



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:02 AM UTC

PDB ID : 6GCU / pdb_00006gcu
Title : MET receptor in complex with InlB internalin domain and DARPin A3A
Authors : Meyer, T.; Andres, F.; Iamele, L.; Gherardi, E.; Pluckthun, A.; Niemann, H.H.
Deposited on : 2018-04-19
Resolution : 6.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

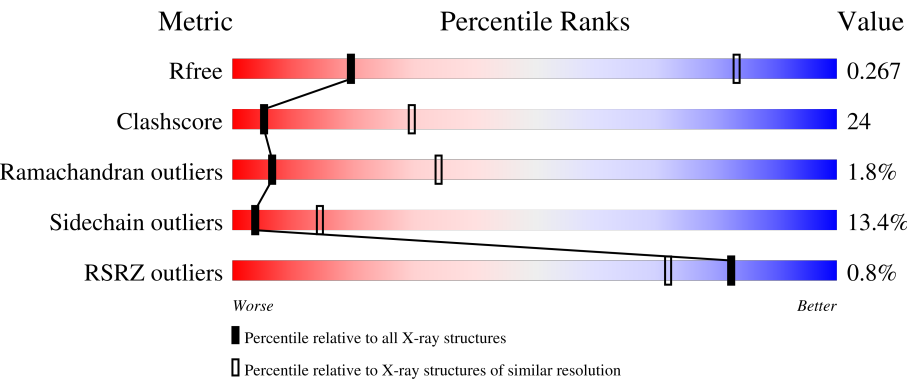
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1143 (8.00-4.00)
Clashscore	190562	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	727	% 49%34%9%7%
1	D	727	% 51%33%8%7%
2	B	289	% 50%45%.
2	E	289	% 52%42%5%
3	C	173	80%9%10%

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Mol	Chain	Length	Quality of chain
3	F	173	% 80% 8% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17448 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 Hepatocyte growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	675	Total	C	N	O	S	0	0	0
			5314	3370	904	1002	38			
1	D	675	Total	C	N	O	S	0	0	0
			5314	3370	904	1002	38			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLU	-	expression tag	UNP P08581
A	23	THR	-	expression tag	UNP P08581
A	24	ARG	-	expression tag	UNP P08581
A	742	LEU	-	expression tag	UNP P08581
A	743	HIS	-	expression tag	UNP P08581
A	744	HIS	-	expression tag	UNP P08581
A	745	HIS	-	expression tag	UNP P08581
A	746	HIS	-	expression tag	UNP P08581
A	747	HIS	-	expression tag	UNP P08581
A	748	HIS	-	expression tag	UNP P08581
D	22	GLU	-	expression tag	UNP P08581
D	23	THR	-	expression tag	UNP P08581
D	24	ARG	-	expression tag	UNP P08581
D	742	LEU	-	expression tag	UNP P08581
D	743	HIS	-	expression tag	UNP P08581
D	744	HIS	-	expression tag	UNP P08581
D	745	HIS	-	expression tag	UNP P08581
D	746	HIS	-	expression tag	UNP P08581
D	747	HIS	-	expression tag	UNP P08581
D	748	HIS	-	expression tag	UNP P08581

- Molecule 2 is a protein called Internalin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	286	Total	C	N	O	S	0	0	0
			2252	1435	378	437	2			
2	E	286	Total	C	N	O	S	0	0	0
			2252	1435	378	437	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	33	GLY	-	expression tag	UNP P25147
B	34	ALA	-	expression tag	UNP P25147
B	35	MET	-	expression tag	UNP P25147
E	33	GLY	-	expression tag	UNP P25147
E	34	ALA	-	expression tag	UNP P25147
E	35	MET	-	expression tag	UNP P25147

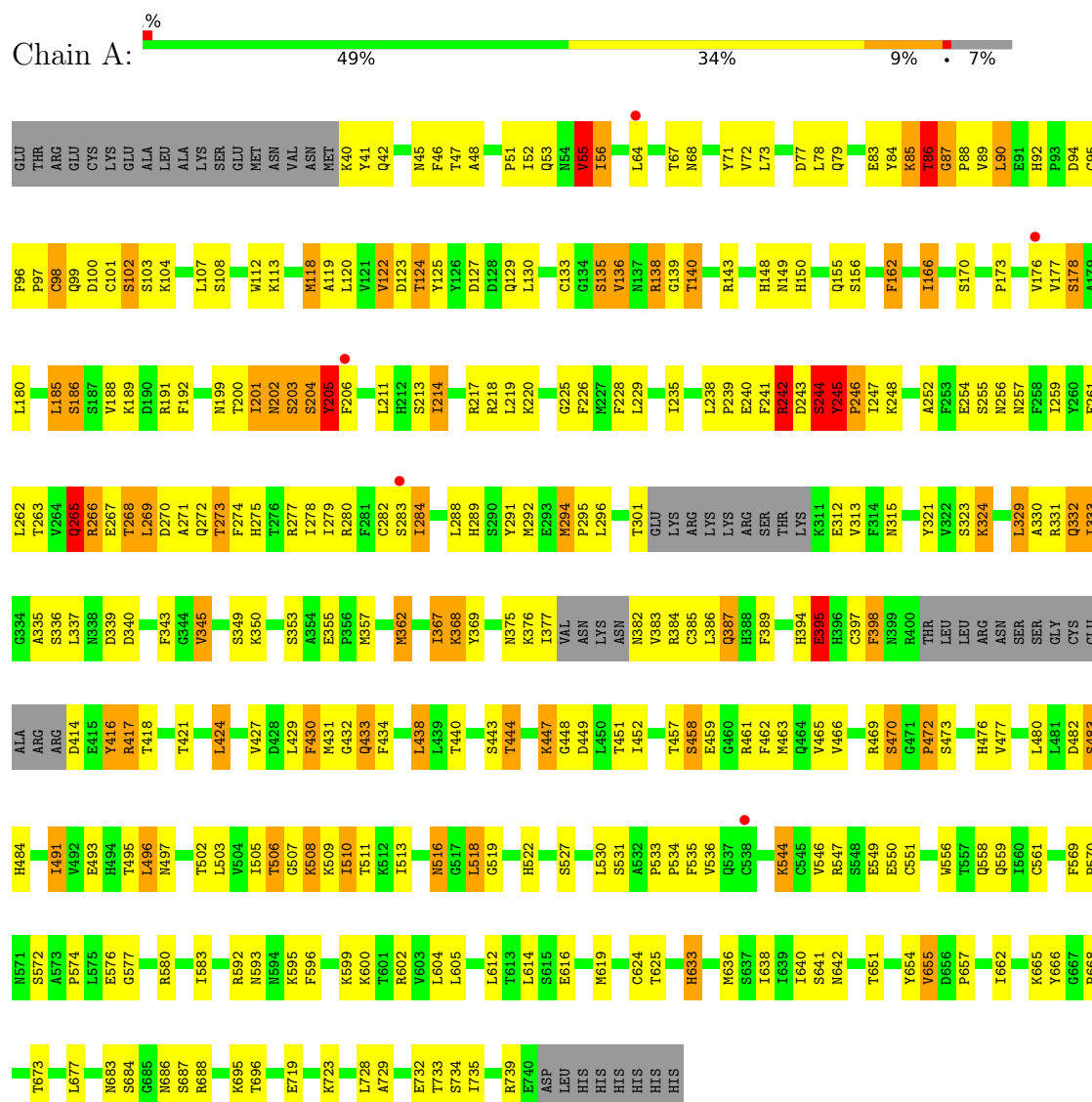
- Molecule 3 is a protein called DARPin A3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	155	Total	C	N	O	S	0	0	0
			1158	717	208	231	2			
3	F	155	Total	C	N	O	S	0	0	0
			1158	717	208	231	2			

