2:E:23:LYS:HB3	1.92	0.51
3:F:44:CYS:HB3	3:F:78:CYS:SG	2.51	0.51
1:J:83:ASP:O	1:J:105:LEU:HD23	2.11	0.51
1:J:147:VAL:HG13	1:J:197:VAL:HG12	1.92	0.51
1:A:151:VAL:HG13	1:A:154:ALA:HB3	1.92	0.51
2:E:40:ALA:HA	2:E:92:ALA:HB2	1.91	0.51
2:E:199:LYS:HZ1	2:E:200:THR:HG22	1.75	0.51
2:K:40:ALA:HA	2:K:92:ALA:HB2	1.91	0.51
2:B:17:SER:HB2	2:B:84:SER:HA	1.92	0.51
3:C:34:HIS:HB3	3:C:89:LEU:O	2.11	0.51
1:D:113:ALA:HB1	1:D:202:LEU:HD21	1.92	0.51
2:K:5:VAL:HB	2:K:23:LYS:HB3	1.92	0.51
1:A:141:TYR:CE1	1:A:142:PRO:HG3	2.46	0.51
2:B:68:VAL:HG12	2:B:69:THR:N	2.26	0.51
1:A:29:LEU:HD12	1:A:72:PHE:CE1	2.46	0.51
2:E:55:VAL:HG12	2:E:57:ILE:HG12	1.93	0.51
3:C:42:ASN:O	3:F:58:HIS:NE2	2.39	0.50
1:D:53:SER:HB3	1:D:65:GLY:O	2.11	0.50
2:E:40:ALA:HB3	2:E:43:GLN:HB2	1.92	0.50
2:K:158:THR:OG1	2:K:206:ASP:HB3	2.11	0.50
3:L:66:ASN:ND2	3:L:74:ALA:H	2.09	0.50
1:D:83:ASP:O	1:D:105:LEU:HD23	2.11	0.50
3:F:91:TYR:HE2	3:F:96:PRO:HG3	1.76	0.50
3:L:30:TRP:C	3:L:32:TRP:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:92:VAL:O	3:L:95:THR:HG23	2.11	0.50
1:G:29:LEU:HD12	1:G:72:PHE:CE1	2.46	0.50
1:G:29:LEU:HB2	1:G:72:PHE:HZ	1.77	0.50
1:D:36:TRP:CD2	1:D:74:LEU:HB2	2.47	0.50
2:H:62:GLN:O	2:H:65:LYS:HB2	2.12	0.50
3:F:66:ASN:ND2	3:F:74:ALA:H	2.10	0.50
1:G:49:ILE:HD13	1:G:74:LEU:HD11	1.93	0.50
2:H:68:VAL:HG12	2:H:69:THR:N	2.26	0.50
1:J:113:ALA:HB1	1:J:202:LEU:HD21	1.92	0.50
1:J:196:GLU:HG2	1:J:207:THR:OG1	2.12	0.50
3:L:91:TYR:HE2	3:L:96:PRO:HG3	1.76	0.50
2:B:201:TYR:HD2	2:B:218:VAL:HG23	1.76	0.50
1:D:155:LEU:HD13	1:D:156:GLN:H	1.77	0.50
3:L:44:CYS:HB3	3:L:78:CYS:SG	2.51	0.50
3:I:34:HIS:HB3	3:I:89:LEU:O	2.11	0.50
2:B:54:ILE:CD1	2:B:74:GLU:HG2	2.41	0.50
1:D:49:ILE:HD12	1:D:74:LEU:HD13	1.92	0.50
1:D:101:GLN:H	1:D:101:GLN:NE2	2.10	0.50
1:D:196:GLU:HG2	1:D:207:THR:OG1	2.12	0.49
1:G:106:GLU:HG3	1:G:174:TYR:HH	1.74	0.49
1:J:36:TRP:CD2	1:J:74:LEU:HB2	2.47	0.49
1:J:53:SER:HB3	1:J:65:GLY:O	2.11	0.49
2:B:130:PRO:C	2:B:131:LEU:HD12	2.37	0.49
2:E:199:LYS:NZ	2:E:200:THR:HG22	2.28	0.49
1:J:191:LYS:HE2	1:J:211:ASN:HB3	1.93	0.49
2:E:40:ALA:HA	2:E:92:ALA:CB	2.43	0.49
2:E:126:PRO:HB2	2:E:149:VAL:HG13	1.95	0.49
1:A:29:LEU:HB2	1:A:72:PHE:HZ	1.77	0.49
2:H:201:TYR:HD2	2:H:218:VAL:HG23	1.76	0.49
2:K:40:ALA:HA	2:K:92:ALA:CB	2.43	0.49
2:E:64:PHE:HB3	2:E:68:VAL:HG23	1.94	0.49
2:B:18:VAL:HG11	2:B:116:VAL:HG11	1.94	0.49
2:K:55:VAL:HG12	2:K:57:ILE:HG12	1.93	0.49
2:H:18:VAL:HG11	2:H:116:VAL:HG11	1.94	0.49
2:H:130:PRO:C	2:H:131:LEU:HD12	2.37	0.49
1:A:49:ILE:HD13	1:A:74:LEU:HD11	1.93	0.49
1:A:167:GLN:HB2	1:A:174:TYR:CE1	2.48	0.49
1:D:51:GLY:O	1:D:52:ALA:HB2	2.12	0.49
1:G:164:VAL:O	2:H:174:PRO:HG2	2.13	0.49
3:I:42:ASN:O	3:L:58:HIS:NE2	2.39	0.49
1:A:117:PHE:CZ	2:B:143:ALA:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LYS:HE3	1:A:190:HIS:HE1	1.78	0.49
3:F:30:TRP:C	3:F:32:TRP:H	2.20	0.49
1:J:51:GLY:O	1:J:52:ALA:HB2	2.12	0.49
1:J:155:LEU:HD13	1:J:156:GLN:H	1.77	0.49
2:K:52:ILE:HD12	2:K:57:ILE:HG13	1.94	0.49
2:K:64:PHE:HB3	2:K:68:VAL:HG23	1.94	0.49
1:G:215:CYS:HB2	2:H:220:SER:HB3	1.95	0.48
1:J:188:GLU:HA	1:J:212:ARG:NH1	2.26	0.48
2:K:144:ALA:O	2:K:145:LEU:HD23	2.12	0.48
2:B:62:GLN:O	2:B:65:LYS:HB2	2.12	0.48
1:D:161:GLN:NE2	2:E:178:GLN:HG2	2.28	0.48
1:G:12:SER:HB3	1:G:106:GLU:OE2	2.13	0.48
2:H:50:GLY:O	2:H:58:ALA:HB1	2.13	0.48
2:K:199:LYS:NZ	2:K:200:THR:HG22	2.28	0.48
1:A:189:LYS:HE3	1:A:190:HIS:CE1	2.48	0.48
2:E:144:ALA:O	2:E:145:LEU:HD23	2.12	0.48
1:G:48:LEU:HB3	1:G:49:ILE:HD12	1.96	0.48
1:G:117:PHE:CZ	2:H:143:ALA:HA	2.48	0.48
2:K:177:LEU:HD13	2:K:178:GLN:O	2.14	0.48
