



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:02 PM EDT

PDB ID : 3EOY / pdb_00003eoy
Title : Structure of Reovirus sigma1 in Complex with Its Receptor Junctional Adhesion Molecule-A
Authors : Kirchner, E.; Guglielmi, K.M.; Dermody, T.S.; Stehle, T.
Deposited on : 2008-09-29
Resolution : 3.40 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

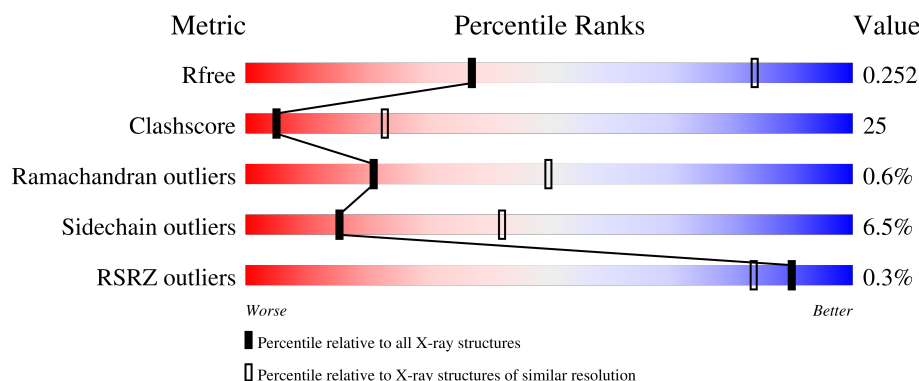
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	165	 60% 32% 5% ..
1	B	165	 60% 29% 7% ..
1	C	165	 61% 33% 5% .
1	D	165	 49% 40% 8% ..
1	E	165	 64% 29% . . .

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Mol	Chain	Length	Quality of chain
1	F	165	57%36%. .
2	G	104	% 60%34%5%. .
2	H	104	% 48%46%. .
2	I	104	42%50%6%. .
2	J	104	2% 48%43%7%. .
2	K	104	53%41%. .
2	L	104	% 50%42%5%. .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12227 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 Outer capsid protein sigma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1241	794	209	233	5			
1	B	160	Total	C	N	O	S	0	0	0
			1234	789	208	232	5			
1	C	162	Total	C	N	O	S	0	0	0
			1247	797	210	235	5			
1	D	162	Total	C	N	O	S	0	0	0
			1249	798	210	236	5			
1	E	160	Total	C	N	O	S	0	0	0
			1234	789	208	232	5			
1	F	160	Total	C	N	O	S	0	0	0
			1234	789	208	232	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	GLY	-	expression tag	UNP P03528
A	292	SER	-	expression tag	UNP P03528
A	408	THR	ALA	SEE REMARK 999	UNP P03528
B	291	GLY	-	expression tag	UNP P03528
B	292	SER	-	expression tag	UNP P03528
B	408	THR	ALA	SEE REMARK 999	UNP P03528
C	291	GLY	-	expression tag	UNP P03528
C	292	SER	-	expression tag	UNP P03528
C	408	THR	ALA	SEE REMARK 999	UNP P03528
D	291	GLY	-	expression tag	UNP P03528
D	292	SER	-	expression tag	UNP P03528
D	408	THR	ALA	SEE REMARK 999	UNP P03528
E	291	GLY	-	expression tag	UNP P03528
E	292	SER	-	expression tag	UNP P03528
E	408	THR	ALA	SEE REMARK 999	UNP P03528
F	291	GLY	-	expression tag	UNP P03528
F	292	SER	-	expression tag	UNP P03528

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Chain	Residue	Modelled	Actual	Comment	Reference
F	408	THR	ALA	SEE REMARK 999	UNP P03528

- Molecule 2 is a protein called Junctional adhesion molecule A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	102	Total	C	N	O	S	0	0	0
			798	500	132	162	4			
2	H	102	Total	C	N	O	S	0	0	0
			798	500	132	162	4			
2	I	102	Total	C	N	O	S	0	0	0
			798	500	132	162	4			
2	J	102	Total	C	N	O	S	0	0	0
			798	500	132	162	4			
2	K	102	Total	C	N	O	S	0	0	0
			798	500	132	162	4			
2	L	102	Total	C	N	O	S	0	0	0
			798	500	132	162	4			

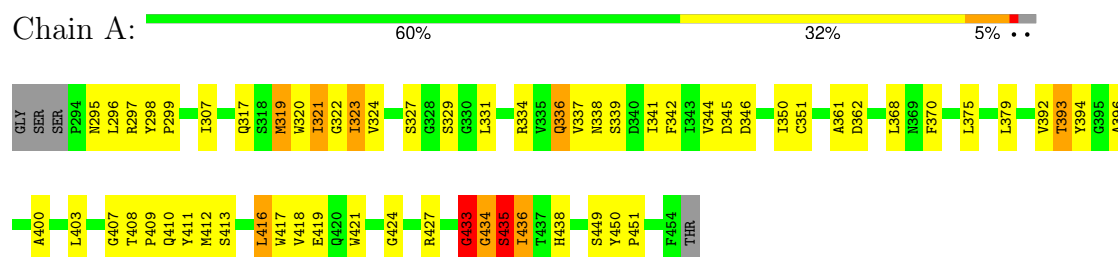
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	26	GLY	-	expression tag	UNP Q9Y624
G	27	SER	-	expression tag	UNP Q9Y624
H	26	GLY	-	expression tag	UNP Q9Y624
H	27	SER	-	expression tag	UNP Q9Y624
I	26	GLY	-	expression tag	UNP Q9Y624
I	27	SER	-	expression tag	UNP Q9Y624
J	26	GLY	-	expression tag	UNP Q9Y624
J	27	SER	-	expression tag	UNP Q9Y624
K	26	GLY	-	expression tag	UNP Q9Y624
K	27	SER	-	expression tag	UNP Q9Y624
L	26	GLY	-	expression tag	UNP Q9Y624
L	27	SER	-	expression tag	UNP Q9Y624

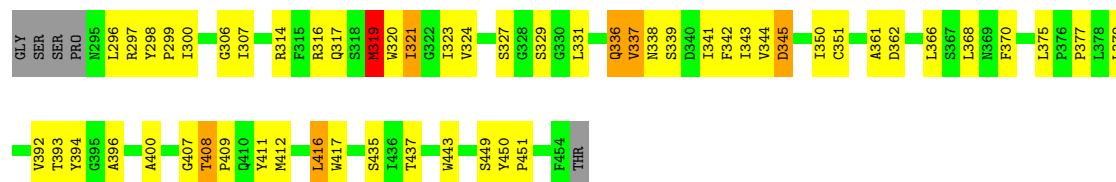
3 Residue-property plots

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.

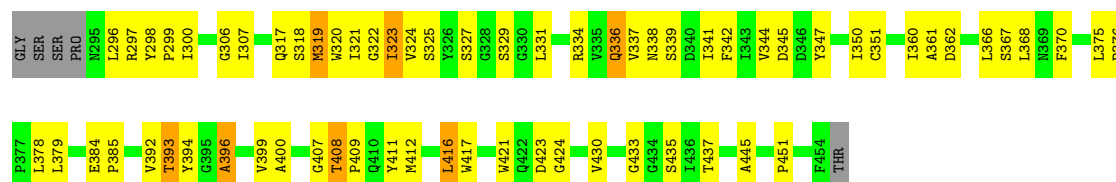
• Molecule 1: Outer capsid protein sigma-1



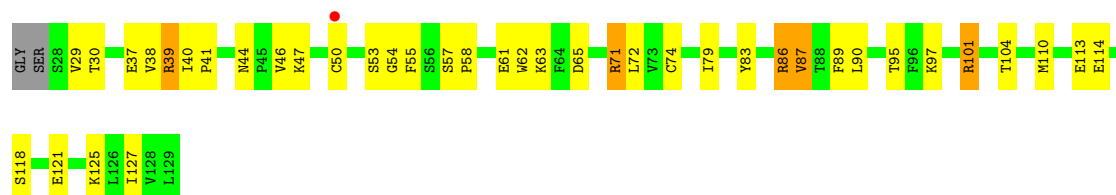
- Molecule 1: Outer capsid protein sigma-1



- Molecule 1: Outer capsid protein sigma-1



- Molecule 2: Junctional adhesion molecule A



- Molecule 2: Junctional adhesion molecule A

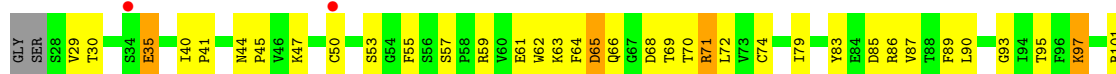


- Molecule 2: Junctional adhesion molecule A





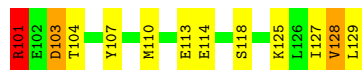
- Molecule 2: Junctional adhesion molecule A



- Molecule 2: Junctional adhesion molecule A



- Molecule 2: Junctional adhesion molecule A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.94Å 124.34Å 130.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.40 30.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (30.00-3.40) 90.0 (30.00-3.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 3.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.252 0.210 , 0.252	Depositor DCC
R_{free} test set	2187 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12227	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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