3 Residue-property plots [i](#)

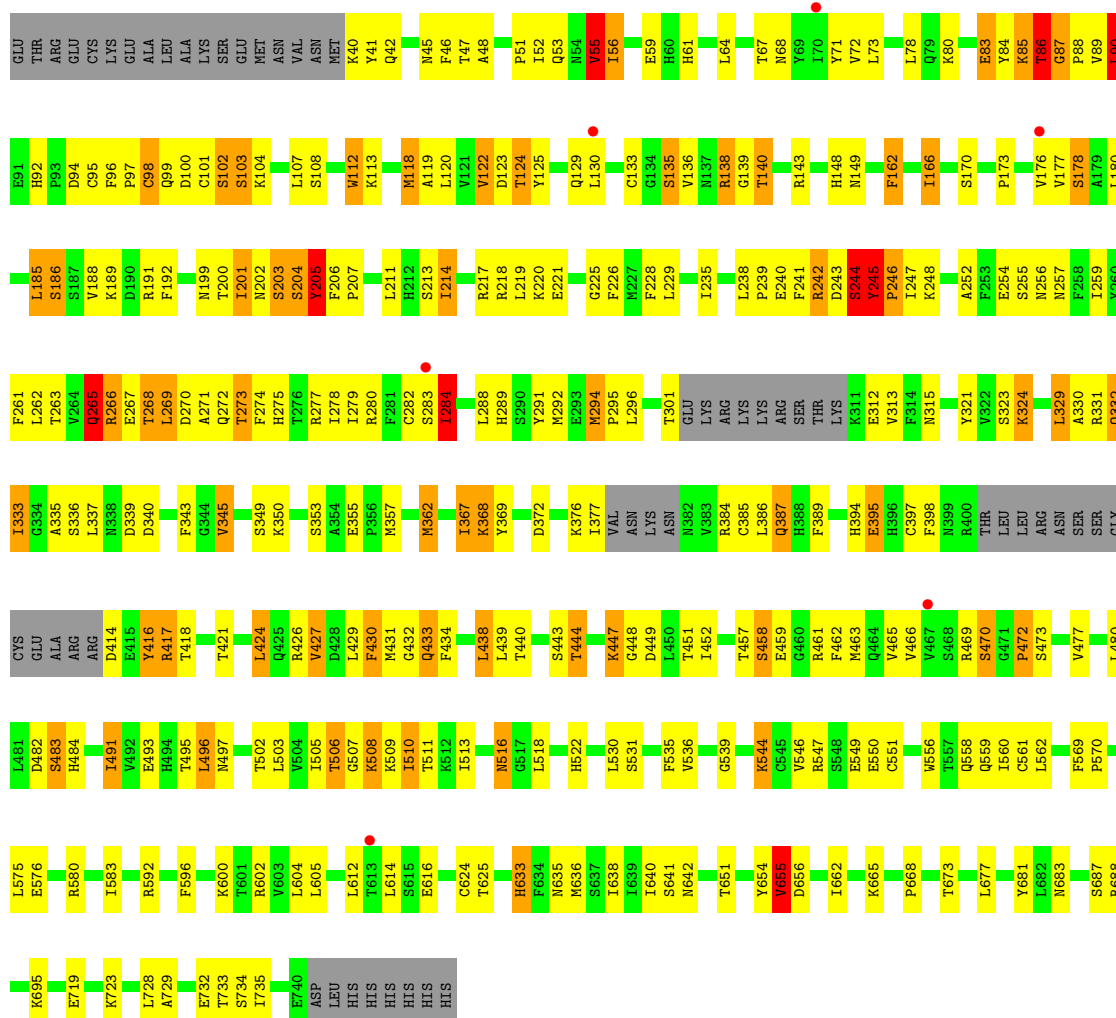
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Hepatocyte growth factor receptor

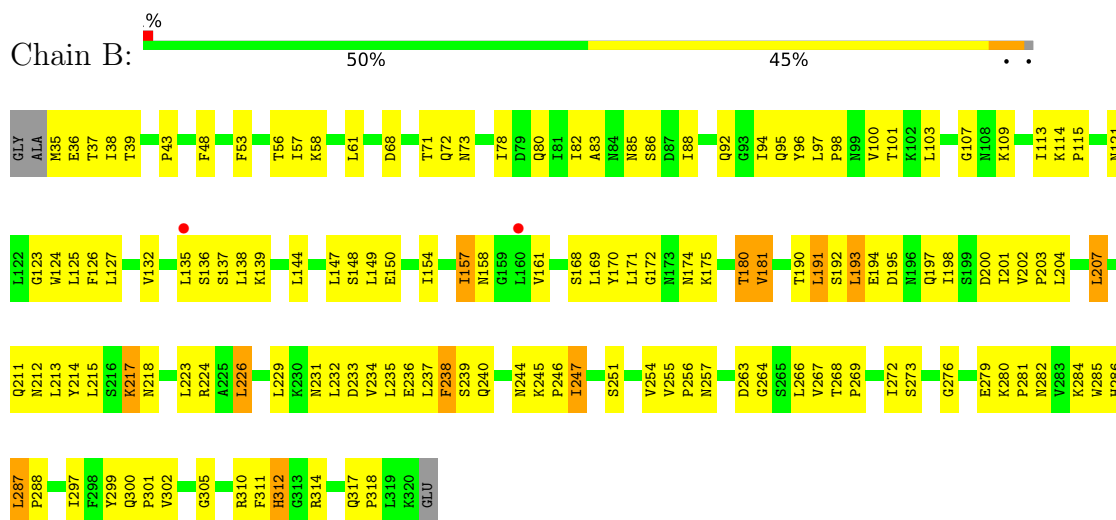


• Molecule 1: Hepatocyte growth factor receptor

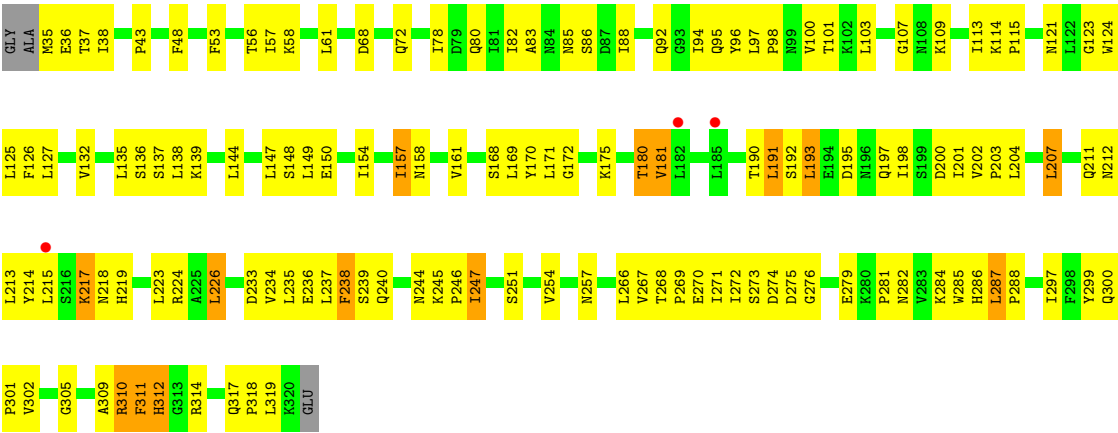




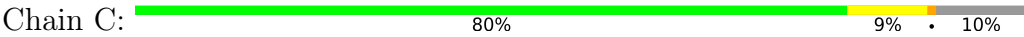
• Molecule 2: Internalin B



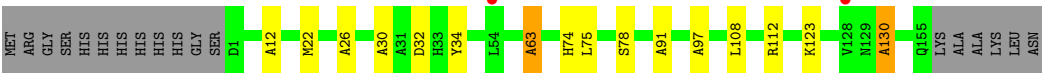
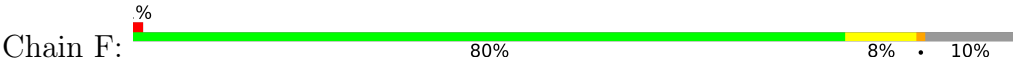
• Molecule 2: Internalin B



● Molecule 3: DARPin A3A



● Molecule 3: DARPin A3A



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	144.87Å 144.87Å 128.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.15 – 6.00 48.15 – 6.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.15-6.00) 99.7 (48.15-6.00)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 6.15Å)	Xtriage
Refinement program	PHENIX (dev_3071: ???)	Depositor
R, R_{free}	0.263 , 0.271 0.261 , 0.267	Depositor DCC
R_{free} test set	340 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	248.6	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 326.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l 0.042 for h,-h-k,-l 0.043 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	17448	wwPDB-VP
Average B, all atoms (Å ²)	317.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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	0.64	2/5439 (0.0%)	1.37	27/7377 (0.4%)
1	D	0.62	1/5439 (0.0%)	1.03	21/7377 (0.3%)
2	B	0.30	0/2288	0.77	4/3105 (0.1%)
2	E	0.31	0/2288	0.84	8/3105 (0.3%)
3	C	1.22	3/1175 (0.3%)	1.31	4/1594 (0.3%)
3	F	1.23	3/1175 (0.3%)	1.31	4/1594 (0.3%)
All	All	0.68	9/17804 (0.1%)	1.14	68/24152 (0.3%)

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	4
1	D	0	5
3	C	0	2
3	F	0	2
All	All	0	13

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	63	ALA	C-N	-30.70	0.92	1.33
3	F	63	ALA	C-N	-30.65	0.92	1.33
3	C	97	ALA	C-N	-16.18	1.11	1.33
3	F	97	ALA	C-N	-16.17	1.11	1.33
1	A	655	VAL	C-N	15.53	1.54	1.33
1	D	655	VAL	C-N	13.97	1.62	1.33
3	F	130	ALA	C-N	12.03	1.50	1.33
1	A	382	ASN	N-CA	-12.00	1.23	1.46
3	C	130	ALA	C-N	11.96	1.50	1.33