1:A:164:VAL:O	2:B:174:PRO:HG2	2.13	0.48
2:B:125:GLY:HA3	2:B:152:TYR:HA	1.96	0.48
2:E:5:VAL:O	2:E:23:LYS:N	2.46	0.48
2:E:177:LEU:HD13	2:E:178:GLN:O	2.14	0.48
1:D:6:GLN:HG3	1:D:101:GLN:OE1	2.13	0.48
1:D:143:ARG:HG2	1:D:143:ARG:O	2.14	0.48
2:E:68:VAL:HG22	2:E:83:LEU:HD13	1.95	0.48
2:H:54:ILE:CD1	2:H:74:GLU:HG2	2.41	0.48
2:K:30:SER:C	2:K:32:ASN:H	2.21	0.48
1:A:48:LEU:HB3	1:A:49:ILE:HD12	1.96	0.48
1:A:106:GLU:HG3	1:A:174:TYR:HH	1.79	0.48
2:E:52:ILE:HD12	2:E:57:ILE:HG13	1.94	0.48
1:G:189:LYS:HE3	1:G:190:HIS:CE1	2.48	0.48
1:J:140:PHE:HE1	1:J:143:ARG:HA	1.79	0.48
2:B:144:ALA:C	2:B:145:LEU:HD22	2.39	0.48
2:E:30:SER:C	2:E:32:ASN:H	2.21	0.48
1:G:117:PHE:CE1	2:H:143:ALA:HA	2.49	0.48
2:K:5:VAL:O	2:K:23:LYS:N	2.46	0.48
2:K:52:ILE:HD11	2:K:103:VAL:CG2	2.44	0.48
1:A:12:SER:HB3	1:A:106:GLU:OE2	2.13	0.48
1:D:188:GLU:HA	1:D:212:ARG:NH1	2.26	0.48
1:G:189:LYS:HE3	1:G:190:HIS:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:53:PRO:C	2:K:55:VAL:H	2.21	0.48
1:A:140:PHE:CD2	1:A:140:PHE:N	2.82	0.48
1:G:167:GLN:HB2	1:G:174:TYR:CE1	2.48	0.48
3:I:20:LEU:HD12	3:I:21:TYR:N	2.28	0.48
1:J:149:TRP:CD2	1:J:180:LEU:HD22	2.49	0.48
2:K:126:PRO:HB2	2:K:149:VAL:HG13	1.95	0.48
1:A:117:PHE:CE1	2:B:143:ALA:HA	2.49	0.47
3:C:2:LEU:HD13	3:C:52:ARG:HH21	1.79	0.47
3:C:81:GLN:HG3	3:C:110:LYS:HD3	1.96	0.47
1:J:101:GLN:NE2	1:J:101:GLN:H	2.10	0.47
2:K:214:VAL:HG12	2:K:215:ASP:N	2.28	0.47
1:A:215:CYS:HB2	2:B:220:SER:HB3	1.95	0.47
2:E:52:ILE:HD11	2:E:103:VAL:CG2	2.44	0.47
3:I:81:GLN:HG3	3:I:110:LYS:HD3	1.96	0.47
2:B:50:GLY:O	2:B:58:ALA:HB1	2.13	0.47
1:G:37:TYR:HH	2:H:107:MET:H	1.62	0.47
1:G:150:LYS:HE3	1:G:196:GLU:HB2	1.97	0.47
2:B:40:ALA:HA	2:B:92:ALA:CB	2.44	0.47
1:D:149:TRP:CD2	1:D:180:LEU:HD22	2.49	0.47
2:E:178:GLN:C	2:E:180:SER:H	2.22	0.47
1:G:34:LEU:HD13	1:G:35:ALA:H	1.79	0.47
1:G:126:LEU:C	1:G:128:SER:H	2.22	0.47
3:I:69:ASN:N	3:I:70:PRO:HD3	2.30	0.47
1:J:143:ARG:O	1:J:143:ARG:HG2	2.14	0.47
1:J:161:GLN:NE2	2:K:178:GLN:HG2	2.28	0.47
2:K:178:GLN:C	2:K:180:SER:H	2.22	0.47
3:C:57:THR:O	3:C:61:VAL:HG23	2.14	0.47
2:E:177:LEU:HD23	2:E:183:TYR:CE1	2.49	0.47
2:E:214:VAL:HG12	2:E:215:ASP:N	2.28	0.47
2:H:40:ALA:HA	2:H:92:ALA:CB	2.44	0.47
2:K:27:TYR:HD2	2:K:28:THR:HG23	1.80	0.47
1:A:150:LYS:HE3	1:A:196:GLU:HB2	1.97	0.47
2:B:20:VAL:HG13	2:B:114:THR:HG21	1.96	0.47
1:J:6:GLN:HG3	1:J:101:GLN:OE1	2.13	0.47
1:A:199:HIS:ND1	1:A:200:GLN:N	2.63	0.47
2:B:2:VAL:HB	2:B:109:TYR:CD1	2.50	0.47
2:B:18:VAL:HG12	2:B:86:LEU:HD11	1.97	0.47
3:C:20:LEU:HD12	3:C:21:TYR:N	2.28	0.47
1:D:140:PHE:HE1	1:D:143:ARG:HA	1.79	0.47
2:E:53:PRO:C	2:E:55:VAL:H	2.21	0.47
2:H:125:GLY:HA3	2:H:152:TYR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:144:ALA:C	2:H:145:LEU:HD22	2.39	0.47
3:I:57:THR:O	3:I:61:VAL:HG23	2.14	0.47
2:K:177:LEU:HD23	2:K:183:TYR:CE1	2.49	0.47
1:D:149:TRP:CE3	1:D:180:LEU:HD22	2.50	0.47
1:G:140:PHE:N	1:G:140:PHE:CD2	2.82	0.47
1:G:177:SER:HB2	2:H:173:PHE:CZ	2.50	0.47
1:A:142:PRO:C	1:A:144:GLU:N	2.73	0.47
2:H:127:SER:HB2	2:H:150:LYS:HB3	1.96	0.47
1:A:34:LEU:HD22	1:A:90:GLN:O	2.15	0.47
1:A:126:LEU:C	1:A:128:SER:H	2.22	0.47
1:D:202:LEU:HB3	1:D:204:SER:O	2.15	0.47
1:G:34:LEU:HD22	1:G:90:GLN:O	2.15	0.47
1:G:199:HIS:ND1	1:G:200:GLN:N	2.63	0.47
2:H:18:VAL:HG12	2:H:86:LEU:HD11	1.97	0.47
1:J:108:LYS:HA	1:J:141:TYR:OH	2.15	0.47
2:K:68:VAL:HG22	2:K:83:LEU:HD13	1.95	0.47
2:B:127:SER:HB2	2:B:150:LYS:HB3	1.96	0.46
3:F:79:VAL:O	3:F:109:CYS:SG	2.73	0.46
2:H:20:VAL:HG13	2:H:114:THR:HG21	1.96	0.46
3:F:18:ARG:O	3:F:42:ASN:HB3	2.15	0.46