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	0.69	2/1277 (0.2%)	1.11	11/1742 (0.6%)
1	B	0.69	2/1269 (0.2%)	1.10	10/1731 (0.6%)
1	C	0.63	1/1283 (0.1%)	1.09	13/1751 (0.7%)
1	D	0.77	3/1285 (0.2%)	1.19	11/1752 (0.6%)
1	E	0.59	1/1269 (0.1%)	1.01	7/1731 (0.4%)
1	F	0.59	1/1269 (0.1%)	1.00	9/1731 (0.5%)
2	G	0.54	0/814	0.91	0/1104
2	H	0.73	2/814 (0.2%)	1.08	3/1104 (0.3%)
2	I	0.55	0/814	0.97	3/1104 (0.3%)
2	J	0.75	0/814	1.11	3/1104 (0.3%)
2	K	0.58	0/814	0.97	2/1104 (0.2%)
2	L	0.59	0/814	1.00	3/1104 (0.3%)
All	All	0.65	12/12536 (0.1%)	1.06	75/17062 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
2	J	0	2
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	GLY	C-O	-7.75	1.18	1.23
1	A	435	SER	CA-CB	-7.72	1.43	1.54
1	D	337	VAL	CA-CB	-6.85	1.45	1.54
1	E	319	MET	SD-CE	5.88	1.94	1.79
1	B	406	GLY	CA-C	5.86	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	376	PRO	CA-C	5.79	1.57	1.52
1	D	295	ASN	CA-CB	5.64	1.63	1.53
1	F	396	ALA	CA-CB	5.60	1.62	1.53
1	B	408	THR	CA-C	-5.54	1.45	1.52
2	H	68	ASP	CA-CB	5.38	1.58	1.53
1	D	453	SER	CA-CB	-5.36	1.45	1.53
2	H	66	GLN	CA-C	-5.22	1.45	1.53

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	SER	N-CA-CB	-10.99	92.75	110.55
1	B	407	GLY	N-CA-C	10.63	138.37	113.18
1	A	435	SER	N-CA-C	10.50	121.73	108.19
1	D	453	SER	CB-CA-C	-10.14	93.32	109.84
1	C	376	PRO	N-CA-C	-9.56	99.04	110.70
1	A	434	GLY	N-CA-C	-9.35	88.88	111.04
2	J	118	SER	N-CA-C	8.45	123.96	107.57
1	B	408	THR	CA-C-N	8.33	128.34	119.76
1	B	408	THR	C-N-CA	8.33	128.34	119.76
1	B	408	THR	N-CA-C	-8.25	91.58	109.81
1	D	337	VAL	N-CA-CB	-8.19	97.71	111.23
1	D	295	ASN	N-CA-CB	7.02	121.18	110.44
1	D	393	THR	N-CA-C	-6.96	102.19	110.41
1	B	393	THR	N-CA-C	-6.96	102.20	110.41
1	E	393	THR	N-CA-C	-6.71	102.22	110.61
1	F	393	THR	N-CA-C	-6.67	102.28	110.61
2	J	119	TYR	N-CA-C	6.64	120.28	109.59
1	F	345	ASP	CB-CA-C	-6.59	108.26	117.23
1	D	378	LEU	N-CA-C	6.58	120.20	110.46
1	C	408	THR	CA-C-N	6.41	126.91	119.99
1	C	408	THR	C-N-CA	6.41	126.91	119.99
2	L	101	ARG	CB-CA-C	-6.28	100.37	110.79
1	B	406	GLY	N-CA-C	-6.24	98.39	113.18
1	C	393	THR	N-CA-C	-6.19	102.87	110.61
1	C	345	ASP	CB-CA-C	-6.13	109.52	116.63
1	C	323	ILE	N-CA-C	6.06	116.59	107.80
1	F	411	TYR	N-CA-C	6.05	119.50	109.46
1	A	433	GLY	O-C-N	6.02	130.53	122.70
1	E	411	TYR	N-CA-C	6.02	119.33	109.76
1	B	411	TYR	N-CA-C	5.99	119.40	109.46
2	J	97	LYS	N-CA-C	-5.98	104.84	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	411	TYR	N-CA-C	5.97	119.26	109.76
1	A	393	THR	N-CA-C	-5.95	103.17	110.61
1	E	323	ILE	N-CA-C	5.94	116.48	108.17
1	D	295	ASN	CB-CA-C	-5.91	99.37	110.01
1	A	433	GLY	CA-C-N	-5.90	114.81	121.83
1	A	433	GLY	C-N-CA	-5.90	114.81	121.83
1	D	345	ASP	CB-CA-C	-5.89	109.21	117.23
2	L	103	ASP	N-CA-C	5.87	120.14	112.92
1	E	408	THR	CA-C-N	5.74	126.18	119.99
1	E	408	THR	C-N-CA	5.74	126.18	119.99
1	C	411	TYR	N-CA-C	5.68	118.80	109.76
1	A	345	ASP	CB-CA-C	-5.66	110.06	116.63
1	F	307	ILE	CB-CA-C	-5.64	105.14	111.23
1	F	323	ILE	N-CA-C	5.56	115.86	107.80
1	B	323	ILE	N-CA-C	5.55	115.85	107.80
1	B	345	ASP	CB-CA-C	-5.54	110.20	116.63
1	F	318	SER	N-CA-C	5.54	115.34	108.19
1	C	293	SER	CA-C-N	5.53	125.05	119.19
1	C	293	SER	C-N-CA	5.53	125.05	119.19
1	F	408	THR	CA-C-N	5.50	125.92	119.99
1	F	408	THR	C-N-CA	5.50	125.92	119.99
2	K	97	LYS	N-CA-C	-5.48	105.31	111.28
1	E	345	ASP	CB-CA-C	-5.46	109.80	117.23
1	D	296	LEU	N-CA-C	5.43	117.76	108.90
1	A	295	ASN	N-CA-C	-5.39	106.29	112.92
1	C	307	ILE	CB-CA-C	-5.36	105.51	111.35
2	I	40	ILE	CA-C-N	5.32	125.26	119.78
2	I	40	ILE	C-N-CA	5.32	125.26	119.78
1	C	384	GLU	CA-C-N	5.31	125.21	119.85
1	C	384	GLU	C-N-CA	5.31	125.21	119.85
1	D	356	ASP	N-CA-C	-5.29	100.47	108.46
1	A	323	ILE	N-CA-C	5.26	115.53	108.17
1	A	411	TYR	N-CA-C	5.25	118.18	109.46
2	K	115	GLY	N-CA-C	-5.25	107.75	114.37
1	F	367	SER	N-CA-C	5.25	116.97	108.41
1	E	337	VAL	N-CA-C	5.25	115.92	108.42
1	C	378	LEU	N-CA-C	5.24	117.63	110.24
1	D	323	ILE	N-CA-C	5.23	115.49	108.17
1	B	367	SER	N-CA-C	5.21	116.90	108.41
2	H	67	GLY	CA-C-N	-5.21	114.12	121.83
2	H	67	GLY	C-N-CA	-5.21	114.12	121.83
2	I	115	GLY	N-CA-C	-5.20	107.82	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	128	VAL	N-CA-C	-5.12	101.08	108.87
2	H	49	SER	N-CA-C	5.10	117.06	108.96

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	433	GLY	Peptide
1	D	453	SER	Mainchain
2	J	115	GLY	Peptide
2	J	119	TYR	Sidechain

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	1241	0	1193	52	0
1	B	1234	0	1185	52	0
1	C	1247	0	1197	41	0
1	D	1249	0	1200	89	0
1	E	1234	0	1185	54	0
1	F	1234	0	1185	54	0
2	G	798	0	775	47	0
2	H	798	0	775	46	0
2	I	798	0	775	58	0
2	J	798	0	775	52	0
2	K	798	0	775	48	0
2	L	798	0	775	58	0
All	All	12227	0	11795	595	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 25.