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	655	VAL	O-C-N	53.83	172.18	122.12
1	A	655	VAL	CA-C-N	-34.04	76.34	122.98
1	A	655	VAL	C-N-CA	-34.04	76.34	122.98
3	F	63	ALA	CA-C-N	24.80	155.93	120.71
3	F	63	ALA	C-N-CA	24.80	155.93	120.71
3	C	63	ALA	CA-C-N	24.59	155.63	120.71
3	C	63	ALA	C-N-CA	24.59	155.63	120.71
1	A	382	ASN	N-CA-CB	22.45	148.66	110.50
3	F	63	ALA	O-C-N	-22.35	94.80	122.96
3	C	63	ALA	O-C-N	-22.10	95.12	122.96
1	A	382	ASN	N-CA-C	-18.98	57.87	111.00
3	C	30	ALA	O-C-N	-16.92	102.75	123.06
3	F	30	ALA	O-C-N	-16.87	102.82	123.06
2	E	238	PHE	N-CA-C	12.56	129.29	109.07
2	B	238	PHE	N-CA-C	12.55	129.28	109.07
2	E	310	ARG	N-CA-C	12.46	132.59	107.41
1	D	245	TYR	N-CA-C	10.50	117.67	108.22
1	A	245	TYR	N-CA-C	10.43	117.61	108.22
1	D	655	VAL	O-C-N	-7.30	114.93	123.03
1	D	516	ASN	N-CA-C	7.12	121.66	112.12
1	D	430	PHE	N-CA-C	-7.05	104.70	113.38
1	A	516	ASN	N-CA-C	7.00	121.50	112.12
1	A	383	VAL	N-CA-C	6.82	117.71	107.75
1	A	430	PHE	N-CA-C	-6.65	105.20	113.38
1	A	102	SER	N-CA-C	-6.61	104.79	112.92
1	D	102	SER	N-CA-C	-6.57	104.84	112.92
1	D	452	ILE	N-CA-C	6.15	116.73	107.75
1	A	332	GLN	N-CA-C	6.10	118.01	111.36
1	A	452	ILE	N-CA-C	6.09	116.64	107.75
1	D	332	GLN	N-CA-C	6.08	117.99	111.36
2	E	274	ASP	CB-CA-C	6.05	119.57	111.82
2	E	309	ALA	N-CA-C	6.01	119.01	109.81
2	E	311	PHE	N-CA-CB	5.87	119.23	109.60
1	D	289	HIS	CA-C-N	-5.76	114.05	122.06
1	D	289	HIS	C-N-CA	-5.76	114.05	122.06
1	A	289	HIS	CA-C-N	-5.71	114.12	122.06
1	A	289	HIS	C-N-CA	-5.71	114.12	122.06
1	A	166	ILE	N-CA-C	5.62	116.84	112.12
1	A	86	THR	N-CA-C	-5.56	106.26	113.16
1	D	86	THR	N-CA-C	-5.56	106.27	113.16
1	A	46	PHE	N-CA-C	5.48	118.55	109.46
1	D	46	PHE	N-CA-C	5.46	118.52	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	TYR	CB-CA-C	5.44	117.40	110.22
1	A	101	CYS	N-CA-C	5.41	117.02	107.61
1	D	245	TYR	CB-CA-C	5.41	117.36	110.22
2	B	245	LYS	CA-C-N	5.40	126.59	119.84
2	B	245	LYS	C-N-CA	5.40	126.59	119.84
1	D	101	CYS	N-CA-C	5.38	116.97	107.61
1	D	90	LEU	N-CA-C	5.38	117.49	108.73
1	A	90	LEU	N-CA-C	5.37	117.49	108.73
1	D	166	ILE	N-CA-C	5.35	116.62	112.12
2	E	245	LYS	CA-C-N	5.34	126.52	119.84
2	E	245	LYS	C-N-CA	5.34	126.52	119.84
1	D	135	SER	CA-C-N	-5.31	117.72	123.08
1	D	135	SER	C-N-CA	-5.31	117.72	123.08
1	D	125	TYR	N-CA-C	-5.20	105.52	111.14
2	B	238	PHE	N-CA-CB	-5.18	102.44	110.57
1	A	125	TYR	N-CA-C	-5.16	105.57	111.14
2	E	238	PHE	N-CA-CB	-5.14	102.50	110.57
1	A	136	VAL	CB-CA-C	5.12	116.30	111.44
1	A	135	SER	CA-C-N	-5.11	117.92	123.08
1	A	135	SER	C-N-CA	-5.11	117.92	123.08
1	D	473	SER	N-CA-C	5.08	117.27	110.35
1	A	55	VAL	N-CA-C	5.08	115.23	108.27
1	A	202	ASN	N-CA-C	5.07	119.19	112.30
1	D	284	ILE	N-CA-C	5.07	115.57	108.17
1	A	473	SER	N-CA-C	5.05	117.22	110.35
1	D	55	VAL	N-CA-C	5.05	115.19	108.27

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	SER	Peptide
1	A	244	SER	Peptide
1	A	265	GLN	Peptide
1	A	274	PHE	Peptide
3	C	130	ALA	Mainchain
3	C	63	ALA	Mainchain
1	D	135	SER	Peptide
1	D	244	SER	Peptide
1	D	265	GLN	Peptide
1	D	274	PHE	Peptide
1	D	655	VAL	Mainchain

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Mol	Chain	Res	Type	Group
3	F	130	ALA	Mainchain
3	F	63	ALA	Mainchain

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	5314	0	5162	317	23
1	D	5314	0	5159	330	17
2	B	2252	0	2322	193	14
2	E	2252	0	2322	182	5
3	C	1158	0	1132	32	11
3	F	1158	0	1130	33	9
All	All	17448	0	17227	847	44

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 24.