3:I:2:LEU:HD13	3:I:52:ARG:HH21	1.79	0.46
1:J:141:TYR:CE1	1:J:142:PRO:HG3	2.50	0.46
3:C:69:ASN:N	3:C:70:PRO:HD3	2.30	0.46
1:D:33:TYR:CB	1:D:93:ALA:HB2	2.44	0.46
1:D:141:TYR:CE1	1:D:142:PRO:HG3	2.50	0.46
2:H:74:GLU:O	3:L:51:LEU:HD22	2.15	0.46
1:J:149:TRP:CE3	1:J:180:LEU:HD22	2.50	0.46
1:A:21:LEU:HD22	1:A:103:THR:HG21	1.97	0.46
2:B:74:GLU:O	3:F:51:LEU:HD22	2.16	0.46
3:F:4:THR:O	3:F:8:PHE:HB2	2.16	0.46
3:F:50:TYR:CD1	3:F:51:LEU:HG	2.51	0.46
1:J:24:ARG:HB3	1:J:24:ARG:NH1	2.30	0.46
1:D:108:LYS:HA	1:D:141:TYR:OH	2.15	0.46
2:E:199:LYS:HE2	2:E:199:LYS:HA	1.97	0.46
1:G:21:LEU:HD22	1:G:103:THR:HG21	1.97	0.46
2:H:68:VAL:CG1	2:H:69:THR:N	2.79	0.46
2:K:199:LYS:HA	2:K:199:LYS:HE2	1.96	0.46
1:A:4:LEU:HD11	1:A:91:GLN:HB3	1.98	0.46
1:A:177:SER:HB2	2:B:173:PHE:CZ	2.50	0.46
1:D:196:GLU:CA	1:D:207:THR:HG23	2.46	0.46
3:L:4:THR:O	3:L:8:PHE:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ARG:HD3	1:A:60:PRO:O	2.15	0.46
1:G:151:VAL:HG13	1:G:151:VAL:O	2.16	0.46
2:H:2:VAL:HB	2:H:109:TYR:CD1	2.50	0.46
2:H:64:PHE:HB3	2:H:68:VAL:HG23	1.98	0.46
2:E:27:TYR:HD2	2:E:28:THR:HG23	1.80	0.46
1:G:55:ARG:HD3	1:G:60:PRO:O	2.15	0.46
1:J:202:LEU:HB3	1:J:204:SER:O	2.15	0.46
3:C:60:THR:CG2	2:E:54:ILE:HD12	2.46	0.46
2:H:74:GLU:C	3:L:51:LEU:HD22	2.40	0.46
3:L:18:ARG:O	3:L:42:ASN:HB3	2.15	0.46
2:B:177:LEU:HG	2:B:183:TYR:CE1	2.51	0.46
2:E:212:THR:C	2:E:213:LYS:HD3	2.41	0.46
2:H:32:ASN:O	2:H:53:PRO:HG2	2.16	0.46
2:H:159:VAL:HG13	2:H:205:VAL:HG22	1.98	0.46
3:L:50:TYR:CD1	3:L:51:LEU:HG	2.51	0.46
3:L:79:VAL:O	3:L:109:CYS:SG	2.73	0.46
1:A:151:VAL:HG13	1:A:151:VAL:O	2.16	0.45
2:B:74:GLU:C	3:F:51:LEU:HD22	2.40	0.45
1:D:162:GLU:HA	1:D:178:SER:HA	1.97	0.45
1:G:4:LEU:HD11	1:G:91:GLN:HB3	1.98	0.45
2:B:32:ASN:O	2:B:53:PRO:HG2	2.16	0.45
1:D:35:ALA:HB3	1:D:90:GLN:HE21	1.80	0.45
1:G:142:PRO:C	1:G:144:GLU:N	2.73	0.45
3:I:60:THR:CG2	2:K:54:ILE:HD12	2.46	0.45
1:J:35:ALA:HB3	1:J:90:GLN:HE21	1.80	0.45
1:J:109:ARG:NH1	1:J:112:ALA:HB2	2.32	0.45
2:K:212:THR:C	2:K:213:LYS:HD3	2.41	0.45
1:A:34:LEU:HD13	1:A:35:ALA:H	1.79	0.45
2:B:159:VAL:HG13	2:B:205:VAL:HG22	1.98	0.45
1:D:141:TYR:CG	1:D:142:PRO:HA	2.52	0.45
2:E:68:VAL:CG2	2:E:83:LEU:HD13	2.46	0.45
1:G:12:SER:HB3	1:G:106:GLU:OE1	2.16	0.45
2:H:177:LEU:HG	2:H:183:TYR:CE1	2.51	0.45
2:H:208:LYS:N	2:H:209:PRO:CD	2.80	0.45
1:J:33:TYR:CB	1:J:93:ALA:HB2	2.44	0.45
1:J:196:GLU:CA	1:J:207:THR:HG23	2.45	0.45
3:L:14:ASN:HB3	3:L:52:ARG:NE	2.32	0.45
1:D:67:GLY:HA3	1:D:72:PHE:HA	1.99	0.45
2:H:18:VAL:HG12	2:H:86:LEU:HD21	1.98	0.45
1:A:131:ALA:HB3	1:A:182:LEU:O	2.16	0.45
2:H:208:LYS:HB2	2:H:209:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:39:TYR:CD2	3:L:86:LEU:HD22	2.51	0.45
1:A:12:SER:HB3	1:A:106:GLU:OE1	2.16	0.45
2:E:128:VAL:HG21	2:E:214:VAL:HB	1.99	0.45
3:F:14:ASN:HB3	3:F:52:ARG:NE	2.32	0.45
1:J:162:GLU:HA	1:J:178:SER:HA	1.97	0.45
2:K:52:ILE:HA	2:K:53:PRO:HD3	1.73	0.45
1:A:37:TYR:OH	1:A:90:GLN:NE2	2.50	0.45
1:G:131:ALA:HB3	1:G:182:LEU:O	2.16	0.45
2:K:68:VAL:CG2	2:K:83:LEU:HD13	2.46	0.45
2:B:64:PHE:HB3	2:B:68:VAL:HG23	1.98	0.45
2:B:68:VAL:CG1	2:B:69:THR:N	2.79	0.45
3:F:66:ASN:HD22	3:F:74:ALA:H	1.65	0.45
1:G:37:TYR:OH	1:G:90:GLN:NE2	2.50	0.45
1:G:155:LEU:HD12	1:G:155:LEU:N	2.32	0.45
3:L:64:LEU:HD12	3:L:64:LEU:O	2.17	0.45
2:E:208:LYS:N	2:E:209:PRO:CD	2.79	0.45
3:F:64:LEU:HD12	3:F:64:LEU:O	2.17	0.45
1:G:12:SER:O	1:G:13:LEU:HD23	2.16	0.45
1:G:33:TYR:CE1	3:I:94:ARG:HD3	2.52	0.45
3:C:80:PRO:HB3	3:C:106:VAL:HG13	1.99	0.45
1:D:28:SER:OG	1:D:69:GLY:HA2	2.17	0.45
1:D:164:VAL:HG12	1:D:165:THR:N	2.32	0.45