All (595) 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:J:57:SER:O	2:J:114:GLU:HB2	1.34	1.22
2:G:86:ARG:HG3	2:G:86:ARG:HH11	1.13	1.10
1:D:454:PHE:HD2	1:D:455:THR:N	1.54	1.05
1:D:376:PRO:HA	1:D:378:LEU:H	1.19	1.05
1:A:412:MET:HE2	1:A:435:SER:HA	1.45	0.97
1:D:454:PHE:CD2	1:D:455:THR:N	2.36	0.92
1:A:433:GLY:O	1:B:411:TYR:CD1	2.24	0.91
1:D:300:ILE:HD11	1:E:300:ILE:HD12	1.53	0.91
1:D:336:GLN:HG2	1:D:337:VAL:H	1.37	0.90
1:D:412:MET:HE2	1:D:435:SER:HA	1.53	0.90
1:D:322:GLY:O	1:D:337:VAL:HG12	1.74	0.87
1:B:423:ASP:OD1	2:H:80:THR:HB	1.75	0.87
1:D:454:PHE:HD2	1:D:455:THR:H	1.15	0.87
1:D:376:PRO:HA	1:D:378:LEU:N	1.88	0.86
2:J:86:ARG:HA	2:J:97:LYS:HE2	1.56	0.85
1:D:451:PRO:HG3	1:E:344:VAL:HG21	1.59	0.85
2:L:39:ARG:HH11	2:L:39:ARG:HB3	1.42	0.85
1:E:319:MET:HE1	1:E:338:ASN:HD22	1.40	0.83
1:F:319:MET:HE1	1:F:338:ASN:HD22	1.40	0.83
2:G:86:ARG:HG3	2:G:86:ARG:NH1	1.84	0.83
1:D:344:VAL:HG21	1:F:451:PRO:HG3	1.60	0.82
2:K:39:ARG:HH11	2:K:39:ARG:HB3	1.44	0.82
2:I:47:LYS:HG3	2:I:95:THR:HG22	1.62	0.81
2:L:114:GLU:OE2	2:L:114:GLU:HA	1.81	0.81
2:H:47:LYS:HG3	2:H:95:THR:HG22	1.64	0.80
1:A:451:PRO:HG3	1:B:344:VAL:HG21	1.64	0.80
2:G:86:ARG:HA	2:G:97:LYS:HE2	1.63	0.79
1:F:423:ASP:OD1	2:L:80:THR:HB	1.81	0.79
2:J:64:PHE:CZ	2:J:66:GLN:HB2	2.19	0.77
1:B:341:ILE:HD11	1:B:350:ILE:HG23	1.66	0.77
1:B:319:MET:HE1	1:B:338:ASN:HD22	1.50	0.77
2:L:74:CYS:HB2	2:L:79:ILE:HD13	1.64	0.77
1:B:451:PRO:HG3	1:C:344:VAL:HG21	1.67	0.76
2:I:68:ASP:HB3	2:L:69:THR:CB	2.15	0.76
1:D:300:ILE:HD11	1:E:300:ILE:CD1	2.15	0.76
2:J:69:THR:HG22	2:J:70:THR:H	1.50	0.76
1:C:423:ASP:OD1	2:I:80:THR:HB	1.86	0.76
2:L:35:GLU:HG2	2:L:38:VAL:HG22	1.69	0.75
1:A:344:VAL:HG21	1:C:451:PRO:HG3	1.68	0.75
1:D:336:GLN:HG2	1:D:337:VAL:N	2.00	0.75
2:K:39:ARG:HH11	2:K:39:ARG:CB	1.99	0.75
1:E:321:ILE:N	1:E:321:ILE:HD12	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:59:ARG:HD2	2:J:114:GLU:OE2	1.86	0.75
1:B:341:ILE:CD1	1:B:350:ILE:HG23	2.17	0.74
2:L:39:ARG:HB3	2:L:39:ARG:NH1	2.01	0.74
1:D:321:ILE:HG22	1:D:336:GLN:OE1	1.87	0.74
2:H:114:GLU:OE2	2:H:114:GLU:HA	1.88	0.73
2:K:113:GLU:HG3	2:K:114:GLU:N	2.03	0.73
2:L:39:ARG:HH11	2:L:39:ARG:CB	2.01	0.73
2:I:74:CYS:HB2	2:I:79:ILE:HD13	1.71	0.72
2:I:113:GLU:HG3	2:I:114:GLU:H	1.53	0.72
2:J:35:GLU:HG3	2:J:35:GLU:O	1.89	0.72
2:J:113:GLU:HB2	2:J:118:SER:HB2	1.69	0.72
2:J:104:THR:HG23	2:J:127:ILE:HA	1.70	0.72
1:A:435:SER:O	1:A:436:ILE:HG22	1.90	0.72
1:D:322:GLY:O	1:D:337:VAL:CG1	2.37	0.72
2:G:104:THR:HG23	2:G:127:ILE:HA	1.72	0.72
1:F:375:LEU:HD12	1:F:376:PRO:HD2	1.70	0.71
2:G:113:GLU:HG3	2:G:114:GLU:N	2.07	0.70
2:L:129:LEU:N	2:L:129:LEU:HD12	2.06	0.70
1:A:433:GLY:O	1:B:411:TYR:CE1	2.43	0.70
1:D:321:ILE:CG2	1:D:336:GLN:OE1	2.39	0.70
2:H:74:CYS:HB2	2:H:79:ILE:HD13	1.71	0.70
1:D:300:ILE:CD1	1:E:300:ILE:HD12	2.21	0.69
1:C:319:MET:HE1	1:C:338:ASN:HD22	1.57	0.69
2:I:47:LYS:CG	2:I:95:THR:HG22	2.21	0.69
1:C:412:MET:HE2	1:C:435:SER:HA	1.73	0.69
2:K:113:GLU:HG3	2:K:114:GLU:H	1.57	0.69
2:H:104:THR:HG23	2:H:127:ILE:HA	1.75	0.69
2:L:113:GLU:HG3	2:L:114:GLU:N	2.08	0.69
2:I:39:ARG:HG3	2:I:127:ILE:HB	1.74	0.68
2:H:113:GLU:HG3	2:H:114:GLU:H	1.59	0.68
2:I:114:GLU:HA	2:I:114:GLU:OE2	1.93	0.68
2:L:104:THR:HG23	2:L:127:ILE:HA	1.76	0.68
1:B:389:ASN:HD22	1:B:389:ASN:H	1.40	0.68
1:D:320:TRP:HB2	1:D:341:ILE:HD11	1.75	0.67
1:D:321:ILE:HD12	1:D:321:ILE:N	2.08	0.67
2:I:113:GLU:HG3	2:I:114:GLU:N	2.09	0.67
1:D:454:PHE:O	1:D:455:THR:HG23	1.94	0.67
2:I:86:ARG:HA	2:I:97:LYS:HE2	1.76	0.67
1:A:435:SER:C	1:A:436:ILE:CG2	2.67	0.67
1:D:344:VAL:HB	1:F:347:TYR:OH	1.95	0.67
2:G:113:GLU:HG3	2:G:114:GLU:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:GLN:HG3	1:F:342:PHE:CE1	2.29	0.67
2:G:47:LYS:HG3	2:G:95:THR:HG22	1.76	0.67
1:F:416:LEU:C	1:F:416:LEU:HD23	2.20	0.66
2:J:114:GLU:OE2	2:J:114:GLU:HA	1.94	0.66
2:I:66:GLN:HG2	2:I:66:GLN:O	1.95	0.66
2:K:74:CYS:HB2	2:K:79:ILE:HD13	1.77	0.66
2:L:113:GLU:HG3	2:L:114:GLU:H	1.60	0.66
1:D:337:VAL:HG13	1:D:337:VAL:O	1.96	0.65
2:H:113:GLU:HG3	2:H:114:GLU:N	2.11	0.65
1:A:413:SER:O	1:A:433:GLY:HA2	1.96	0.65
1:B:416:LEU:HD23	1:B:416:LEU:C	2.22	0.65
2:J:69:THR:HG22	2:J:70:THR:N	2.11	0.65
1:E:319:MET:HB3	1:E:375:LEU:HD22	1.79	0.64
1:D:416:LEU:C	1:D:416:LEU:HD23	2.22	0.64
1:D:347:TYR:OH	1:E:344:VAL:HB	1.96	0.64
2:H:47:LYS:CG	2:H:95:THR:HG22	2.27	0.64
1:E:379:LEU:HB3	2:K:61:GLU:OE2	1.98	0.64
2:H:35:GLU:HG2	2:H:38:VAL:HG22	1.79	0.63
2:I:37:GLU:HG2	2:I:125:LYS:HB3	1.80	0.63
1:B:321:ILE:HD12	1:B:321:ILE:N	2.13	0.63
1:B:297:ARG:NH1	1:C:306:GLY:HA3	2.13	0.63
1:E:416:LEU:C	1:E:416:LEU:HD23	2.23	0.63
2:K:38:VAL:HG11	2:K:46:VAL:HG21	1.81	0.63
1:F:323:ILE:HG21	1:F:334:ARG:HD2	1.79	0.63
2:I:68:ASP:HB3	2:L:69:THR:HG21	1.78	0.63
1:C:379:LEU:HB3	2:I:61:GLU:OE2	1.99	0.62
2:I:42:GLU:HB2	2:I:129:LEU:O	1.98	0.62
2:L:47:LYS:HG3	2:L:95:THR:HG22	1.80	0.62
1:D:396:ALA:HA	1:D:417:TRP:HB3	1.80	0.62
1:E:319:MET:CB	1:E:375:LEU:HD22	2.29	0.62
1:A:396:ALA:HA	1:A:417:TRP:HB3	1.80	0.61
2:I:104:THR:HG23	2:I:127:ILE:HA	1.81	0.61
2:J:74:CYS:HB2	2:J:79:ILE:HD13	1.82	0.61
2:H:113:GLU:HB2	2:H:118:SER:HB2	1.82	0.61
2:G:113:GLU:HB2	2:G:118:SER:HB2	1.81	0.61
2:K:104:THR:HG23	2:K:127:ILE:HA	1.81	0.61
1:C:416:LEU:C	1:C:416:LEU:HD23	2.26	0.60
2:G:74:CYS:HB2	2:G:79:ILE:HD13	1.82	0.60
2:J:71:ARG:HH11	2:J:71:ARG:HB3	1.66	0.60
2:L:41:PRO:HB2	2:L:44:ASN:ND2	2.15	0.60
1:D:319:MET:HE1	1:D:338:ASN:HD22	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ILE:HD13	1:A:370:PHE:HZ	1.67	0.60
2:G:113:GLU:CB	2:G:118:SER:HB2	2.32	0.59
1:C:321:ILE:N	1:C:321:ILE:HD12	2.16	0.59
2:H:106:THR:HG21	2:H:123:LYS:HE3	1.82	0.59
2:K:47:LYS:HG3	2:K:95:THR:HG22	1.83	0.59
2:H:41:PRO:HB2	2:H:44:ASN:ND2	2.17	0.59
2:G:38:VAL:HG11	2:G:46:VAL:HG21	1.85	0.59
2:L:42:GLU:OE1	2:L:101:ARG:NH1	2.36	0.59
2:I:68:ASP:HB3	2:L:69:THR:CG2	2.31	0.59
1:F:317:GLN:HG3	1:F:342:PHE:CD1	2.36	0.59
1:F:321:ILE:N	1:F:321:ILE:HD12	2.17	0.59
1:E:298:TYR:CD2	2:K:114:GLU:HB3	2.38	0.58
2:G:86:ARG:HH11	2:G:86:ARG:CG	2.02	0.58
1:F:396:ALA:HA	1:F:417:TRP:HB3	1.85	0.58
1:D:392:VAL:HG23	1:D:394:TYR:H	1.67	0.58
2:G:39:ARG:HB3	2:G:39:ARG:HH11	1.68	0.58
1:D:296:LEU:HD23	1:E:307:ILE:HB	1.85	0.57
2:G:41:PRO:HB2	2:G:44:ASN:ND2	2.19	0.57
2:I:47:LYS:CB	2:I:95:THR:HG22	2.33	0.57
2:H:113:GLU:CB	2:H:118:SER:HB2	2.34	0.57
1:D:297:ARG:NH1	1:E:306:GLY:HA3	2.19	0.57
2:G:61:GLU:HG2	2:G:110:MET:HE3	1.85	0.57
1:F:350:ILE:HD13	1:F:370:PHE:HZ	1.69	0.57
2:G:30:THR:CG2	2:G:53:SER:HB3	2.34	0.57
2:G:114:GLU:HA	2:G:114:GLU:OE2	2.04	0.57
2:H:64:PHE:CZ	2:H:66:GLN:HB2	2.39	0.57
1:C:317:GLN:HG3	1:C:342:PHE:CE1	2.40	0.56
1:E:451:PRO:HG3	1:F:344:VAL:HG21	1.85	0.56
1:D:355:PHE:CZ	1:D:446:MET:CE	2.88	0.56
1:E:320:TRP:HB2	1:E:341:ILE:HD11	1.87	0.56
2:L:40:ILE:HG13	2:L:41:PRO:HD2	1.87	0.56
1:D:379:LEU:HB3	2:J:61:GLU:OE2	2.05	0.56
1:E:396:ALA:HA	1:E:417:TRP:HB3	1.87	0.56