All (847) 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:732:GLU:OE2	1:D:723:LYS:NZ	1.60	1.35
2:B:264:GLY:HA3	2:E:180:THR:CG2	1.57	1.31
1:D:602:ARG:NH2	2:E:170:TYR:OH	1.66	1.28
1:D:372:ASP:HB3	2:E:275:ASP:OD1	1.14	1.27
1:D:41:TYR:HE1	1:D:522:HIS:CD2	1.52	1.27
1:A:127:ASP:OD1	3:C:45:LYS:NZ	1.68	1.26
1:D:41:TYR:CE1	1:D:522:HIS:HD2	1.53	1.26
1:A:531:SER:OG	1:A:596:PHE:CE2	1.85	1.24
1:D:41:TYR:CE1	1:D:522:HIS:CD2	2.26	1.22
1:D:560:ILE:HG23	1:D:562:LEU:CD1	1.70	1.19
1:D:191:ARG:NH2	3:F:74:HIS:HB3	1.54	1.19
1:A:735:ILE:HG13	1:D:735:ILE:CG2	1.72	1.18
1:A:735:ILE:HG21	1:D:735:ILE:CG1	1.74	1.17
1:D:470:SER:OG	2:E:238:PHE:HB3	1.44	1.17
1:D:614:LEU:HD12	2:E:234:VAL:HG23	1.29	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:ILE:HD12	1:D:735:ILE:HD12	1.22	1.15
1:A:602:ARG:NH2	2:B:170:TYR:OH	1.80	1.14
1:D:376:LYS:HD2	2:E:275:ASP:HB3	1.18	1.12
1:D:614:LEU:CD1	2:E:234:VAL:CG2	2.26	1.12
1:D:614:LEU:HD13	2:E:234:VAL:CG2	1.79	1.11
1:D:560:ILE:HG23	1:D:562:LEU:HD11	1.17	1.11
1:D:560:ILE:CG2	1:D:562:LEU:CD1	2.28	1.10
2:B:264:GLY:HA3	2:E:180:THR:HG21	1.18	1.09
1:A:614:LEU:HB2	2:B:233:ASP:OD2	1.53	1.08
1:A:735:ILE:CG1	1:D:735:ILE:HG21	1.84	1.08
1:D:614:LEU:CD1	2:E:234:VAL:HG21	1.83	1.08
1:A:245:TYR:HB2	1:A:246:PRO:HD3	1.36	1.07
1:A:599:LYS:NZ	2:B:214:TYR:CD2	2.05	1.06
1:D:560:ILE:CG2	1:D:562:LEU:HD11	1.86	1.05
1:D:559:GLN:O	1:D:561:CYS:N	1.89	1.05
1:A:191:ARG:HH22	3:C:74:HIS:C	1.65	1.04
1:A:735:ILE:HG21	1:D:735:ILE:HG13	1.05	1.04
1:A:655:VAL:HG23	1:A:657:PRO:HD3	1.39	1.04
1:D:245:TYR:HB2	1:D:246:PRO:HD3	1.36	1.04
1:D:41:TYR:OH	1:D:522:HIS:NE2	1.91	1.03
1:A:602:ARG:HH21	2:B:168:SER:HB3	1.23	1.03
1:D:604:LEU:HD11	2:E:124:TRP:CZ2	1.94	1.02
2:B:224:ARG:HD3	2:E:180:THR:HG23	1.40	1.01
1:D:191:ARG:HH21	3:F:74:HIS:HB3	1.25	1.01
1:D:614:LEU:HD13	2:E:234:VAL:HG21	1.03	1.01
2:B:264:GLY:CA	2:E:180:THR:HG21	1.89	1.00
2:B:301:PRO:HB3	2:B:310:ARG:HG2	1.43	1.00
1:D:372:ASP:CB	2:E:275:ASP:OD1	2.09	1.00
1:A:191:ARG:HH12	3:C:75:LEU:HA	1.26	0.99
1:A:191:ARG:NH2	3:C:74:HIS:HB3	1.78	0.99
1:A:191:ARG:HH21	3:C:74:HIS:HB3	1.29	0.98
1:D:191:ARG:HH22	3:F:74:HIS:C	1.69	0.98
1:A:191:ARG:NH2	3:C:74:HIS:C	2.23	0.97
1:A:641:SER:HB3	2:B:124:TRP:CZ3	2.01	0.96
1:A:376:LYS:O	1:A:377:ILE:C	2.09	0.95
1:A:447:LYS:HD2	1:A:535:PHE:CB	1.95	0.95
1:A:604:LEU:CD1	2:B:124:TRP:CZ2	2.50	0.94
2:B:264:GLY:HA3	2:E:180:THR:HG22	1.49	0.94
1:A:600:LYS:HE3	2:B:126:PHE:CE1	2.03	0.93
1:A:735:ILE:CG2	1:D:735:ILE:CD1	2.46	0.93
2:B:193:LEU:HD22	2:B:198:ILE:HD11	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TYR:OH	1:A:522:HIS:CD2	2.21	0.92
1:D:576:GLU:CD	1:D:729:ALA:HB2	1.95	0.92
1:D:614:LEU:CD1	2:E:234:VAL:HG23	1.95	0.92
1:D:470:SER:HG	2:E:238:PHE:HB3	1.29	0.91
1:A:735:ILE:HG13	1:D:735:ILE:HG21	0.95	0.91
1:A:735:ILE:HG23	1:D:735:ILE:CD1	2.00	0.91
1:D:148:HIS:CE1	3:F:12:ALA:HA	2.06	0.91
1:A:531:SER:OG	1:A:596:PHE:HE2	1.32	0.91
1:D:85:LYS:H	1:D:85:LYS:HD2	1.35	0.91
1:D:426:ARG:CZ	2:E:271:ILE:HG23	2.00	0.91
2:E:193:LEU:HD22	2:E:198:ILE:HD11	1.51	0.90
1:A:447:LYS:HD2	1:A:535:PHE:HB3	1.50	0.90
1:A:85:LYS:H	1:A:85:LYS:HD2	1.35	0.90
1:A:735:ILE:CG2	1:D:735:ILE:HG13	1.98	0.90
1:A:127:ASP:CG	3:C:45:LYS:HZ1	1.79	0.90
2:B:301:PRO:CB	2:B:310:ARG:HG2	2.02	0.89
1:A:256:ASN:HD22	1:A:367:ILE:HD11	1.38	0.88
1:D:604:LEU:CD1	2:E:124:TRP:CZ2	2.57	0.88
1:D:427:VAL:HG23	2:E:270:GLU:OE2	1.73	0.88
1:A:127:ASP:CG	3:C:45:LYS:NZ	2.30	0.88
1:D:469:ARG:NE	2:E:299:TYR:CE2	2.40	0.88
1:D:256:ASN:HD22	1:D:367:ILE:HD11	1.38	0.87
1:A:430:PHE:O	1:A:431:MET:HG2	1.74	0.87
1:D:191:ARG:NH2	3:F:74:HIS:CB	2.37	0.87
1:A:723:LYS:NZ	1:D:732:GLU:OE2	2.08	0.87
1:D:430:PHE:O	1:D:431:MET:HG2	1.75	0.87
1:D:191:ARG:HH12	3:F:75:LEU:HA	1.39	0.86
1:A:735:ILE:HG23	1:D:735:ILE:HD12	1.58	0.86
1:D:191:ARG:CZ	3:F:108:LEU:HD13	2.05	0.86
1:A:124:THR:HG22	3:C:34:TYR:HE2	1.40	0.86
1:D:576:GLU:HB3	1:D:728:LEU:HB2	1.58	0.86
1:A:604:LEU:HD11	2:B:124:TRP:CZ2	2.10	0.85
1:A:735:ILE:CD1	1:D:735:ILE:HG23	2.07	0.85
1:A:574:PRO:HB2	1:A:729:ALA:HB2	1.57	0.84
1:D:426:ARG:NH2	2:E:271:ILE:HG23	1.93	0.84
1:D:516:ASN:C	1:D:535:PHE:HE1	1.85	0.84
1:D:600:LYS:HZ1	2:E:126:PHE:HE1	1.22	0.84
1:D:600:LYS:HE3	2:E:126:PHE:CE1	2.13	0.83
1:A:332:GLN:NE2	1:A:469:ARG:H	1.77	0.83
1:D:191:ARG:NH2	3:F:74:HIS:C	2.36	0.83
1:A:614:LEU:CD1	2:B:212:ASN:OD1	2.27	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:GLN:NE2	1:D:469:ARG:H	1.77	0.82
1:A:516:ASN:O	1:A:535:PHE:HE1	1.59	0.82
1:D:531:SER:OG	1:D:596:PHE:CE2	2.32	0.82
1:A:269:LEU:H	1:A:269:LEU:CD2	1.92	0.82
1:A:614:LEU:HD11	2:B:212:ASN:OD1	1.77	0.82
1:D:41:TYR:CZ	1:D:522:HIS:CD2	2.68	0.82
1:D:376:LYS:O	1:D:377:ILE:C	2.22	0.82
1:D:560:ILE:CG2	1:D:562:LEU:HD12	2.10	0.82
1:D:269:LEU:H	1:D:269:LEU:CD2	1.92	0.81
1:D:600:LYS:NZ	2:E:126:PHE:HE1	1.77	0.81
1:A:469:ARG:NE	2:B:299:TYR:CE2	2.48	0.81