1:A:97:ILE:HG13	2:B:104:LEU:HG	1.99	0.44
3:F:39:TYR:CD2	3:F:86:LEU:HD22	2.52	0.44
3:I:80:PRO:HB3	3:I:106:VAL:HG13	1.99	0.44
1:J:107:ILE:HD13	1:J:107:ILE:C	2.43	0.44
2:K:208:LYS:N	2:K:209:PRO:CD	2.79	0.44
2:B:208:LYS:HB2	2:B:209:PRO:HD3	1.99	0.44
1:G:97:ILE:HG13	2:H:104:LEU:HG	1.99	0.44
3:I:86:LEU:O	3:I:88:ILE:HG23	2.17	0.44
1:J:28:SER:OG	1:J:69:GLY:HA2	2.17	0.44
1:A:12:SER:O	1:A:13:LEU:HD23	2.16	0.44
2:B:208:LYS:N	2:B:209:PRO:CD	2.80	0.44
1:J:81:PRO:C	1:J:83:ASP:H	2.26	0.44
1:G:142:PRO:C	1:G:144:GLU:H	2.26	0.44
1:J:21:LEU:HG	1:J:103:THR:HG21	2.00	0.44
2:K:32:ASN:O	2:K:53:PRO:HG2	2.18	0.44
2:H:124:LYS:O	2:H:152:TYR:HA	2.17	0.44
1:J:107:ILE:HG22	1:J:167:GLN:NE2	2.33	0.44
1:A:155:LEU:HD12	1:A:155:LEU:N	2.32	0.44
2:B:18:VAL:HG12	2:B:86:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:32:ASN:O	2:E:53:PRO:HG2	2.18	0.44
2:H:81:MET:HE2	2:H:81:MET:C	2.43	0.44
3:C:86:LEU:O	3:C:88:ILE:HG23	2.17	0.44
1:D:80:GLU:O	1:D:83:ASP:HB2	2.17	0.44
2:E:97:ALA:HA	2:E:109:TYR:O	2.18	0.44
1:G:6:GLN:OE1	1:G:88:TYR:HA	2.18	0.44
1:J:150:LYS:HB2	1:J:194:ALA:HB3	2.00	0.44
1:J:164:VAL:HG12	1:J:165:THR:N	2.32	0.44
2:K:159:VAL:HG22	2:K:205:VAL:HG13	2.00	0.44
1:A:6:GLN:OE1	1:A:88:TYR:HA	2.18	0.44
1:A:141:TYR:HA	1:A:143:ARG:H	1.82	0.44
1:D:33:TYR:N	1:D:51:GLY:HA2	2.33	0.44
1:D:109:ARG:NH1	1:D:112:ALA:HB2	2.32	0.44
1:D:194:ALA:HB2	1:D:209:SER:HB3	2.00	0.44
3:F:35:GLU:OE1	3:F:36:PRO:HA	2.18	0.44
1:G:40:LYS:HB2	1:G:43:GLN:OE1	2.18	0.44
1:D:150:LYS:HB2	1:D:194:ALA:HB3	2.00	0.44
1:G:141:TYR:HA	1:G:143:ARG:H	1.82	0.44
1:G:141:TYR:CD2	1:G:142:PRO:HA	2.53	0.44
1:J:49:ILE:HD13	1:J:65:GLY:N	2.33	0.44
1:J:67:GLY:HA3	1:J:72:PHE:HA	1.99	0.44
1:J:80:GLU:O	1:J:83:ASP:HB2	2.17	0.44
2:K:201:TYR:O	2:K:217:ARG:HA	2.18	0.44
1:A:141:TYR:CD2	1:A:142:PRO:HA	2.53	0.43
1:A:159:ASN:OD1	1:A:182:LEU:HD23	2.18	0.43
1:D:8:PRO:HG2	1:D:11:LEU:HB2	2.00	0.43
2:E:52:ILE:HA	2:E:53:PRO:HD3	1.73	0.43
2:K:147:CYS:HB2	2:K:161:TRP:CH2	2.53	0.43
2:K:181:GLY:C	2:K:182:LEU:HD12	2.43	0.43
1:A:142:PRO:C	1:A:144:GLU:H	2.26	0.43
2:B:81:MET:C	2:B:81:MET:HE2	2.43	0.43
3:C:15:CYS:O	3:C:52:ARG:NH2	2.51	0.43
1:J:8:PRO:HG2	1:J:11:LEU:HB2	2.00	0.43
1:J:141:TYR:CG	1:J:142:PRO:HA	2.52	0.43
1:J:149:TRP:HB2	1:J:155:LEU:HG	2.00	0.43
3:L:35:GLU:OE1	3:L:36:PRO:HA	2.18	0.43
1:A:40:LYS:HB2	1:A:43:GLN:OE1	2.18	0.43
1:A:136:LEU:O	1:A:137:LEU:HG	2.19	0.43
2:B:124:LYS:O	2:B:152:TYR:HA	2.17	0.43
1:D:107:ILE:HD13	1:D:107:ILE:C	2.43	0.43
1:D:107:ILE:HG22	1:D:167:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:124:LYS:HD2	2:E:182:LEU:HD21	2.01	0.43
2:E:181:GLY:C	2:E:182:LEU:HD12	2.43	0.43
3:I:15:CYS:O	3:I:52:ARG:NH2	2.51	0.43
1:A:49:ILE:HD13	1:A:74:LEU:CD1	2.49	0.43
1:A:141:TYR:CG	1:A:142:PRO:HA	2.53	0.43
2:B:196:LEU:C	2:B:198:THR:H	2.27	0.43
1:D:149:TRP:HB2	1:D:155:LEU:HG	2.00	0.43
3:I:83:LEU:HA	3:I:105:VAL:O	2.18	0.43
1:A:33:TYR:CE1	3:C:94:ARG:HD3	2.52	0.43
1:D:81:PRO:C	1:D:83:ASP:H	2.26	0.43
2:E:162:ASN:ND2	2:E:201:TYR:HA	2.27	0.43
3:F:6:TYR:CD1	3:F:6:TYR:C	2.97	0.43
2:H:126:PRO:HA	2:H:152:TYR:HB3	2.01	0.43
1:J:143:ARG:HB2	1:J:174:TYR:CD2	2.54	0.43
1:D:24:ARG:HB3	1:D:24:ARG:NH1	2.30	0.43
2:E:123:THR:HG22	2:E:210:SER:HB3	1.99	0.43
3:F:46:GLY:HA2	3:F:47:PRO:HD3	1.91	0.43
1:J:132:SER:OG	1:J:181:THR:HG23	2.19	0.43
2:K:134:CYS:HB2	2:K:220:SER:OG	2.18	0.43
2:K:155:GLU:OE2	2:K:175:ALA:HB3	2.19	0.43
3:C:83:LEU:HA	3:C:105:VAL:O	2.18	0.43
1:G:136:LEU:O	1:G:137:LEU:HG	2.19	0.43
1:G:159:ASN:OD1	1:G:182:LEU:HD23	2.18	0.43
3:I:68:LEU:HD12	3:I:68:LEU:N	2.34	0.43