1:F:412:MET:HE2	1:F:435:SER:HA	1.86	0.56
2:L:86:ARG:HB2	2:L:97:LYS:HG2	1.87	0.56
1:D:297:ARG:HG2	1:D:297:ARG:HH11	1.71	0.56
1:D:454:PHE:HD2	1:D:455:THR:CA	2.19	0.56
2:I:47:LYS:HB2	2:I:95:THR:HG22	1.88	0.56
1:A:319:MET:HE1	1:A:338:ASN:HD22	1.71	0.56
2:I:68:ASP:HB3	2:L:69:THR:HB	1.85	0.56
2:J:47:LYS:HG3	2:J:95:THR:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:113:GLU:CB	2:J:118:SER:HB2	2.35	0.56
1:D:296:LEU:HD22	1:D:300:ILE:HG22	1.88	0.56
1:B:396:ALA:HA	1:B:417:TRP:HB3	1.88	0.55
1:F:323:ILE:HG22	1:F:334:ARG:HG2	1.87	0.55
1:F:379:LEU:HB3	2:L:61:GLU:OE2	2.06	0.55
2:K:47:LYS:HB2	2:K:95:THR:HG22	1.88	0.55
2:L:35:GLU:CG	2:L:38:VAL:HG22	2.34	0.55
2:L:83:TYR:HD2	2:L:87:VAL:HG21	1.71	0.55
1:A:329:SER:HB2	1:A:361:ALA:HB2	1.88	0.55
1:B:298:TYR:CD1	1:B:299:PRO:HA	2.42	0.55
1:D:329:SER:HB3	1:D:361:ALA:HB2	1.87	0.55
2:K:29:VAL:HB	2:K:55:PHE:CE1	2.41	0.55
2:K:39:ARG:HB3	2:K:39:ARG:NH1	2.17	0.55
2:J:64:PHE:CE2	2:J:66:GLN:HB2	2.41	0.55
1:A:412:MET:HE3	1:A:434:GLY:H	1.70	0.55
2:H:35:GLU:HG2	2:H:38:VAL:CG2	2.37	0.55
2:K:50:CYS:HB2	2:K:62:TRP:CZ2	2.42	0.55
1:A:320:TRP:HB2	1:A:341:ILE:HD11	1.88	0.55
1:A:319:MET:CB	1:A:375:LEU:HD22	2.37	0.55
1:E:394:TYR:CZ	1:E:451:PRO:HD3	2.41	0.55
2:I:38:VAL:HG11	2:I:46:VAL:HG21	1.89	0.54
1:B:324:VAL:HG22	1:B:368:LEU:HD22	1.89	0.54
1:D:347:TYR:HH	1:E:344:VAL:HB	1.71	0.54
2:J:85:ASP:O	2:J:97:LYS:HE2	2.07	0.54
1:B:396:ALA:HB1	1:C:445:ALA:O	2.07	0.54
2:L:61:GLU:OE1	2:L:63:LYS:HE3	2.08	0.54
1:D:350:ILE:HD13	1:D:370:PHE:HZ	1.72	0.54
2:J:57:SER:HB2	2:J:114:GLU:HB3	1.89	0.54
2:L:50:CYS:HB2	2:L:62:TRP:CZ2	2.43	0.54
1:D:355:PHE:CD1	1:D:355:PHE:N	2.74	0.53
1:D:316:ARG:HD3	1:D:343:ILE:HD12	1.89	0.53
2:I:68:ASP:CG	2:L:69:THR:HG21	2.33	0.53
2:H:50:CYS:HB2	2:H:62:TRP:CZ2	2.43	0.53
2:I:41:PRO:HB2	2:I:44:ASN:ND2	2.24	0.53
2:K:114:GLU:OE2	2:K:114:GLU:HA	2.07	0.53
1:C:350:ILE:HD13	1:C:370:PHE:HZ	1.74	0.53
1:D:371:VAL:O	2:J:63:LYS:NZ	2.38	0.53
1:E:317:GLN:HG3	1:E:342:PHE:CE1	2.44	0.53
1:A:321:ILE:HG23	1:A:338:ASN:CG	2.33	0.53
1:E:297:ARG:NH1	1:F:306:GLY:HA3	2.23	0.53
1:B:341:ILE:HD13	1:B:350:ILE:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ARG:HB3	1:B:343:ILE:HB	1.90	0.53
1:C:396:ALA:HA	1:C:417:TRP:HB3	1.91	0.53
1:D:393:THR:HA	1:D:417:TRP:CD1	2.45	0.52
2:L:57:SER:O	2:L:114:GLU:HG2	2.09	0.52
1:D:436:ILE:HG12	1:D:437:THR:N	2.23	0.52
2:G:86:ARG:HA	2:G:97:LYS:CE	2.36	0.52
1:B:431:GLU:CG	1:B:432:GLY:N	2.73	0.52
1:D:316:ARG:HB3	1:D:343:ILE:HB	1.92	0.52
1:C:317:GLN:HG3	1:C:342:PHE:CD1	2.44	0.52
1:E:392:VAL:HG23	1:E:394:TYR:H	1.74	0.52
2:L:40:ILE:HD11	2:L:44:ASN:HB3	1.92	0.52
1:A:298:TYR:CD1	1:A:299:PRO:HA	2.45	0.52
2:H:47:LYS:HB2	2:H:95:THR:HG22	1.91	0.52
1:A:337:VAL:HG22	1:A:338:ASN:N	2.23	0.52
1:A:346:ASP:OD2	1:B:345:ASP:OD1	2.27	0.52
1:B:340:ASP:O	1:B:341:ILE:HD13	2.10	0.52
1:A:394:TYR:CZ	1:A:451:PRO:HD3	2.45	0.52
2:G:37:GLU:HG3	2:G:125:LYS:HB3	1.92	0.52
2:H:47:LYS:CB	2:H:95:THR:HG22	2.40	0.52
2:I:35:GLU:HG2	2:I:38:VAL:HG22	1.92	0.52
1:F:337:VAL:HG22	1:F:338:ASN:N	2.25	0.51
2:J:57:SER:CB	2:J:114:GLU:CB	2.88	0.51
1:A:403:LEU:HD22	1:A:438:HIS:CD2	2.44	0.51
1:E:329:SER:HB2	1:E:361:ALA:HB2	1.91	0.51
2:J:71:ARG:HH11	2:J:71:ARG:CB	2.22	0.51
2:K:113:GLU:CB	2:K:118:SER:HB2	2.40	0.51
1:F:394:TYR:CZ	1:F:451:PRO:HD3	2.46	0.51
1:A:324:VAL:HG22	1:A:368:LEU:HD22	1.92	0.51
1:E:317:GLN:HG3	1:E:342:PHE:CD1	2.46	0.51
1:E:394:TYR:CE1	1:E:450:TYR:HA	2.46	0.51
2:G:113:GLU:CG	2:G:114:GLU:H	2.24	0.51
1:C:375:LEU:O	1:C:378:LEU:HB2	2.11	0.51
1:C:416:LEU:HD12	1:C:430:VAL:HG22	1.91	0.51
2:I:68:ASP:CB	2:L:69:THR:HG21	2.39	0.51
2:K:47:LYS:CG	2:K:95:THR:HG22	2.40	0.51
1:B:382:ASP:OD1	2:H:59:ARG:NH1	2.44	0.51
1:D:320:TRP:C	1:D:321:ILE:HD12	2.36	0.51
2:K:41:PRO:HB2	2:K:44:ASN:ND2	2.26	0.51
1:A:416:LEU:C	1:A:416:LEU:HD23	2.36	0.51
2:G:50:CYS:HB2	2:G:62:TRP:CZ2	2.46	0.51
2:G:83:TYR:HD2	2:G:87:VAL:HG21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:129:LEU:HD12	2:L:129:LEU:H	1.76	0.51
1:A:319:MET:HB2	1:A:375:LEU:HD22	1.93	0.51
2:G:40:ILE:HG13	2:G:41:PRO:HD2	1.93	0.51
2:J:50:CYS:HB2	2:J:62:TRP:CZ2	2.46	0.51
1:D:372:THR:CG2	2:J:70:THR:HG21	2.42	0.50
2:K:103:ASP:HB3	2:K:107:TYR:OH	2.12	0.50
2:G:47:LYS:CG	2:G:95:THR:HG22	2.40	0.50
2:J:90:LEU:HB2	2:J:93:GLY:O	2.11	0.50
1:A:344:VAL:HB	1:C:347:TYR:OH	2.11	0.50
1:E:396:ALA:HB1	1:F:445:ALA:O	2.12	0.50
2:K:63:LYS:HD2	2:K:110:MET:HE1	1.93	0.50
1:A:394:TYR:CE1	1:A:450:TYR:HA	2.47	0.50
1:A:379:LEU:HB3	2:G:61:GLU:OE2	2.11	0.50
1:A:435:SER:C	1:A:436:ILE:HG23	2.37	0.50
1:D:376:PRO:CA	1:D:378:LEU:H	2.08	0.50
1:A:307:ILE:HB	1:C:296:LEU:HD23	1.92	0.50
2:H:110:MET:HG2	2:H:121:GLU:HG3	1.93	0.50
2:K:100:THR:O	2:K:128:VAL:HG21	2.11	0.50
2:K:103:ASP:O	2:K:126:LEU:HD23	2.12	0.50
2:H:63:LYS:HD2	2:H:110:MET:HE1	1.94	0.50
1:D:303:VAL:O	1:D:304:SER:C	2.55	0.49
1:B:379:LEU:HB3	2:H:61:GLU:OE2	2.11	0.49
1:E:320:TRP:C	1:E:321:ILE:HD12	2.37	0.49
2:I:86:ARG:HA	2:I:97:LYS:CE	2.42	0.49
2:K:55:PHE:HB3	2:K:58:PRO:HB3	1.94	0.49
2:K:61:GLU:OE1	2:K:63:LYS:HE3	2.12	0.49
1:D:347:TYR:CZ	1:E:344:VAL:HB	2.48	0.49
1:D:379:LEU:HD11	2:J:112:SER:HB3	1.94	0.49
1:D:412:MET:HE2	1:D:435:SER:CA	2.35	0.49
1:E:297:ARG:HH11	1:E:297:ARG:HG2	1.76	0.49
1:D:394:TYR:CZ	1:D:451:PRO:HD3	2.47	0.49
2:G:113:GLU:CG	2:G:114:GLU:N	2.75	0.49
2:I:64:PHE:CZ	2:I:66:GLN:HB2	2.47	0.49
2:K:47:LYS:CB	2:K:95:THR:HG22	2.42	0.49
1:F:350:ILE:HD13	1:F:370:PHE:CZ	2.48	0.49
1:F:421:TRP:CZ2	1:F:424:GLY:HA2	2.47	0.49
2:J:69:THR:CG2	2:J:70:THR:H	2.23	0.49
2:L:89:PHE:CG	2:L:90:LEU:N	2.80	0.49
1:F:296:LEU:HD22	1:F:300:ILE:HG22	1.94	0.49
2:L:75:TYR:CD2	2:L:80:THR:HG22	2.47	0.49
1:D:369:ASN:OD1	1:D:371:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:GLU:HG2	1:A:427:ARG:NH2	2.28	0.49
2:I:57:SER:O	2:I:114:GLU:HG2	2.13	0.49
2:L:63:LYS:CD	2:L:110:MET:HE1	2.43	0.49
1:B:385:PRO:HG3	1:B:450:TYR:CE2	2.47	0.48
1:E:350:ILE:HD13	1:E:370:PHE:HZ	1.77	0.48
1:F:323:ILE:HD13	1:F:336:GLN:HA	1.95	0.48
2:L:30:THR:CG2	2:L:53:SER:HB3	2.43	0.48
1:B:327:SER:HA	1:B:331:LEU:O	2.13	0.48
1:E:342:PHE:HE2	1:E:351:CYS:HG	1.60	0.48
2:I:42:GLU:N	2:I:129:LEU:O	2.46	0.48
2:I:63:LYS:CD	2:I:110:MET:HE1	2.43	0.48
2:J:41:PRO:HB2	2:J:44:ASN:ND2	2.28	0.48
1:D:385:PRO:HG3	1:D:450:TYR:CE2	2.48	0.48
2:I:86:ARG:HA	2:I:97:LYS:CD	2.43	0.48
2:J:57:SER:O	2:J:114:GLU:CB	2.30	0.48
2:L:61:GLU:HG2	2:L:110:MET:HE3	1.94	0.48
2:H:60:VAL:HG22	2:H:111:VAL:HG22	1.95	0.48
2:K:106:THR:HG21	2:K:123:LYS:HE3	1.95	0.48
2:K:113:GLU:CG	2:K:114:GLU:N	2.75	0.48
2:L:89:PHE:O	2:L:90:LEU:HG	2.14	0.48
2:L:129:LEU:N	2:L:129:LEU:CD1	2.76	0.48
1:E:412:MET:HE2	1:E:435:SER:HA	1.95	0.48
2:K:63:LYS:CD	2:K:110:MET:HE1	2.43	0.48
2:L:113:GLU:CB	2:L:118:SER:HB2	2.44	0.48
1:A:350:ILE:HD13	1:A:370:PHE:CZ	2.47	0.48
2:H:40:ILE:HD11	2:H:44:ASN:HB3	1.94	0.48
2:L:113:GLU:HB2	2:L:118:SER:HB2	1.95	0.48