2:E:157:ILE:HG12	2:E:181:VAL:HG11	1.62	0.81
1:A:735:ILE:CG1	1:D:735:ILE:CG2	2.50	0.81
1:A:574:PRO:CB	1:A:729:ALA:HB2	2.10	0.81
2:B:157:ILE:HG12	2:B:181:VAL:HG11	1.62	0.81
1:A:735:ILE:CG2	1:D:735:ILE:CG1	2.58	0.81
1:A:239:PRO:HA	1:A:242:ARG:HD2	1.64	0.80
1:A:162:PHE:C	1:A:162:PHE:HD1	1.89	0.79
1:A:735:ILE:CG2	1:D:735:ILE:HD12	2.12	0.79
1:A:245:TYR:HB2	1:A:246:PRO:CD	2.12	0.79
1:A:735:ILE:HG21	1:D:735:ILE:CD1	2.12	0.79
1:D:162:PHE:C	1:D:162:PHE:HD1	1.89	0.79
2:E:226:LEU:H	2:E:226:LEU:HD12	1.48	0.79
1:D:600:LYS:CE	2:E:126:PHE:CE1	2.66	0.79
1:D:239:PRO:HA	1:D:242:ARG:HD2	1.64	0.79
1:D:530:LEU:HD12	1:D:561:CYS:SG	2.22	0.79
2:B:301:PRO:HA	2:B:310:ARG:HA	1.64	0.78
1:D:191:ARG:HH22	3:F:74:HIS:HB3	1.46	0.78
1:A:572:SER:OG	1:A:684:SER:HB3	1.83	0.78
1:D:469:ARG:NE	2:E:299:TYR:CD2	2.52	0.78
2:B:285:TRP:HB3	2:B:287:LEU:HD13	1.66	0.78
1:A:315:ASN:HD21	1:A:349:SER:HB2	1.49	0.78
1:A:431:MET:SD	2:B:310:ARG:NH1	2.57	0.78
1:D:191:ARG:NH2	3:F:108:LEU:CD1	2.47	0.78
1:A:516:ASN:O	1:A:535:PHE:CE1	2.37	0.77
1:A:602:ARG:NH2	2:B:168:SER:HB3	1.97	0.77
1:A:129:GLN:HE22	1:A:143:ARG:HE	1.31	0.77
1:A:600:LYS:CE	2:B:126:PHE:CE1	2.68	0.77
1:D:129:GLN:HE22	1:D:143:ARG:HE	1.31	0.77
1:D:655:VAL:HB	1:D:681:TYR:CG	2.20	0.77
1:A:470:SER:OG	2:B:238:PHE:HB3	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:ILE:HB	2:B:317:GLN:HE21	1.49	0.77
1:D:604:LEU:HD11	2:E:124:TRP:HZ2	1.50	0.77
1:D:516:ASN:HB3	1:D:535:PHE:CE1	2.20	0.77
2:E:247:ILE:HB	2:E:317:GLN:HE21	1.49	0.77
2:B:226:LEU:HD12	2:B:226:LEU:H	1.48	0.76
1:A:162:PHE:C	1:A:162:PHE:CD1	2.63	0.76
1:D:560:ILE:HG23	1:D:562:LEU:CG	2.15	0.76
1:D:245:TYR:HB2	1:D:246:PRO:CD	2.12	0.76
2:B:224:ARG:NH1	2:E:202:VAL:HB	2.00	0.76
1:D:516:ASN:O	1:D:535:PHE:CE1	2.38	0.76
1:D:315:ASN:HD21	1:D:349:SER:HB2	1.49	0.75
1:A:600:LYS:HD2	2:B:170:TYR:CZ	2.21	0.75
2:E:285:TRP:HB3	2:E:287:LEU:HD13	1.66	0.75
1:D:427:VAL:CG2	2:E:270:GLU:OE2	2.34	0.75
1:D:516:ASN:CB	1:D:535:PHE:CE1	2.70	0.75
1:D:221:GLU:OE2	3:F:112:ARG:NH2	2.18	0.75
1:A:572:SER:OG	1:A:684:SER:CB	2.35	0.75
2:B:113:ILE:HG13	2:B:137:SER:HB2	1.68	0.75
1:D:469:ARG:HE	2:E:299:TYR:HE2	1.33	0.75
1:D:516:ASN:C	1:D:535:PHE:CE1	2.65	0.75
1:D:191:ARG:NE	3:F:108:LEU:CD1	2.50	0.74
1:A:516:ASN:OD1	1:A:535:PHE:CD1	2.40	0.74
1:A:191:ARG:NH2	3:C:74:HIS:O	2.20	0.74
1:D:505:ILE:HG13	1:D:510:ILE:HD12	1.70	0.74
1:D:426:ARG:NH1	2:E:271:ILE:CG2	2.50	0.74
1:A:505:ILE:HG13	1:A:510:ILE:HD12	1.70	0.74
1:D:191:ARG:NE	3:F:108:LEU:HD13	2.01	0.74
1:A:332:GLN:HE22	1:A:469:ARG:H	1.34	0.74
1:D:162:PHE:C	1:D:162:PHE:CD1	2.63	0.74
2:E:113:ILE:HG13	2:E:137:SER:HB2	1.68	0.73
1:D:560:ILE:HG22	1:D:562:LEU:HD12	1.69	0.73
2:B:224:ARG:HD3	2:E:180:THR:CG2	2.18	0.73
1:D:332:GLN:HE22	1:D:469:ARG:H	1.34	0.73
1:A:52:ILE:HD13	1:A:64:LEU:HD22	1.72	0.72
1:A:447:LYS:HD2	1:A:535:PHE:HB2	1.71	0.72
1:A:600:LYS:HD3	2:B:170:TYR:CE2	2.24	0.72
1:A:614:LEU:HD12	2:B:233:ASP:OD2	1.90	0.72
1:D:331:ARG:HG2	2:E:314:ARG:NH2	2.04	0.72
1:A:245:TYR:CB	1:A:246:PRO:HD3	2.18	0.72
1:D:600:LYS:NZ	2:E:126:PHE:CE1	2.56	0.72
1:A:600:LYS:HA	2:B:170:TYR:OH	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:ARG:HH21	3:F:108:LEU:HD11	1.55	0.71
1:A:599:LYS:HE3	2:B:234:VAL:HG11	1.72	0.71
2:B:247:ILE:HB	2:B:317:GLN:NE2	2.05	0.71
1:A:600:LYS:HE3	2:B:126:PHE:HE1	1.53	0.71
2:E:247:ILE:HB	2:E:317:GLN:NE2	2.05	0.71
1:A:97:PRO:HG2	1:A:162:PHE:HE2	1.56	0.70
1:A:191:ARG:NH2	3:C:74:HIS:CB	2.54	0.70
1:D:426:ARG:NH1	2:E:271:ILE:HG23	2.07	0.70
1:D:602:ARG:HH21	2:E:168:SER:HB3	1.57	0.70
1:D:41:TYR:OH	1:D:522:HIS:CD2	2.43	0.70
1:D:614:LEU:HD12	2:E:234:VAL:CG2	1.97	0.70
1:D:191:ARG:CZ	3:F:108:LEU:CD1	2.70	0.70
1:A:636:MET:HE1	1:A:654:TYR:HD2	1.56	0.70
1:D:52:ILE:HD13	1:D:64:LEU:HD22	1.71	0.70
1:D:331:ARG:CG	2:E:314:ARG:HH22	2.04	0.69
1:D:655:VAL:HB	1:D:681:TYR:CD1	2.27	0.69
1:A:600:LYS:CE	2:B:126:PHE:HE1	2.05	0.69
1:D:636:MET:HE1	1:D:654:TYR:HD2	1.56	0.69
1:A:531:SER:OG	1:A:596:PHE:CD2	2.44	0.69
1:A:735:ILE:CD1	1:D:735:ILE:HD12	2.13	0.69
2:B:80:GLN:HE21	2:B:82:ILE:HD11	1.58	0.69
1:D:41:TYR:CZ	1:D:522:HIS:NE2	2.61	0.69
1:A:191:ARG:HD3	3:C:78:SER:OG	1.93	0.69
1:D:600:LYS:CE	2:E:126:PHE:HE1	2.06	0.69
1:A:431:MET:HE3	1:A:472:PRO:HA	1.73	0.69
2:E:80:GLN:HE21	2:E:82:ILE:HD11	1.58	0.69
1:A:476:HIS:ND1	1:A:533:PRO:HG2	2.08	0.68
1:D:97:PRO:HG2	1:D:162:PHE:HE2	1.56	0.68
1:D:191:ARG:HH21	3:F:108:LEU:CD1	2.07	0.68
1:D:602:ARG:HH22	2:E:170:TYR:HH	1.41	0.68
1:D:191:ARG:HE	3:F:108:LEU:CD1	2.07	0.67
2:B:204:LEU:HA	2:B:207:LEU:HD22	1.77	0.67
1:D:275:HIS:CE1	1:D:295:PRO:HB3	2.30	0.67
1:D:191:ARG:HH22	3:F:74:HIS:CB	2.01	0.66
1:D:614:LEU:HD11	2:E:212:ASN:OD1	1.95	0.66
2:E:254:VAL:HG22	2:E:284:LYS:HG2	1.78	0.66
1:A:275:HIS:CE1	1:A:295:PRO:HB3	2.30	0.66
1:A:614:LEU:CB	2:B:233:ASP:OD2	2.38	0.66
2:B:202:VAL:HB	2:E:224:ARG:HH12	1.61	0.66