1:J:194:ALA:HB2	1:J:209:SER:HB3	2.00	0.43
2:K:123:THR:HG22	2:K:210:SER:HB3	1.99	0.43
2:B:126:PRO:HA	2:B:152:TYR:HB3	2.01	0.43
1:D:49:ILE:HD13	1:D:65:GLY:N	2.33	0.43
1:D:150:LYS:O	1:D:193:TYR:HA	2.19	0.43
2:E:4:LEU:HA	2:E:23:LYS:O	2.18	0.43
2:E:159:VAL:HG22	2:E:205:VAL:HG13	2.00	0.43
2:E:201:TYR:O	2:E:217:ARG:HA	2.18	0.43
1:D:21:LEU:HG	1:D:103:THR:HG21	2.00	0.43
1:G:92:TYR:CD2	2:H:105:ASP:HA	2.54	0.43
1:J:31:SER:O	1:J:32:SER:HB2	2.19	0.43
1:J:90:GLN:HE21	1:J:90:GLN:HB3	1.51	0.43
1:D:31:SER:O	1:D:32:SER:HB2	2.19	0.43
2:E:134:CYS:HB2	2:E:220:SER:OG	2.18	0.43
1:J:33:TYR:N	1:J:51:GLY:HA2	2.33	0.43
2:K:148:LEU:HD12	2:K:149:VAL:H	1.84	0.43
2:K:192:PRO:HG2	2:K:195:SER:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:ASN:HD22	2:B:32:ASN:HA	1.70	0.42
2:E:133:PRO:HD3	2:E:145:LEU:HD13	2.01	0.42
2:E:155:GLU:OE2	2:E:175:ALA:HB3	2.19	0.42
1:G:141:TYR:CG	1:G:142:PRO:HA	2.53	0.42
1:J:150:LYS:O	1:J:193:TYR:HA	2.19	0.42
1:J:162:GLU:HB3	1:J:178:SER:CB	2.49	0.42
2:K:124:LYS:HD2	2:K:182:LEU:HD21	2.01	0.42
1:D:132:SER:OG	1:D:181:THR:HG23	2.19	0.42
2:E:38:ARG:HE	2:E:46:GLU:CD	2.28	0.42
2:H:128:VAL:CG2	2:H:214:VAL:HG11	2.50	0.42
2:H:196:LEU:C	2:H:198:THR:H	2.27	0.42
2:K:97:ALA:HA	2:K:109:TYR:O	2.18	0.42
2:K:128:VAL:HG21	2:K:214:VAL:HB	1.99	0.42
1:A:21:LEU:HD12	1:A:74:LEU:HD23	2.01	0.42
1:A:92:TYR:CD2	2:B:105:ASP:HA	2.54	0.42
2:B:191:VAL:HA	2:B:192:PRO:HD3	1.91	0.42
1:D:143:ARG:HB2	1:D:174:TYR:CD2	2.54	0.42
1:D:165:THR:HG22	1:D:175:SER:H	1.84	0.42
1:G:21:LEU:HD12	1:G:74:LEU:HD23	2.01	0.42
2:H:124:LYS:HD3	2:H:124:LYS:C	2.45	0.42
2:K:162:ASN:ND2	2:K:201:TYR:HA	2.27	0.42
3:L:66:ASN:HD22	3:L:74:ALA:H	1.65	0.42
2:B:124:LYS:HD3	2:B:124:LYS:C	2.45	0.42
2:E:147:CYS:HB2	2:E:161:TRP:CH2	2.54	0.42
2:E:160:SER:OG	2:E:204:ASN:HB2	2.20	0.42
1:G:49:ILE:HD13	1:G:74:LEU:CD1	2.49	0.42
1:J:165:THR:HG22	1:J:175:SER:H	1.84	0.42
1:A:3:VAL:O	1:A:3:VAL:HG23	2.18	0.42
3:C:68:LEU:N	3:C:68:LEU:HD12	2.34	0.42
1:D:162:GLU:HB3	1:D:178:SER:CB	2.49	0.42
3:I:28:LEU:HB3	3:I:30:TRP:NE1	2.35	0.42
2:B:160:SER:O	2:B:204:ASN:HB3	2.20	0.42
1:D:155:LEU:CD1	1:D:157:SER:H	2.32	0.42
1:G:37:TYR:HE1	1:G:90:GLN:HE21	1.67	0.42
1:J:155:LEU:CD1	1:J:157:SER:H	2.32	0.42
1:A:194:ALA:HB1	1:A:207:THR:HG22	2.02	0.42
3:C:57:THR:CG2	2:E:54:ILE:HG22	2.50	0.42
2:E:30:SER:C	2:E:32:ASN:N	2.78	0.42
2:E:112:GLN:HG2	2:E:113:GLY:O	2.20	0.42
2:E:160:SER:HG	2:E:204:ASN:HB2	1.85	0.42
3:I:2:LEU:HD13	3:I:15:CYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:4:LEU:HA	2:K:23:LYS:O	2.18	0.42
2:K:97:ALA:HB2	2:K:110:TRP:CD2	2.55	0.42
2:B:40:ALA:HA	2:B:92:ALA:HB2	2.02	0.42
2:B:140:GLU:O	2:B:141:SER:HB3	2.20	0.42
2:B:211:ASN:HD21	2:B:213:LYS:NZ	2.18	0.42
3:C:28:LEU:HB3	3:C:30:TRP:NE1	2.35	0.42
2:H:32:ASN:HD22	2:H:32:ASN:HA	1.70	0.42
2:H:211:ASN:HD21	2:H:213:LYS:NZ	2.18	0.42
1:J:47:LEU:HD22	2:K:108:ASP:HB3	2.01	0.42
2:K:38:ARG:HE	2:K:46:GLU:CD	2.28	0.42
2:K:160:SER:OG	2:K:204:ASN:HB2	2.19	0.42
1:A:37:TYR:HE1	1:A:90:GLN:HE21	1.67	0.42
1:D:34:LEU:HD13	1:D:34:LEU:C	2.45	0.42
1:D:47:LEU:HD22	2:E:108:ASP:HB3	2.01	0.42
1:D:151:VAL:HG13	1:D:193:TYR:CE2	2.54	0.42
2:E:97:ALA:HB2	2:E:110:TRP:CD2	2.55	0.42
2:K:34:ILE:HG21	2:K:79:THR:HG21	2.02	0.42
2:B:128:VAL:CG2	2:B:214:VAL:HG11	2.50	0.41
2:E:103:VAL:HG12	2:E:104:LEU:HD12	2.01	0.41
2:E:103:VAL:HG12	2:E:104:LEU:HD13	2.02	0.41
3:F:14:ASN:HB3	3:F:15:CYS:H	1.69	0.41
3:F:62:LEU:HD12	3:F:74:ALA:O	2.20	0.41
1:G:11:LEU:O	1:G:105:LEU:HA	2.20	0.41
2:H:140:GLU:O	2:H:141:SER:HB3	2.20	0.41
3:I:80:PRO:HA	3:I:109:CYS:SG	2.60	0.41