1:C:394:TYR:CE1	1:C:450:TYR:HA	2.49	0.48
1:F:329:SER:HB2	1:F:361:ALA:HB2	1.94	0.48
2:L:47:LYS:CG	2:L:95:THR:HG22	2.43	0.48
2:G:61:GLU:OE1	2:G:63:LYS:HE3	2.13	0.48
1:A:296:LEU:HD23	1:B:307:ILE:HB	1.94	0.48
1:E:321:ILE:HG22	1:E:336:GLN:OE1	2.14	0.48
2:G:86:ARG:CG	2:G:86:ARG:O	2.62	0.47
2:I:113:GLU:CG	2:I:114:GLU:H	2.23	0.47
2:K:61:GLU:HG2	2:K:110:MET:HE3	1.95	0.47
1:C:293:SER:HB3	1:C:296:LEU:HD12	1.96	0.47
1:D:454:PHE:CE1	1:E:314:ARG:HB2	2.49	0.47
2:K:100:THR:C	2:K:128:VAL:HG11	2.39	0.47
1:C:399:VAL:O	1:C:399:VAL:HG13	2.15	0.47
1:D:421:TRP:CZ2	1:D:424:GLY:HA2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:320:TRP:HB2	1:F:341:ILE:HD11	1.97	0.47
2:H:38:VAL:HG11	2:H:46:VAL:HG21	1.95	0.47
2:K:35:GLU:HG2	2:K:38:VAL:HG22	1.97	0.47
1:A:435:SER:C	1:A:436:ILE:HG22	2.37	0.47
1:B:296:LEU:HD22	1:B:300:ILE:HG22	1.96	0.47
2:I:107:TYR:N	2:I:107:TYR:CD1	2.81	0.47
2:H:40:ILE:HG13	2:H:41:PRO:HD2	1.96	0.47
2:J:63:LYS:HE3	2:J:110:MET:HE1	1.96	0.47
2:K:89:PHE:O	2:K:90:LEU:HG	2.15	0.47
2:K:113:GLU:CG	2:K:114:GLU:H	2.26	0.47
1:F:324:VAL:HG22	1:F:368:LEU:HD22	1.96	0.47
2:G:63:LYS:HE3	2:G:110:MET:HE1	1.96	0.47
2:I:40:ILE:HG13	2:I:41:PRO:HD2	1.97	0.47
2:J:29:VAL:HB	2:J:55:PHE:CE1	2.50	0.47
2:J:63:LYS:CD	2:J:110:MET:HE1	2.44	0.47
2:K:71:ARG:HH11	2:K:71:ARG:HB3	1.80	0.47
2:L:75:TYR:CD1	2:L:75:TYR:O	2.68	0.47
2:L:103:ASP:HB3	2:L:107:TYR:OH	2.15	0.47
1:C:327:SER:HA	1:C:331:LEU:O	2.14	0.47
1:B:392:VAL:HG23	1:B:394:TYR:H	1.80	0.47
1:C:329:SER:HB2	1:C:361:ALA:HB2	1.97	0.47
1:D:297:ARG:NH1	1:D:297:ARG:HG2	2.28	0.47
2:H:41:PRO:HB2	2:H:44:ASN:HD21	1.80	0.47
2:L:63:LYS:HD2	2:L:110:MET:HE1	1.96	0.47
1:A:297:ARG:HG3	1:B:303:VAL:O	2.13	0.47
1:C:382:ASP:OD1	2:I:59:ARG:NH1	2.48	0.47
1:E:319:MET:CE	1:E:338:ASN:HD22	2.20	0.47
1:E:321:ILE:N	1:E:321:ILE:CD1	2.75	0.47
2:I:71:ARG:HH12	2:I:83:TYR:HE1	1.63	0.47
2:I:113:GLU:CG	2:I:114:GLU:N	2.78	0.47
1:C:298:TYR:CD1	1:C:299:PRO:HA	2.49	0.46
1:C:337:VAL:HG22	1:C:338:ASN:N	2.30	0.46
1:C:384:GLU:OE1	2:I:76:ASN:ND2	2.47	0.46
1:E:296:LEU:HD22	1:E:300:ILE:HG22	1.97	0.46
1:F:342:PHE:HE2	1:F:351:CYS:HG	1.63	0.46
1:B:431:GLU:HG2	1:B:432:GLY:N	2.27	0.46
2:I:89:PHE:O	2:I:90:LEU:HG	2.16	0.46
2:I:66:GLN:O	2:I:66:GLN:CG	2.61	0.46
2:I:113:GLU:CB	2:I:118:SER:HB2	2.45	0.46
1:A:320:TRP:CE2	1:A:322:GLY:HA3	2.50	0.46
1:B:389:ASN:HD22	1:B:389:ASN:N	2.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:TRP:HB2	1:C:341:ILE:HD11	1.98	0.46
1:C:400:ALA:HA	1:C:412:MET:O	2.15	0.46
2:H:63:LYS:CD	2:H:110:MET:HE1	2.45	0.46
1:B:323:ILE:HD13	1:B:336:GLN:HA	1.98	0.46
1:D:378:LEU:O	1:D:379:LEU:HD23	2.15	0.46
1:D:412:MET:HE3	1:D:434:GLY:O	2.16	0.46
2:G:110:MET:HG2	2:G:121:GLU:HG3	1.98	0.46
2:J:83:TYR:HD2	2:J:87:VAL:HG21	1.79	0.46
1:A:317:GLN:HG3	1:A:342:PHE:CD1	2.51	0.46
1:B:317:GLN:HG3	1:B:342:PHE:CE1	2.51	0.46
1:C:316:ARG:HB3	1:C:343:ILE:HB	1.98	0.46
2:J:57:SER:HB2	2:J:114:GLU:CB	2.44	0.46
1:D:403:LEU:HD22	1:D:438:HIS:CD2	2.51	0.46
1:F:408:THR:HA	1:F:409:PRO:HD3	1.78	0.46
2:I:48:LEU:O	2:I:93:GLY:HA3	2.16	0.46
1:E:339:SER:HB2	1:E:351:CYS:O	2.15	0.45
2:H:113:GLU:CG	2:H:114:GLU:N	2.79	0.45
2:J:110:MET:HG2	2:J:121:GLU:HG3	1.98	0.45
2:L:100:THR:O	2:L:128:VAL:HG21	2.16	0.45
1:A:317:GLN:HG3	1:A:342:PHE:CE1	2.52	0.45
1:D:355:PHE:HZ	1:D:446:MET:CE	2.30	0.45
1:D:408:THR:HA	1:D:409:PRO:HD3	1.78	0.45
2:I:41:PRO:HA	2:I:129:LEU:HB2	1.96	0.45
2:J:69:THR:CG2	2:J:70:THR:N	2.79	0.45
1:A:297:ARG:NH1	1:B:306:GLY:HA3	2.31	0.45
2:I:108:THR:HG23	2:I:123:LYS:HG2	1.98	0.45
2:I:121:GLU:HG2	2:I:122:VAL:N	2.32	0.45
2:K:30:THR:CG2	2:K:53:SER:HB3	2.47	0.45
2:K:42:GLU:HG2	2:K:100:THR:HA	1.98	0.45
2:K:45:PRO:HG3	2:K:97:LYS:O	2.17	0.45
2:K:113:GLU:HB2	2:K:118:SER:HB2	1.97	0.45
2:L:46:VAL:HG12	2:L:99:VAL:HG11	1.98	0.45
1:E:298:TYR:CD1	1:E:299:PRO:HA	2.52	0.45
1:E:443:TRP:CD1	1:E:443:TRP:N	2.85	0.45
1:F:393:THR:HA	1:F:417:TRP:CD1	2.52	0.45
2:H:42:GLU:OE1	2:H:101:ARG:HG3	2.17	0.45
2:L:41:PRO:HB2	2:L:44:ASN:HD21	1.79	0.45
1:C:324:VAL:HG22	1:C:368:LEU:HD22	1.98	0.45
2:J:64:PHE:HZ	2:J:66:GLN:OE1	1.98	0.45
1:D:327:SER:HA	1:D:331:LEU:O	2.17	0.45
1:E:296:LEU:HD22	1:E:300:ILE:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:ILE:HD13	1:E:375:LEU:HD11	1.99	0.45
1:F:339:SER:HB2	1:F:351:CYS:O	2.17	0.45
2:J:47:LYS:CG	2:J:95:THR:HG22	2.46	0.45
2:K:31:VAL:HG22	2:K:52:TYR:HB2	1.98	0.45
1:E:297:ARG:NH1	1:E:297:ARG:HG2	2.32	0.45
1:F:327:SER:HA	1:F:331:LEU:O	2.17	0.45
2:G:55:PHE:HB3	2:G:58:PRO:HB3	1.99	0.45
2:J:64:PHE:HE1	2:J:105:GLY:HA3	1.82	0.45
1:A:298:TYR:CG	1:A:299:PRO:HA	2.52	0.44
1:B:329:SER:HB2	1:B:361:ALA:HB2	1.97	0.44
1:F:321:ILE:HA	1:F:337:VAL:O	2.17	0.44
2:H:61:GLU:OE1	2:H:63:LYS:HE3	2.17	0.44
2:K:101:ARG:HA	2:K:128:VAL:HB	1.99	0.44
1:B:298:TYR:CG	1:B:299:PRO:HA	2.52	0.44
1:D:346:ASP:OD2	1:E:345:ASP:OD1	2.35	0.44
1:F:296:LEU:HD22	1:F:300:ILE:CG2	2.47	0.44
2:G:101:ARG:H	2:G:101:ARG:HG2	1.55	0.44
2:K:35:GLU:CG	2:K:38:VAL:HG22	2.47	0.44
2:L:40:ILE:HD11	2:L:44:ASN:CB	2.47	0.44
1:B:319:MET:HB3	1:B:375:LEU:HD22	1.98	0.44
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.80	0.44
1:D:296:LEU:HD13	1:D:301:ALA:C	2.42	0.44
2:H:113:GLU:CG	2:H:114:GLU:H	2.27	0.44
2:I:31:VAL:HG22	2:I:52:TYR:HB2	2.00	0.44
1:C:408:THR:HA	1:C:409:PRO:HD3	1.75	0.44
1:F:298:TYR:CD1	1:F:299:PRO:HA	2.53	0.44
2:H:71:ARG:HB3	2:H:71:ARG:HH11	1.82	0.44
2:I:61:GLU:OE1	2:I:63:LYS:HE3	2.16	0.44
1:D:350:ILE:HD13	1:D:370:PHE:CZ	2.52	0.44
2:H:46:VAL:CG1	2:H:99:VAL:HG11	2.47	0.44
2:J:45:PRO:HG3	2:J:97:LYS:O	2.18	0.44
1:D:344:VAL:HB	1:F:347:TYR:CZ	2.52	0.44
1:D:416:LEU:HD12	1:D:430:VAL:HG22	2.00	0.44
1:E:408:THR:HA	1:E:409:PRO:HD3	1.70	0.44
2:L:46:VAL:CG1	2:L:99:VAL:HG11	2.48	0.44
1:A:319:MET:HB3	1:A:375:LEU:HD22	1.99	0.43
2:J:57:SER:CB	2:J:114:GLU:HB2	2.48	0.43
2:J:117:ASN:C	2:J:117:ASN:ND2	2.76	0.43
2:G:30:THR:HG22	2:G:53:SER:HB3	2.00	0.43
2:H:103:ASP:HB3	2:H:107:TYR:OH	2.17	0.43
1:A:421:TRP:CZ2	1:A:424:GLY:HA2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:360:ILE:O	1:F:360:ILE:HG13	2.17	0.43
1:F:366:LEU:HD12	1:F:366:LEU:HA	1.84	0.43
2:G:29:VAL:HB	2:G:55:PHE:CE1	2.53	0.43
2:I:29:VAL:HB	2:I:55:PHE:CE1	2.53	0.43
2:K:57:SER:O	2:K:114:GLU:HG2	2.18	0.43
2:J:40:ILE:HG13	2:J:41:PRO:HD2	2.00	0.43
1:B:310:SER:O	1:B:313:TYR:HB3	2.18	0.43
1:B:394:TYR:CE1	1:B:450:TYR:HA	2.53	0.43
2:H:83:TYR:HD2	2:H:87:VAL:HG21	1.83	0.43
2:J:57:SER:HB3	2:J:114:GLU:CB	2.48	0.43
2:K:38:VAL:C	2:K:39:ARG:HG3	2.44	0.43
1:C:297:ARG:HG2	1:C:297:ARG:HH11	1.82	0.43
1:D:296:LEU:HD22	1:D:300:ILE:CG2	2.49	0.43
1:D:317:GLN:HG3	1:D:342:PHE:CE1	2.53	0.43
2:H:55:PHE:HB3	2:H:58:PRO:HB3	2.00	0.43
2:I:89:PHE:CG	2:I:90:LEU:N	2.87	0.43
2:G:41:PRO:HB2	2:G:44:ASN:HD21	1.82	0.43
1:C:320:TRP:C	1:C:321:ILE:HD12	2.43	0.43
1:D:451:PRO:HG3	1:E:344:VAL:CG2	2.40	0.43
1:E:400:ALA:HA	1:E:412:MET:O	2.19	0.43