1:A:735:ILE:CD1	1:D:735:ILE:CG2	2.73	0.65
2:B:192:SER:O	2:B:193:LEU:HG	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:576:GLU:OE2	1:D:729:ALA:CB	2.43	0.65
1:D:470:SER:OG	2:E:238:PHE:CB	2.33	0.65
2:E:192:SER:O	2:E:193:LEU:HG	1.96	0.65
1:A:719:GLU:HB3	1:D:735:ILE:HG13	1.79	0.65
2:B:202:VAL:CG1	2:E:224:ARG:NH1	2.60	0.65
2:E:204:LEU:HA	2:E:207:LEU:HD22	1.77	0.65
2:B:254:VAL:HG22	2:B:284:LYS:HG2	1.77	0.65
1:D:431:MET:HE3	1:D:472:PRO:HA	1.79	0.64
1:D:516:ASN:O	1:D:535:PHE:CZ	2.50	0.64
1:D:138:ARG:HA	1:D:138:ARG:HH11	1.62	0.64
1:A:127:ASP:OD2	3:C:45:LYS:NZ	2.29	0.64
1:D:331:ARG:HG3	2:E:314:ARG:HH22	1.62	0.64
2:B:235:LEU:HD12	2:B:236:GLU:H	1.63	0.64
1:D:560:ILE:HG22	1:D:562:LEU:CD1	2.23	0.64
2:E:235:LEU:HD12	2:E:236:GLU:H	1.63	0.64
1:A:191:ARG:NE	3:C:108:LEU:HD13	2.12	0.64
1:A:600:LYS:NZ	2:B:126:PHE:HE1	1.95	0.64
1:A:469:ARG:HD3	2:B:299:TYR:HD2	1.62	0.64
1:A:735:ILE:HD12	1:D:735:ILE:HG23	1.79	0.64
1:A:600:LYS:CD	2:B:170:TYR:CE2	2.81	0.64
2:B:236:GLU:HG2	2:B:238:PHE:CE2	2.32	0.64
1:A:138:ARG:HA	1:A:138:ARG:HH11	1.62	0.64
1:A:604:LEU:HD12	2:B:124:TRP:CZ2	2.31	0.63
2:B:35:MET:HE3	2:B:35:MET:HA	1.79	0.63
1:D:426:ARG:NH1	2:E:271:ILE:HG21	2.12	0.63
1:D:457:THR:HG22	1:D:459:GLU:H	1.63	0.63
1:D:576:GLU:CD	1:D:729:ALA:CB	2.71	0.63
1:A:457:THR:HG22	1:A:459:GLU:H	1.63	0.63
1:A:518:LEU:O	1:A:519:GLY:O	2.17	0.63
2:E:236:GLU:HG2	2:E:238:PHE:CE2	2.33	0.63
1:A:469:ARG:HD3	2:B:299:TYR:CD2	2.34	0.63
2:E:35:MET:HE3	2:E:35:MET:HA	1.79	0.63
1:A:641:SER:CB	2:B:124:TRP:CZ3	2.81	0.63
1:A:269:LEU:H	1:A:269:LEU:HD22	1.63	0.62
1:A:614:LEU:HD11	2:B:212:ASN:CG	2.25	0.62
2:B:36:GLU:HG3	2:B:95:GLN:HB3	1.80	0.62
2:B:202:VAL:HB	2:E:224:ARG:NH1	2.14	0.62
2:B:86:SER:HB2	2:B:88:ILE:HG13	1.81	0.62
1:D:191:ARG:NH2	3:F:74:HIS:O	2.33	0.62
2:E:36:GLU:HG3	2:E:95:GLN:HB3	1.80	0.62
1:D:580:ARG:NH2	1:D:616:GLU:OE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:HIS:CE1	3:C:11:ARG:NH1	2.68	0.62
1:D:600:LYS:HD2	2:E:170:TYR:CZ	2.34	0.62
1:D:604:LEU:CD1	2:E:124:TRP:HZ2	2.09	0.62
1:A:580:ARG:NH2	1:A:616:GLU:OE2	2.33	0.61
2:E:94:ILE:HD12	2:E:97:LEU:HD13	1.82	0.61
2:B:94:ILE:HD12	2:B:97:LEU:HD13	1.82	0.61
1:A:476:HIS:CG	1:A:533:PRO:CG	2.84	0.61
2:B:224:ARG:HH12	2:E:202:VAL:HB	1.65	0.61
1:D:576:GLU:OE2	1:D:729:ALA:HA	2.01	0.61
1:A:482:ASP:HB2	1:A:506:THR:HG21	1.82	0.61
1:D:269:LEU:H	1:D:269:LEU:HD22	1.63	0.61
2:E:86:SER:HB2	2:E:88:ILE:HG13	1.81	0.61
1:A:476:HIS:CG	1:A:533:PRO:HG3	2.35	0.61
2:E:246:PRO:HA	2:E:318:PRO:HB2	1.82	0.61
2:B:53:PHE:O	2:B:57:ILE:HG12	2.01	0.61
1:D:191:ARG:HG2	1:D:191:ARG:HH11	1.66	0.61
1:A:570:PRO:HD3	1:A:686:ASN:HD21	1.67	0.60
1:A:735:ILE:HG13	1:D:719:GLU:HB3	1.83	0.60
1:A:191:ARG:NH1	3:C:75:LEU:HA	2.07	0.60
1:D:283:SER:C	1:D:284:ILE:HG12	2.27	0.60
2:E:157:ILE:HD13	2:E:157:ILE:H	1.66	0.60
1:A:269:LEU:H	1:A:269:LEU:HD23	1.66	0.60
1:A:604:LEU:HD12	2:B:124:TRP:CH2	2.37	0.60
1:D:245:TYR:CB	1:D:246:PRO:HD3	2.18	0.60
2:B:246:PRO:HA	2:B:318:PRO:HB2	1.82	0.60
2:B:264:GLY:CA	2:E:180:THR:CG2	2.50	0.60
1:D:256:ASN:O	1:D:257:ASN:HB2	2.00	0.60
1:D:482:ASP:HB2	1:D:506:THR:HG21	1.82	0.60
1:D:636:MET:HE1	1:D:654:TYR:CD2	2.36	0.60
1:A:191:ARG:HH11	1:A:191:ARG:HG2	1.65	0.60
2:B:279:GLU:HB3	2:B:284:LYS:HE3	1.83	0.60
1:D:191:ARG:CD	3:F:108:LEU:HD22	2.32	0.60
2:E:213:LEU:HD11	2:E:215:LEU:HD21	1.84	0.60
2:E:285:TRP:HB3	2:E:287:LEU:CD1	2.32	0.60
1:A:469:ARG:NE	2:B:299:TYR:CD2	2.70	0.60
1:A:68:ASN:HB3	1:A:87:GLY:HA2	1.84	0.60
1:A:600:LYS:NZ	2:B:148:SER:HB2	2.16	0.60
2:E:53:PHE:O	2:E:57:ILE:HG12	2.01	0.60
2:B:56:THR:HG21	2:B:83:ALA:HB2	1.83	0.60
2:B:157:ILE:HD13	2:B:157:ILE:H	1.66	0.60
1:D:68:ASN:HB3	1:D:87:GLY:HA2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:THR:HG22	3:F:34:TYR:HE2	1.65	0.60
1:A:118:MET:HE2	1:A:118:MET:HA	1.84	0.59
1:A:600:LYS:HZ1	2:B:126:PHE:HE1	1.44	0.59
2:B:213:LEU:HD11	2:B:215:LEU:HD21	1.84	0.59
1:D:118:MET:HE2	1:D:118:MET:HA	1.84	0.59
1:A:256:ASN:O	1:A:257:ASN:HB2	2.00	0.59
1:A:602:ARG:HH22	2:B:170:TYR:HH	1.49	0.59
1:D:191:ARG:HE	3:F:108:LEU:HD11	1.67	0.59
2:E:279:GLU:HB3	2:E:284:LYS:HE3	1.83	0.59
1:A:384:ARG:HD3	1:A:387:GLN:HE22	1.67	0.59
1:A:516:ASN:HA	1:A:535:PHE:CE1	2.37	0.59
1:A:129:GLN:NE2	1:A:143:ARG:HE	2.01	0.59
2:E:56:THR:HG21	2:E:83:ALA:HB2	1.83	0.59
1:A:191:ARG:HE	3:C:108:LEU:CD1	2.16	0.59
1:A:331:ARG:CG	2:B:314:ARG:HH22	2.15	0.59
2:B:285:TRP:HB3	2:B:287:LEU:CD1	2.32	0.59
1:D:324:LYS:HE3	1:D:340:ASP:OD1	2.03	0.59
1:A:614:LEU:HD13	2:B:234:VAL:HG21	1.85	0.59
1:A:636:MET:HE1	1:A:654:TYR:CD2	2.36	0.59
1:A:604:LEU:HG	2:B:124:TRP:HZ2	1.67	0.59
1:D:384:ARG:HD3	1:D:387:GLN:HE22	1.68	0.59
1:A:324:LYS:HE3	1:A:340:ASP:OD1	2.03	0.59
1:A:602:ARG:HH21	2:B:168:SER:CB	2.09	0.58
1:D:214:ILE:HD13	1:D:214:ILE:N	2.18	0.58
1:A:214:ILE:HD13	1:A:214:ILE:N	2.18	0.58
1:A:570:PRO:HD3	1:A:686:ASN:ND2	2.18	0.58