2:K:133:PRO:HD2	2:K:220:SER:HB3	2.02	0.41
3:L:6:TYR:CD1	3:L:6:TYR:C	2.97	0.41
1:A:136:LEU:CD1	2:B:188:VAL:HG21	2.47	0.41
2:B:103:VAL:O	2:B:104:LEU:HD12	2.21	0.41
1:D:111:VAL:HG12	1:D:112:ALA:N	2.36	0.41
1:G:194:ALA:HB1	1:G:207:THR:CG2	2.50	0.41
1:A:140:PHE:CD1	1:A:143:ARG:HA	2.55	0.41
2:B:148:LEU:O	2:B:148:LEU:HG	2.20	0.41
1:D:155:LEU:HD22	1:D:155:LEU:HA	1.90	0.41
1:G:3:VAL:O	1:G:3:VAL:HG23	2.18	0.41
3:I:57:THR:CG2	2:K:54:ILE:HG22	2.50	0.41
1:J:34:LEU:C	1:J:34:LEU:HD13	2.45	0.41
2:B:30:SER:HB2	3:F:50:TYR:OH	2.20	0.41
2:B:55:VAL:HG13	3:C:101:LEU:HG	2.02	0.41
1:D:107:ILE:H	1:D:167:GLN:HE22	1.69	0.41
2:E:133:PRO:HD2	2:E:220:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:192:PRO:HG2	2:E:195:SER:HB2	2.01	0.41
2:H:30:SER:HB2	3:L:50:TYR:OH	2.20	0.41
2:K:112:GLN:HG2	2:K:113:GLY:O	2.20	0.41
1:A:163:SER:HB3	2:B:176:VAL:CG1	2.50	0.41
1:G:140:PHE:CD1	1:G:143:ARG:HA	2.55	0.41
2:K:208:LYS:N	2:K:209:PRO:HD3	2.36	0.41
1:A:11:LEU:O	1:A:105:LEU:HA	2.20	0.41
3:C:80:PRO:HA	3:C:109:CYS:SG	2.60	0.41
1:D:125:GLN:HG3	2:E:129:PHE:CE2	2.56	0.41
2:E:6:GLN:H	2:E:112:GLN:CD	2.29	0.41
2:H:67:ARG:NH2	2:H:83:LEU:HD11	2.35	0.41
2:H:103:VAL:O	2:H:104:LEU:HD12	2.20	0.41
1:J:111:VAL:HG12	1:J:112:ALA:N	2.36	0.41
1:J:137:LEU:N	1:J:137:LEU:HD12	2.35	0.41
2:B:67:ARG:NH2	2:B:83:LEU:HD11	2.35	0.41
3:C:101:LEU:HB3	3:C:104:MET:HG3	2.03	0.41
2:E:34:ILE:HG21	2:E:79:THR:HG21	2.02	0.41
1:G:163:SER:HB3	2:H:176:VAL:CG1	2.50	0.41
3:I:83:LEU:HD23	3:I:103:ASN:CB	2.50	0.41
2:K:103:VAL:O	2:K:104:LEU:HD12	2.21	0.41
2:K:132:ALA:HB1	2:K:133:PRO:HD2	2.03	0.41
1:D:137:LEU:HD12	1:D:137:LEU:N	2.35	0.41
2:E:91:THR:O	2:E:92:ALA:HB2	2.21	0.41
1:G:6:GLN:N	1:G:101:GLN:HE22	2.19	0.41
2:H:12:LYS:HE3	2:H:16:SER:OG	2.20	0.41
2:H:148:LEU:O	2:H:148:LEU:HG	2.20	0.41
2:H:160:SER:O	2:H:204:ASN:HB3	2.20	0.41
2:K:91:THR:O	2:K:92:ALA:HB2	2.21	0.41
3:L:62:LEU:HD12	3:L:74:ALA:O	2.20	0.41
3:C:2:LEU:HD13	3:C:15:CYS:O	2.20	0.41
3:C:90:TYR:O	3:C:97:LYS:HB2	2.21	0.41
1:D:189:LYS:H	1:D:189:LYS:HG3	1.79	0.41
2:E:126:PRO:HB3	2:E:152:TYR:HB3	2.03	0.41
2:H:152:TYR:OH	2:H:185:LEU:HD23	2.21	0.41
3:I:44:CYS:HB3	3:I:78:CYS:SG	2.61	0.41
1:J:34:LEU:O	1:J:51:GLY:O	2.39	0.41
1:J:189:LYS:H	1:J:189:LYS:HG3	1.79	0.41
2:K:103:VAL:HG12	2:K:104:LEU:HD12	2.01	0.41
1:A:194:ALA:HB1	1:A:207:THR:CG2	2.50	0.41
2:B:51:VAL:CG2	2:B:58:ALA:HB2	2.51	0.41
3:C:14:ASN:OD1	3:C:47:PRO:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:57:ILE:HG13	2:E:57:ILE:O	2.21	0.41
3:F:25:ARG:H	3:F:25:ARG:HG2	1.73	0.41
1:G:194:ALA:HB1	1:G:207:THR:HG22	2.02	0.41
2:H:98:SER:OG	2:H:109:TYR:HB2	2.21	0.41
3:I:20:LEU:HD21	3:L:65:TYR:CE2	2.56	0.41
1:J:52:ALA:C	1:J:53:SER:HG	2.29	0.41
1:G:53:SER:OG	1:G:66:SER:HA	2.21	0.40
3:I:101:LEU:HB3	3:I:104:MET:HG3	2.03	0.40
1:J:125:GLN:HG3	2:K:129:PHE:CE2	2.56	0.40
1:A:176:LEU:HD23	1:A:178:SER:N	2.36	0.40
1:A:177:SER:HB2	2:B:173:PHE:CE1	2.57	0.40
2:B:12:LYS:HE3	2:B:16:SER:OG	2.20	0.40
2:E:148:LEU:HD12	2:E:149:VAL:H	1.84	0.40
1:G:59:ILE:HA	1:G:60:PRO:HD3	1.98	0.40
2:H:64:PHE:HB3	2:H:68:VAL:CG2	2.52	0.40
3:I:90:TYR:O	3:I:97:LYS:HB2	2.21	0.40
1:J:5:THR:HB	1:J:24:ARG:HG3	2.03	0.40
1:J:24:ARG:HA	1:J:70:THR:O	2.22	0.40
2:K:57:ILE:HG13	2:K:57:ILE:O	2.21	0.40
1:A:6:GLN:N	1:A:101:GLN:HE22	2.19	0.40
2:B:177:LEU:HD23	2:B:177:LEU:HA	1.89	0.40
3:C:44:CYS:HB3	3:C:78:CYS:SG	2.61	0.40
2:E:103:VAL:O	2:E:104:LEU:HD12	2.21	0.40
2:K:103:VAL:HG12	2:K:104:LEU:HD13	2.02	0.40
2:K:133:PRO:HD3	2:K:145:LEU:HD13	2.01	0.40
2:B:98:SER:OG	2:B:109:TYR:HB2	2.21	0.40
2:B:152:TYR:OH	2:B:185:LEU:HD23	2.21	0.40