2:G:86:ARG:CA	2:G:97:LYS:HE2	2.42	0.43
1:A:327:SER:HA	1:A:331:LEU:O	2.19	0.43
1:A:408:THR:HA	1:A:409:PRO:HD3	1.80	0.43
1:C:303:VAL:O	1:C:304:SER:C	2.61	0.43
1:C:421:TRP:CZ2	1:C:424:GLY:HA2	2.53	0.43
1:D:323:ILE:CG2	1:D:334:ARG:HB2	2.49	0.43
1:C:302:ASP:OD1	1:C:305:GLY:O	2.36	0.42
1:D:355:PHE:HZ	1:D:446:MET:HE1	1.84	0.42
2:L:31:VAL:HG22	2:L:52:TYR:HB2	2.01	0.42
1:A:323:ILE:HD13	1:A:336:GLN:HA	2.00	0.42
1:A:449:SER:O	1:A:450:TYR:HB3	2.18	0.42
1:B:296:LEU:HD22	1:B:300:ILE:CG2	2.49	0.42
1:D:454:PHE:O	1:D:455:THR:CG2	2.64	0.42
1:F:298:TYR:CG	1:F:299:PRO:HA	2.54	0.42
2:G:86:ARG:HA	2:G:97:LYS:HG3	2.00	0.42
2:J:106:THR:HG21	2:J:123:LYS:HE3	2.01	0.42
2:L:107:TYR:N	2:L:107:TYR:CD1	2.87	0.42
1:A:400:ALA:HA	1:A:412:MET:O	2.19	0.42
1:F:320:TRP:C	1:F:321:ILE:HD12	2.44	0.42
2:I:103:ASP:HB3	2:I:107:TYR:OH	2.18	0.42
2:J:89:PHE:O	2:J:90:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:89:PHE:CG	2:K:90:LEU:N	2.87	0.42
2:L:46:VAL:HG12	2:L:99:VAL:CG1	2.50	0.42
2:L:72:LEU:HD21	2:L:75:TYR:HB3	2.00	0.42
1:C:321:ILE:HA	1:C:337:VAL:O	2.19	0.42
1:D:400:ALA:HA	1:D:412:MET:O	2.20	0.42
1:D:443:TRP:CD1	1:D:443:TRP:N	2.88	0.42
1:E:327:SER:HA	1:E:331:LEU:O	2.19	0.42
1:F:297:ARG:HG2	1:F:297:ARG:HH11	1.84	0.42
2:G:89:PHE:CG	2:G:90:LEU:N	2.86	0.42
2:H:57:SER:O	2:H:114:GLU:HG2	2.19	0.42
2:L:75:TYR:CE2	2:L:80:THR:HG22	2.54	0.42
1:B:408:THR:HA	1:B:409:PRO:HD3	1.68	0.42
1:D:419:GLU:HG2	1:D:427:ARG:NH2	2.34	0.42
2:J:30:THR:CG2	2:J:53:SER:HB3	2.50	0.42
1:B:443:TRP:N	1:B:443:TRP:CD1	2.88	0.42
2:J:40:ILE:HA	2:J:41:PRO:HD3	1.87	0.42
1:B:347:TYR:OH	1:C:344:VAL:HB	2.19	0.42
1:E:316:ARG:HB3	1:E:343:ILE:HB	1.99	0.42
1:E:324:VAL:HG22	1:E:368:LEU:HD22	2.01	0.42
1:F:375:LEU:HD12	1:F:376:PRO:CD	2.46	0.42
2:I:63:LYS:HE3	2:I:110:MET:HE1	2.02	0.42
2:J:62:TRP:CE3	2:J:109:CYS:HB2	2.54	0.42
2:K:116:GLY:O	2:K:119:TYR:HE1	2.01	0.42
1:B:366:LEU:HD12	1:B:366:LEU:HA	1.81	0.42
2:G:38:VAL:HG11	2:G:46:VAL:CG2	2.49	0.42
2:H:47:LYS:HB2	2:H:95:THR:CG2	2.50	0.42
1:C:378:LEU:HA	1:C:378:LEU:HD23	1.86	0.42
1:D:320:TRP:HB2	1:D:341:ILE:CD1	2.46	0.42
2:G:86:ARG:O	2:G:87:VAL:HG23	2.20	0.42
2:H:121:GLU:HG2	2:H:122:VAL:N	2.34	0.42
2:L:86:ARG:CB	2:L:97:LYS:HE2	2.50	0.42
2:I:61:GLU:HG2	2:I:110:MET:HE3	2.01	0.42
2:J:47:LYS:HB2	2:J:95:THR:HG22	2.02	0.42
1:B:321:ILE:HD13	1:B:375:LEU:HD11	2.02	0.41
1:D:360:ILE:O	1:D:360:ILE:HG13	2.20	0.41
1:F:384:GLU:HA	1:F:385:PRO:HD3	1.85	0.41
2:H:46:VAL:HG12	2:H:99:VAL:HG11	2.02	0.41
2:K:63:LYS:CE	2:K:110:MET:HE1	2.50	0.41
1:A:393:THR:HA	1:A:417:TRP:CD1	2.55	0.41
1:E:449:SER:O	1:E:450:TYR:HB3	2.19	0.41
1:F:400:ALA:HA	1:F:412:MET:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ILE:HD13	1:C:370:PHE:CZ	2.55	0.41
1:D:326:TYR:CE2	1:D:360:ILE:HA	2.55	0.41
1:D:454:PHE:C	1:D:455:THR:HG23	2.45	0.41
1:F:320:TRP:CZ2	1:F:322:GLY:HA3	2.54	0.41
1:F:416:LEU:HD12	1:F:430:VAL:HG22	2.02	0.41
1:B:317:GLN:HG3	1:B:342:PHE:CD1	2.54	0.41
1:D:317:GLN:HG3	1:D:342:PHE:CD1	2.55	0.41
1:E:366:LEU:HD12	1:E:366:LEU:HA	1.82	0.41
1:F:297:ARG:HA	1:F:297:ARG:HD3	1.92	0.41
2:G:40:ILE:HA	2:G:41:PRO:HD3	1.91	0.41
2:G:89:PHE:O	2:G:90:LEU:HG	2.20	0.41
2:H:89:PHE:CG	2:H:90:LEU:N	2.88	0.41
2:I:42:GLU:HG2	2:I:43:ASN:N	2.35	0.41
2:I:63:LYS:HD2	2:I:110:MET:HE1	2.01	0.41
2:L:113:GLU:CG	2:L:114:GLU:H	2.27	0.41
1:D:384:GLU:HA	1:D:385:PRO:HD3	1.89	0.41
2:I:50:CYS:HB2	2:I:62:TRP:CZ2	2.55	0.41
1:E:321:ILE:HA	1:E:337:VAL:O	2.20	0.41
2:G:29:VAL:HG12	2:G:54:GLY:O	2.20	0.41
2:G:57:SER:O	2:G:114:GLU:HG2	2.21	0.41
2:G:125:LYS:HB2	2:G:125:LYS:HE3	1.82	0.41
2:J:63:LYS:CE	2:J:110:MET:HE1	2.50	0.41
2:L:40:ILE:HG13	2:L:41:PRO:CD	2.49	0.41
1:A:339:SER:HB2	1:A:351:CYS:O	2.19	0.41
2:H:46:VAL:HG12	2:H:99:VAL:CG1	2.51	0.41
1:D:355:PHE:CZ	1:D:446:MET:HE1	2.54	0.41
1:F:399:VAL:O	1:F:399:VAL:HG13	2.21	0.41
1:D:336:GLN:CG	1:D:337:VAL:N	2.78	0.41
1:D:394:TYR:CE1	1:D:450:TYR:HA	2.55	0.41
1:D:418:VAL:HG13	1:D:426:LEU:HD11	2.02	0.41
1:F:378:LEU:HD23	1:F:378:LEU:HA	1.82	0.41
2:I:113:GLU:HB2	2:I:118:SER:HB2	2.03	0.41
2:K:63:LYS:HE3	2:K:110:MET:HE1	2.03	0.41
2:L:29:VAL:HB	2:L:55:PHE:CE1	2.55	0.41
1:A:433:GLY:O	1:B:411:TYR:CG	2.73	0.41
1:B:400:ALA:HA	1:B:412:MET:O	2.20	0.41
1:B:421:TRP:CZ2	1:B:424:GLY:HA2	2.56	0.41
1:D:371:VAL:O	2:J:63:LYS:CE	2.69	0.41
2:H:103:ASP:O	2:H:126:LEU:HD23	2.21	0.41
1:A:323:ILE:CG2	1:A:334:ARG:HB2	2.51	0.40
2:G:86:ARG:HG3	2:G:86:ARG:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:VAL:O	1:B:345:ASP:HB2	2.21	0.40
2:I:101:ARG:H	2:I:101:ARG:HG2	1.53	0.40
1:F:392:VAL:HG23	1:F:394:TYR:H	1.85	0.40
1:F:412:MET:HE3	1:F:433:GLY:O	2.21	0.40
2:J:65:ASP:HB2	2:J:106:THR:O	2.21	0.40
1:A:320:TRP:CZ2	1:A:322:GLY:HA3	2.57	0.40
1:A:392:VAL:HG23	1:A:418:VAL:O	2.22	0.40
1:B:319:MET:CB	1:B:375:LEU:HD22	2.52	0.40
1:D:449:SER:O	1:D:450:TYR:HB3	2.21	0.40
1:F:320:TRP:CE2	1:F:322:GLY:HA3	2.56	0.40
1:F:337:VAL:CG2	1:F:338:ASN:N	2.84	0.40
2:G:71:ARG:HB3	2:G:71:ARG:HH11	1.86	0.40
1:D:324:VAL:HG22	1:D:368:LEU:HD22	2.04	0.40
1:E:298:TYR:CG	1:E:299:PRO:HA	2.56	0.40
1:F:394:TYR:CD1	1:F:394:TYR:C	2.98	0.40
2:H:40:ILE:HD11	2:H:44:ASN:CB	2.51	0.40
2:H:45:PRO:HG3	2:H:97:LYS:O	2.22	0.40
2:I:30:THR:CG2	2:I:53:SER:HB3	2.51	0.40
2:K:61:GLU:HA	2:K:74:CYS:O	2.21	0.40
2:L:86:ARG:HB3	2:L:97:LYS:HE2	2.04	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	159/165 (96%)	140 (88%)	18 (11%)	1 (1%)	21	50
1	B	158/165 (96%)	143 (90%)	14 (9%)	1 (1%)	21	50
1	C	160/165 (97%)	144 (90%)	15 (9%)	1 (1%)	21	50
1	D	160/165 (97%)	139 (87%)	19 (12%)	2 (1%)	9	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	158/165 (96%)	144 (91%)	13 (8%)	1 (1%)	21	50
1	F	158/165 (96%)	143 (90%)	14 (9%)	1 (1%)	21	50
2	G	100/104 (96%)	89 (89%)	10 (10%)	1 (1%)	12	40
2	H	100/104 (96%)	88 (88%)	12 (12%)	0	100	100
2	I	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
2	J	100/104 (96%)	85 (85%)	13 (13%)	2 (2%)	6	25
2	K	100/104 (96%)	91 (91%)	9 (9%)	0	100	100
2	L	100/104 (96%)	89 (89%)	11 (11%)	0	100	100
All	All	1553/1614 (96%)	1385 (89%)	158 (10%)	10 (1%)	21	50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	407	GLY
2	J	116	GLY
2	J	68	ASP
1	C	407	GLY
1	A	407	GLY
1	D	407	GLY
1	F	407	GLY
2	G	87	VAL
1	E	407	GLY
1	D	377	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	135/138 (98%)	127 (94%)	8 (6%)	18	44
1	B	134/138 (97%)	124 (92%)	10 (8%)	12	38
1	C	136/138 (99%)	129 (95%)	7 (5%)	21	48
1	D	136/138 (99%)	124 (91%)	12 (9%)	9	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	134/138 (97%)	127 (95%)	7 (5%)	21	48
1	F	134/138 (97%)	128 (96%)	6 (4%)	24	51
2	G	93/94 (99%)	87 (94%)	6 (6%)	15	42
2	H	93/94 (99%)	87 (94%)	6 (6%)	15	42
2	I	93/94 (99%)	85 (91%)	8 (9%)	10	33
2	J	93/94 (99%)	87 (94%)	6 (6%)	15	42
2	K	93/94 (99%)	88 (95%)	5 (5%)	20	47
2	L	93/94 (99%)	85 (91%)	8 (9%)	10	33
All	All	1367/1392 (98%)	1278 (94%)	89 (6%)	15	42