1:D:600:LYS:HD3	2:E:170:TYR:CE2	2.39	0.58
1:A:600:LYS:NZ	2:B:126:PHE:CE1	2.70	0.58
1:D:576:GLU:OE1	1:D:729:ALA:HB2	2.03	0.58
2:E:157:ILE:CG1	2:E:181:VAL:HG11	2.33	0.58
1:A:191:ARG:CZ	3:C:108:LEU:HD13	2.33	0.58
1:A:599:LYS:HE3	2:B:234:VAL:CG1	2.34	0.58
1:A:191:ARG:HH22	3:C:75:LEU:N	2.01	0.58
1:A:283:SER:C	1:A:284:ILE:HG12	2.27	0.58
1:D:64:LEU:HD11	1:D:73:LEU:HD11	1.86	0.58
2:B:299:TYR:HD1	2:B:301:PRO:HD3	1.69	0.58
1:D:416:TYR:CD1	1:D:416:TYR:N	2.71	0.58
1:A:447:LYS:CD	1:A:535:PHE:CB	2.78	0.57
1:A:527:SER:HA	1:A:561:CYS:SG	2.44	0.57
1:A:547:ARG:NH1	1:A:549:GLU:OE2	2.38	0.57
2:B:136:SER:O	2:B:139:LYS:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:LEU:H	1:D:269:LEU:HD23	1.66	0.57
1:A:41:TYR:OH	1:A:522:HIS:HD2	1.81	0.57
1:A:735:ILE:HG23	1:D:735:ILE:HD11	1.85	0.57
2:B:157:ILE:CG1	2:B:181:VAL:HG11	2.33	0.57
1:D:124:THR:HG23	1:D:124:THR:O	2.04	0.57
1:A:64:LEU:HD11	1:A:73:LEU:HD11	1.86	0.57
1:A:124:THR:HG22	3:C:34:TYR:CE2	2.29	0.57
1:A:191:ARG:HD3	3:C:78:SER:CB	2.34	0.57
1:A:719:GLU:HB3	1:D:735:ILE:CG1	2.35	0.57
1:A:465:VAL:HG12	1:A:466:VAL:N	2.20	0.57
1:D:516:ASN:CA	1:D:535:PHE:CE1	2.87	0.57
2:E:299:TYR:HD1	2:E:301:PRO:HD3	1.69	0.57
1:D:96:PHE:HB3	1:D:97:PRO:HD3	1.87	0.57
1:D:604:LEU:HD12	2:E:124:TRP:CH2	2.40	0.57
1:A:98:CYS:SG	1:A:162:PHE:HB3	2.45	0.56
1:A:614:LEU:HD13	2:B:234:VAL:CG2	2.35	0.56
2:B:148:SER:HA	2:B:170:TYR:HB2	1.88	0.56
1:D:191:ARG:NH2	3:F:108:LEU:HD13	2.16	0.56
1:D:575:LEU:HD11	1:D:656:ASP:HB2	1.85	0.56
2:E:136:SER:O	2:E:139:LYS:HG3	2.05	0.56
1:A:96:PHE:HB3	1:A:97:PRO:HD3	1.88	0.56
1:D:531:SER:HG	1:D:596:PHE:HE2	1.41	0.56
1:D:547:ARG:NH1	1:D:549:GLU:OE2	2.38	0.56
1:A:332:GLN:O	2:B:297:ILE:HG21	2.06	0.56
1:D:641:SER:HB3	2:E:124:TRP:CZ3	2.41	0.56
1:D:465:VAL:HG12	1:D:466:VAL:N	2.20	0.56
1:A:124:THR:O	1:A:124:THR:HG23	2.04	0.56
1:D:98:CYS:SG	1:D:162:PHE:HB3	2.46	0.56
1:D:331:ARG:CG	2:E:314:ARG:NH2	2.66	0.56
1:A:85:LYS:H	1:A:85:LYS:CD	2.08	0.56
1:A:595:LYS:HE2	2:B:236:GLU:OE2	2.05	0.56
1:D:683:ASN:HA	1:D:688:ARG:HE	1.71	0.56
1:A:604:LEU:HD11	2:B:124:TRP:CE2	2.40	0.56
2:B:180:THR:HG23	2:E:224:ARG:HD3	1.87	0.56
1:A:220:LYS:HG3	1:A:225:GLY:O	2.05	0.55
1:A:592:ARG:NH1	2:B:170:TYR:HD2	2.04	0.55
1:A:416:TYR:CD1	1:A:416:TYR:N	2.71	0.55
1:D:220:LYS:HG3	1:D:225:GLY:O	2.06	0.55
2:E:148:SER:HA	2:E:170:TYR:HB2	1.87	0.55
1:A:593:ASN:ND2	2:B:194:GLU:OE2	2.39	0.55
1:A:683:ASN:HA	1:A:688:ARG:HE	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:GLN:NE2	1:D:143:ARG:HE	2.01	0.55
1:A:602:ARG:NE	2:B:168:SER:OG	2.40	0.55
1:A:96:PHE:HB3	1:A:97:PRO:CD	2.37	0.54
1:A:269:LEU:CD2	1:A:269:LEU:N	2.66	0.54
1:D:48:ALA:HB1	1:D:71:TYR:CE2	2.43	0.54
1:D:482:ASP:HB2	1:D:506:THR:CG2	2.37	0.54
1:A:331:ARG:HG2	2:B:314:ARG:NH2	2.22	0.54
2:B:38:ILE:HG13	2:B:38:ILE:O	2.07	0.54
2:B:48:PHE:HA	2:B:92:GLN:O	2.07	0.54
1:D:469:ARG:HD3	2:E:299:TYR:HD2	1.72	0.54
2:E:48:PHE:HA	2:E:92:GLN:O	2.08	0.54
1:A:572:SER:OG	1:A:684:SER:HB2	2.07	0.54
1:A:368:LYS:HD3	1:A:369:TYR:CE1	2.43	0.54
1:A:447:LYS:CD	1:A:535:PHE:HB2	2.37	0.54
1:D:96:PHE:HB3	1:D:97:PRO:CD	2.37	0.54
1:D:516:ASN:OD1	1:D:535:PHE:CZ	2.61	0.54
1:D:733:THR:OG1	1:D:734:SER:N	2.40	0.54
1:A:482:ASP:HB2	1:A:506:THR:CG2	2.37	0.54
2:E:94:ILE:HA	2:E:97:LEU:HD13	1.90	0.54
2:E:299:TYR:CD1	2:E:301:PRO:HD3	2.43	0.54
1:D:482:ASP:O	1:D:484:HIS:N	2.41	0.54
1:A:331:ARG:HG3	2:B:314:ARG:HH22	1.73	0.54
2:B:94:ILE:HA	2:B:97:LEU:HD13	1.90	0.54
2:E:150:GLU:HG2	2:E:172:GLY:H	1.74	0.53
2:E:150:GLU:HG2	2:E:172:GLY:N	2.23	0.53
1:A:191:ARG:NE	3:C:108:LEU:CD1	2.71	0.53
2:B:147:LEU:HD11	2:B:149:LEU:HG	1.90	0.53
2:B:264:GLY:C	2:E:180:THR:HG21	2.33	0.53
2:B:150:GLU:HG2	2:B:172:GLY:H	1.74	0.53
1:D:315:ASN:ND2	1:D:349:SER:HB2	2.22	0.53
1:A:48:ALA:HB1	1:A:71:TYR:CE2	2.43	0.53
1:A:602:ARG:NH2	2:B:170:TYR:CZ	2.74	0.53
1:D:368:LYS:HD3	1:D:369:TYR:CE1	2.43	0.53
1:D:662:ILE:HG22	1:D:677:LEU:HD22	1.91	0.53
2:E:58:LYS:HD2	2:E:58:LYS:C	2.34	0.53
1:A:482:ASP:O	1:A:484:HIS:N	2.41	0.53
2:B:169:LEU:HG	2:B:171:LEU:HG	1.91	0.53
2:B:299:TYR:CD1	2:B:301:PRO:HD3	2.43	0.53
2:E:38:ILE:O	2:E:38:ILE:HG13	2.07	0.53
1:A:719:GLU:HB2	1:D:735:ILE:HG12	1.90	0.53
1:A:41:TYR:CZ	1:A:522:HIS:HD2	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:ILE:HG22	1:A:677:LEU:HD22	1.91	0.53
2:B:150:GLU:HG2	2:B:172:GLY:N	2.23	0.53
1:A:600:LYS:CD	2:B:170:TYR:CZ	2.92	0.53
1:D:604:LEU:HD12	2:E:124:TRP:CZ2	2.44	0.53
1:A:55:VAL:CG2	1:A:64:LEU:HD23	2.40	0.52
1:A:96:PHE:CB	1:A:97:PRO:HD3	2.39	0.52
2:B:58:LYS:HD2	2:B:58:LYS:C	2.34	0.52
2:B:113:ILE:HG13	2:B:137:SER:CB	2.39	0.52
2:E:113:ILE:HG13	2:E:137:SER:CB	2.39	0.52
1:A:476:HIS:CG	1:A:533:PRO:HG2	2.43	0.52
1:D:560:ILE:HG23	1:D:562:LEU:HG	1.89	0.52
2:E:147:LEU:HD11	2:E:149:LEU:HG	1.91	0.52
1:D:55:VAL:CG2	1:D:64:LEU:HD23	2.40	0.52
1:A:345:VAL:HG22	1:A:362:MET:HB2	1.92	0.52
2:E:299:TYR:HE1	2:E:301:PRO:HG3	1.74	0.52