3:C:20:LEU:HD21	3:F:65:TYR:CE2	2.56	0.40
3:C:84:GLU:HB3	3:C:85:PRO:HD2	2.04	0.40
2:E:132:ALA:HB1	2:E:133:PRO:HD2	2.03	0.40
2:E:150:LYS:NZ	2:E:178:GLN:HE22	2.20	0.40
1:G:90:GLN:HG2	1:G:91:GLN:N	2.37	0.40
1:G:177:SER:HB2	2:H:173:PHE:CE1	2.56	0.40
3:I:14:ASN:OD1	3:I:47:PRO:HB2	2.21	0.40
3:I:58:HIS:NE2	3:L:42:ASN:O	2.50	0.40
3:I:80:PRO:CB	3:I:83:LEU:HD11	2.49	0.40
3:I:84:GLU:HB3	3:I:85:PRO:HD2	2.04	0.40
3:I:106:VAL:HG23	3:L:58:HIS:NE2	2.36	0.40
1:J:48:LEU:C	1:J:49:ILE:HG13	2.46	0.40
1:A:6:GLN:H	1:A:101:GLN:HE22	1.69	0.40
1:A:53:SER:OG	1:A:66:SER:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLN:HG2	1:A:91:GLN:N	2.37	0.40
2:B:2:VAL:HG22	2:B:28:THR:HG21	2.03	0.40
1:D:149:TRP:CE2	1:D:180:LEU:HB2	2.57	0.40
3:F:101:LEU:N	3:F:101:LEU:CD1	2.85	0.40
2:H:20:VAL:CG1	2:H:114:THR:HG21	2.52	0.40
2:H:150:LYS:HG3	2:H:151:ASP:N	2.37	0.40
1:J:130:THR:CB	1:J:183:SER:HA	2.51	0.40
3:L:101:LEU:HD23	3:L:104:MET:HE2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASP:OD1	1:J:109:ARG:NH2[4_455]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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	213/215 (99%)	177 (83%)	35 (16%)	1 (0%)	24	57
1	D	213/215 (99%)	171 (80%)	41 (19%)	1 (0%)	24	57
1	G	213/215 (99%)	177 (83%)	35 (16%)	1 (0%)	24	57
1	J	213/215 (99%)	171 (80%)	41 (19%)	1 (0%)	24	57
2	B	212/225 (94%)	177 (84%)	29 (14%)	6 (3%)	4	20
2	E	212/225 (94%)	185 (87%)	25 (12%)	2 (1%)	14	44
2	H	212/225 (94%)	177 (84%)	29 (14%)	6 (3%)	4	20
2	K	212/225 (94%)	185 (87%)	25 (12%)	2 (1%)	14	44
3	C	110/112 (98%)	94 (86%)	16 (14%)	0	100	100
3	F	110/112 (98%)	96 (87%)	13 (12%)	1 (1%)	14	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	110/112 (98%)	94 (86%)	16 (14%)	0	100	100
3	L	110/112 (98%)	96 (87%)	13 (12%)	1 (1%)	14	44
All	All	2140/2208 (97%)	1800 (84%)	318 (15%)	22 (1%)	12	41

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	26	GLY
2	H	26	GLY
2	E	133	PRO
2	K	133	PRO
3	L	47	PRO
1	A	158	GLY
2	B	133	PRO
1	D	26	SER
2	E	156	PRO
3	F	47	PRO
1	G	158	GLY
2	H	133	PRO
1	J	26	SER
2	K	156	PRO
2	B	101	GLY
2	B	166	LEU
2	H	101	GLY
2	H	166	LEU
2	B	155	GLU
2	B	156	PRO
2	H	155	GLU
2	H	156	PRO

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	185/185 (100%)	169 (91%)	16 (9%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	185/185 (100%)	170 (92%)	15 (8%)	11	36
1	G	185/185 (100%)	169 (91%)	16 (9%)	10	34
1	J	185/185 (100%)	170 (92%)	15 (8%)	11	36
2	B	184/192 (96%)	170 (92%)	14 (8%)	12	39
2	E	184/192 (96%)	168 (91%)	16 (9%)	9	34
2	H	184/192 (96%)	170 (92%)	14 (8%)	12	39
2	K	184/192 (96%)	168 (91%)	16 (9%)	9	34
3	C	102/102 (100%)	91 (89%)	11 (11%)	6	25
3	F	102/102 (100%)	92 (90%)	10 (10%)	7	29
3	I	102/102 (100%)	91 (89%)	11 (11%)	6	25
3	L	102/102 (100%)	92 (90%)	10 (10%)	7	29
All	All	1884/1916 (98%)	1720 (91%)	164 (9%)	9	34

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	12	SER
1	A	20	THR
1	A	53	SER
1	A	78	ARG
1	A	80	GLU
1	A	86	VAL
1	A	106	GLU
1	A	109	ARG
1	A	118	ILE
1	A	146	LYS
1	A	151	VAL
1	A	152	ASP
1	A	170	LYS
1	A	182	LEU
1	A	198	THR
2	B	18	VAL
2	B	69	THR
2	B	81	MET
2	B	96	CYS
2	B	115	LEU
2	B	119	SER

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Mol	Chain	Res	Type
2	B	120	SER
2	B	124	LYS
2	B	139	SER
2	B	140	GLU
2	B	155	GLU
2	B	158	THR
2	B	177	LEU
2	B	190	THR
3	C	13	GLU
3	C	16	CYS
3	C	26	GLN
3	C	33	VAL
3	C	47	PRO
3	C	56	THR
3	C	62	LEU
3	C	77	CYS
3	C	95	THR
3	C	99	GLU
3	C	109	CYS
1	D	6	GLN
1	D	7	SER
1	D	24	ARG
1	D	78	ARG
1	D	80	GLU
1	D	90	GLN
1	D	101	GLN
1	D	107	ILE