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	MET
1	A	321	ILE
1	A	336	GLN
1	A	362	ASP
1	A	410	GLN
1	A	416	LEU
1	A	435	SER
1	A	436	ILE
1	B	319	MET
1	B	321	ILE
1	B	336	GLN
1	B	375	LEU
1	B	382	ASP
1	B	389	ASN
1	B	408	THR
1	B	416	LEU
1	B	431	GLU
1	B	437	THR
1	C	304	SER
1	C	319	MET
1	C	336	GLN
1	C	362	ASP
1	C	375	LEU
1	C	416	LEU
1	C	437	THR
1	D	294	PRO

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Mol	Chain	Res	Type
1	D	295	ASN
1	D	300	ILE
1	D	303	VAL
1	D	319	MET
1	D	336	GLN
1	D	337	VAL
1	D	355	PHE
1	D	375	LEU
1	D	416	LEU
1	D	436	ILE
1	D	437	THR
1	E	319	MET
1	E	321	ILE
1	E	336	GLN
1	E	362	ASP
1	E	377	PRO
1	E	416	LEU
1	E	437	THR
1	F	319	MET
1	F	325	SER
1	F	336	GLN
1	F	362	ASP
1	F	416	LEU
1	F	437	THR
2	G	39	ARG
2	G	65	ASP
2	G	71	ARG
2	G	72	LEU
2	G	86	ARG
2	G	101	ARG
2	H	35	GLU
2	H	39	ARG
2	H	65	ASP
2	H	71	ARG
2	H	72	LEU
2	H	74	CYS
2	I	37	GLU
2	I	39	ARG
2	I	65	ASP
2	I	69	THR
2	I	71	ARG
2	I	72	LEU