1	D	109	ARG
1	D	144	GLU
1	D	155	LEU
1	D	182	LEU
1	D	189	LYS
1	D	198	THR
1	D	214	GLU
2	E	35	SER
2	E	48	MET
2	E	55	VAL
2	E	56	ASP
2	E	71	THR
2	E	74	GLU
2	E	79	THR
2	E	96	CYS

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Mol	Chain	Res	Type
2	E	99	THR
2	E	105	ASP
2	E	117	THR
2	E	124	LYS
2	E	140	GLU
2	E	199	LYS
2	E	208	LYS
2	E	213	LYS
3	F	16	CYS
3	F	25	ARG
3	F	33	VAL
3	F	62	LEU
3	F	75	SER
3	F	77	CYS
3	F	81	GLN
3	F	95	THR
3	F	107	LYS
3	F	109	CYS
1	G	6	GLN
1	G	12	SER
1	G	20	THR
1	G	53	SER
1	G	78	ARG
1	G	80	GLU
1	G	86	VAL
1	G	106	GLU
1	G	109	ARG
1	G	118	ILE
1	G	146	LYS
1	G	151	VAL
1	G	152	ASP
1	G	170	LYS
1	G	182	LEU
1	G	198	THR
2	H	18	VAL
2	H	69	THR
2	H	81	MET
2	H	96	CYS
2	H	115	LEU
2	H	119	SER
2	H	120	SER
2	H	124	LYS

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Mol	Chain	Res	Type
2	H	139	SER
2	H	140	GLU
2	H	155	GLU
2	H	158	THR
2	H	177	LEU
2	H	190	THR
3	I	13	GLU
3	I	16	CYS
3	I	26	GLN
3	I	33	VAL
3	I	47	PRO
3	I	56	THR
3	I	62	LEU
3	I	77	CYS
3	I	95	THR
3	I	99	GLU
3	I	109	CYS
1	J	6	GLN
1	J	7	SER
1	J	24	ARG
1	J	78	ARG
1	J	80	GLU
1	J	90	GLN
1	J	101	GLN
1	J	107	ILE
1	J	109	ARG
1	J	144	GLU
1	J	155	LEU
1	J	182	LEU
1	J	189	LYS
1	J	198	THR
1	J	214	GLU
2	K	35	SER
2	K	48	MET
2	K	55	VAL
2	K	56	ASP
2	K	71	THR
2	K	74	GLU
2	K	79	THR
2	K	96	CYS
2	K	99	THR
2	K	105	ASP

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Mol	Chain	Res	Type
2	K	117	THR
2	K	124	LYS
2	K	140	GLU
2	K	199	LYS
2	K	208	LYS
2	K	213	LYS
3	L	16	CYS
3	L	25	ARG
3	L	33	VAL
3	L	62	LEU
3	L	75	SER
3	L	77	CYS
3	L	81	GLN
3	L	95	THR
3	L	107	LYS
3	L	109	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	90	GLN
1	A	139	ASN
1	A	153	ASN
1	A	156	GLN
1	A	159	ASN
1	A	161	GLN
1	A	190	HIS
2	B	32	ASN
2	B	39	GLN
2	B	43	GLN
2	B	62	GLN
2	B	171	HIS
2	B	178	GLN
2	B	211	ASN
3	C	10	ASN
3	C	26	GLN
3	C	103	ASN
1	D	27	GLN
1	D	38	GLN
1	D	39	GLN
1	D	90	GLN

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Mol	Chain	Res	Type
1	D	138	ASN
1	D	153	ASN
1	D	161	GLN
1	D	167	GLN
1	D	190	HIS
2	E	32	ASN
2	E	39	GLN
2	E	43	GLN
2	E	171	HIS
2	E	178	GLN
2	E	204	ASN
2	E	207	HIS
2	E	211	ASN
3	F	66	ASN
3	F	69	ASN
3	F	81	GLN
1	G	39	GLN
1	G	90	GLN
1	G	139	ASN
1	G	153	ASN
1	G	156	GLN
1	G	159	ASN
1	G	161	GLN
1	G	190	HIS
2	H	1	GLN
2	H	32	ASN
2	H	39	GLN
2	H	43	GLN
2	H	62	GLN
2	H	171	HIS
2	H	178	GLN
2	H	211	ASN
3	I	10	ASN
3	I	69	ASN
3	I	103	ASN
1	J	27	GLN
1	J	38	GLN
1	J	39	GLN
1	J	90	GLN
1	J	138	ASN
1	J	153	ASN
1	J	161	GLN

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Mol	Chain	Res	Type
1	J	167	GLN
1	J	190	HIS
2	K	32	ASN
2	K	39	GLN
2	K	43	GLN
2	K	171	HIS
2	K	178	GLN
2	K	204	ASN
2	K	207	HIS
2	K	211	ASN
3	L	66	ASN
3	L	81	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	215/215 (100%)	-1.15	0 100 100	18, 81, 158, 184	0
1	D	215/215 (100%)	-1.11	0 100 100	29, 87, 152, 179	0
1	G	215/215 (100%)	-1.12	0 100 100	18, 81, 158, 184	0
1	J	215/215 (100%)	-1.12	0 100 100	29, 87, 152, 179	0
2	B	216/225 (96%)	-1.12	0 100 100	25, 78, 157, 171	0
2	E	216/225 (96%)	-1.14	0 100 100	26, 85, 150, 176	0
2	H	216/225 (96%)	-1.12	0 100 100	25, 78, 157, 171	0
2	K	216/225 (96%)	-1.13	0 100 100	26, 85, 150, 176	0
3	C	112/112 (100%)	-1.16	0 100 100	4, 42, 101, 131	0
3	F	112/112 (100%)	-1.20	0 100 100	16, 45, 95, 123	0
3	I	112/112 (100%)	-1.16	0 100 100	4, 42, 101, 131	0
3	L	112/112 (100%)	-1.16	0 100 100	16, 45, 95, 123	0
All	All	2172/2208 (98%)	-1.13	0 100 100	4, 74, 152, 184	0

There are no RSRZ outliers to report.

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.