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Mol	Chain	Res	Type
2	I	74	CYS
2	I	101	ARG
2	J	35	GLU
2	J	65	ASP
2	J	71	ARG
2	J	72	LEU
2	J	101	ARG
2	J	114	GLU
2	K	39	ARG
2	K	65	ASP
2	K	71	ARG
2	K	72	LEU
2	K	119	TYR
2	L	28	SER
2	L	39	ARG
2	L	65	ASP
2	L	72	LEU
2	L	74	CYS
2	L	85	ASP
2	L	101	ARG
2	L	125	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	ASN
1	A	422	GLN
1	B	295	ASN
1	B	332	ASN
1	B	338	ASN
1	B	388	HIS
1	B	389	ASN
1	B	410	GLN
1	B	422	GLN
1	C	336	GLN
1	C	338	ASN
1	C	410	GLN
1	C	422	GLN
1	D	338	ASN
1	D	410	GLN
1	E	295	ASN
1	E	336	GLN

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Mol	Chain	Res	Type
1	E	338	ASN
1	E	410	GLN
1	F	295	ASN
1	F	332	ASN
1	F	336	GLN
1	F	338	ASN
1	F	388	HIS
1	F	410	GLN
2	G	32	HIS
2	G	44	ASN
2	H	44	ASN
2	I	44	ASN
2	J	43	ASN
2	J	117	ASN
2	K	44	ASN
2	L	44	ASN
2	L	66	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	161/165 (97%)	-0.15	0	100 100	32, 55, 76, 83	0
1	B	160/165 (96%)	-0.22	0	100 100	34, 47, 66, 75	0
1	C	162/165 (98%)	-0.17	0	100 100	36, 53, 75, 82	0
1	D	162/165 (98%)	-0.04	0	100 100	39, 59, 91, 95	0
1	E	160/165 (96%)	-0.12	0	100 100	34, 56, 72, 77	0
1	F	160/165 (96%)	-0.04	0	100 100	41, 60, 81, 88	0
2	G	102/104 (98%)	0.37	1 (0%)	79 66	70, 94, 111, 116	0
2	H	102/104 (98%)	0.05	1 (0%)	79 66	45, 61, 79, 85	0
2	I	102/104 (98%)	-0.06	0	100 100	39, 66, 88, 101	0
2	J	102/104 (98%)	0.30	2 (1%)	65 49	52, 73, 92, 104	0
2	K	102/104 (98%)	0.05	0	100 100	48, 66, 79, 89	0
2	L	102/104 (98%)	0.08	1 (0%)	79 66	46, 69, 90, 94	0
All	All	1577/1614 (97%)	-0.02	5 (0%)	90 84	32, 60, 92, 116	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	34	SER	2.4
2	J	50	CYS	2.3
2	G	50	CYS	2.1
2	H	50	CYS	2.1
2	L	85	ASP	2.0

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

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

6.3 Carbohydrates [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.