1:A:56:ILE:HD11	1:A:120:LEU:O	2.09	0.52
1:D:426:ARG:HH12	2:E:271:ILE:CG2	2.22	0.52
1:D:583:ILE:HD13	1:D:640:ILE:HD11	1.90	0.52
1:D:96:PHE:CB	1:D:97:PRO:HD3	2.39	0.52
1:D:191:ARG:HH22	3:F:74:HIS:CA	2.21	0.52
1:D:544:LYS:HB3	1:D:546:VAL:HG23	1.92	0.52
2:B:213:LEU:HD12	2:B:214:TYR:H	1.74	0.52
1:D:266:ARG:O	1:D:267:GLU:C	2.53	0.52
1:D:600:LYS:CD	2:E:170:TYR:CE2	2.93	0.52
1:D:614:LEU:CD1	2:E:212:ASN:OD1	2.57	0.52
1:A:544:LYS:HB3	1:A:546:VAL:HG23	1.92	0.52
1:A:593:ASN:HD21	2:B:194:GLU:CD	2.18	0.52
2:B:169:LEU:HD11	2:B:171:LEU:HD21	1.91	0.52
2:B:251:SER:HA	2:B:287:LEU:O	2.10	0.52
2:E:169:LEU:HD11	2:E:171:LEU:HD21	1.91	0.52
2:E:251:SER:HA	2:E:287:LEU:O	2.10	0.52
1:A:583:ILE:HD13	1:A:640:ILE:HD11	1.90	0.52
1:D:56:ILE:HD11	1:D:120:LEU:O	2.09	0.52
1:D:332:GLN:O	2:E:297:ILE:HG21	2.10	0.52
1:A:633:HIS:HB3	1:A:636:MET:HE2	1.92	0.51
2:B:202:VAL:CB	2:E:224:ARG:HH12	2.22	0.51
2:B:299:TYR:HE1	2:B:301:PRO:HG3	1.74	0.51
1:D:430:PHE:C	1:D:431:MET:HG2	2.34	0.51
1:A:235:ILE:HG23	1:A:389:PHE:CD1	2.46	0.51
1:A:288:LEU:O	1:A:417:ARG:NH2	2.44	0.51
1:D:345:VAL:HG22	1:D:362:MET:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:CYS:SG	1:A:556:TRP:HB2	2.50	0.51
1:D:41:TYR:HH	1:D:522:HIS:CE1	2.16	0.51
1:A:430:PHE:C	1:A:431:MET:HG2	2.34	0.51
1:D:551:CYS:SG	1:D:556:TRP:HB2	2.50	0.51
1:D:576:GLU:OE2	1:D:729:ALA:HB2	2.05	0.51
2:E:169:LEU:HG	2:E:171:LEU:HG	1.91	0.51
2:E:213:LEU:HD12	2:E:214:TYR:H	1.74	0.51
1:A:329:LEU:HD12	1:A:451:THR:HG21	1.93	0.51
1:A:350:LYS:HG3	1:A:357:MET:HG3	1.93	0.51
1:A:577:GLY:O	1:A:728:LEU:HB2	2.11	0.51
1:A:732:GLU:OE2	1:D:723:LYS:CE	2.54	0.51
1:A:735:ILE:HD12	1:D:735:ILE:CD1	2.16	0.51
1:A:192:PHE:CE1	1:A:218:ARG:NH1	2.79	0.51
1:D:192:PHE:CE1	1:D:218:ARG:NH1	2.79	0.51
1:D:633:HIS:HB3	1:D:636:MET:HE2	1.92	0.51
1:A:576:GLU:OE1	1:A:576:GLU:N	2.43	0.51
2:B:263:ASP:O	2:E:180:THR:HG22	2.10	0.51
1:D:288:LEU:O	1:D:417:ARG:NH2	2.44	0.51
1:D:447:LYS:HD2	1:D:535:PHE:HB3	1.93	0.51
2:E:223:LEU:HD11	2:E:311:PHE:CG	2.46	0.51
2:B:266:LEU:HD13	2:B:281:PRO:HB3	1.93	0.50
1:A:614:LEU:HD12	2:B:212:ASN:OD1	2.11	0.50
2:B:223:LEU:HD11	2:B:311:PHE:CG	2.46	0.50
1:D:569:PHE:CD1	1:D:570:PRO:HA	2.47	0.50
1:A:469:ARG:CD	2:B:299:TYR:CD2	2.94	0.50
1:D:235:ILE:HG23	1:D:389:PHE:CD1	2.46	0.50
1:A:569:PHE:CD1	1:A:570:PRO:HA	2.47	0.50
1:D:516:ASN:O	1:D:535:PHE:HE1	1.83	0.50
2:E:266:LEU:HD13	2:E:281:PRO:HB3	1.93	0.50
1:A:266:ARG:O	1:A:267:GLU:C	2.53	0.50
2:B:127:LEU:HD13	2:B:132:VAL:HG21	1.94	0.50
2:E:53:PHE:HB2	2:E:88:ILE:HG23	1.94	0.50
1:A:86:THR:O	1:A:87:GLY:O	2.30	0.50
2:B:125:LEU:HD12	2:B:126:PHE:N	2.27	0.50
1:D:426:ARG:HH12	2:E:271:ILE:HG21	1.75	0.50
2:E:218:ASN:O	2:E:240:GLN:HA	2.12	0.50
1:A:733:THR:OG1	1:A:734:SER:N	2.40	0.50
2:B:123:GLY:O	2:B:144:LEU:HD12	2.12	0.50
1:D:576:GLU:OE1	1:D:576:GLU:N	2.42	0.50
2:E:272:ILE:HG22	2:E:273:SER:N	2.27	0.50
1:A:191:ARG:NH1	1:A:191:ARG:HG2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:THR:O	1:D:87:GLY:O	2.30	0.49
1:D:118:MET:HA	1:D:118:MET:CE	2.42	0.49
1:D:124:THR:HG22	3:F:34:TYR:CE2	2.46	0.49
1:D:350:LYS:HG3	1:D:357:MET:HG3	1.93	0.49
1:A:592:ARG:HH12	2:B:170:TYR:HD2	1.60	0.49
2:B:218:ASN:O	2:B:240:GLN:HA	2.12	0.49
1:D:191:ARG:NH2	3:F:74:HIS:CA	2.74	0.49
2:E:127:LEU:HD13	2:E:132:VAL:HG21	1.94	0.49
2:E:123:GLY:O	2:E:144:LEU:HD12	2.12	0.49
1:D:576:GLU:OE2	1:D:729:ALA:CA	2.59	0.49
1:D:614:LEU:HB2	2:E:233:ASP:OD2	2.12	0.49
1:D:655:VAL:CG1	1:D:681:TYR:CD1	2.96	0.49
1:A:375:ASN:O	1:A:376:LYS:C	2.55	0.49
1:D:269:LEU:HD23	1:D:269:LEU:N	2.27	0.49
1:A:118:MET:HA	1:A:118:MET:CE	2.43	0.49
1:A:559:GLN:O	1:A:561:CYS:N	2.46	0.49
2:B:272:ILE:HG22	2:B:273:SER:N	2.27	0.49
1:A:719:GLU:CB	1:D:735:ILE:CG1	2.90	0.49
1:D:238:LEU:HD12	1:D:241:PHE:HE2	1.78	0.49
2:E:85:ASN:HA	2:E:107:GLY:O	2.13	0.49
2:B:202:VAL:CB	2:E:224:ARG:NH1	2.76	0.49
2:E:244:ASN:HB2	2:E:317:GLN:OE1	2.13	0.49
1:D:51:PRO:HA	1:D:508:LYS:HB3	1.95	0.48
2:B:244:ASN:HB2	2:B:317:GLN:OE1	2.13	0.48
1:D:191:ARG:NH2	3:F:108:LEU:HD11	2.18	0.48
2:E:125:LEU:HD12	2:E:126:PHE:N	2.28	0.48
2:E:238:PHE:CE1	2:E:310:ARG:HB2	2.49	0.48
1:A:580:ARG:HG2	1:A:625:THR:HG22	1.95	0.48
2:B:235:LEU:HD12	2:B:236:GLU:N	2.27	0.48
1:D:139:GLY:O	1:D:176:VAL:N	2.45	0.48
1:A:191:ARG:HH21	3:C:108:LEU:CD1	2.25	0.48
1:A:735:ILE:CG1	1:D:719:GLU:HB3	2.44	0.48
1:A:92:HIS:ND1	1:A:94:ASP:HB2	2.28	0.48
1:A:315:ASN:ND2	1:A:349:SER:HB2	2.22	0.48
1:A:438:LEU:HB3	1:A:458:SER:OG	2.13	0.48
1:D:191:ARG:HG2	1:D:191:ARG:NH1	2.28	0.48
1:A:55:VAL:HG22	1:A:64:LEU:HD23	1.96	0.48
2:B:53:PHE:HB2	2:B:88:ILE:HG23	1.94	0.48
2:B:114:LYS:N	2:B:115:PRO:CD	2.76	0.48
1:D:85:LYS:H	1:D:85:LYS:CD	2.08	0.48
1:D:329:LEU:HD12	1:D:451:THR:HG21	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:PRO:O	1:A:226:PHE:HB2	2.14	0.48
2:B:190:THR:HG22	2:B:191:LEU:N	2.29	0.48
2:E:114:LYS:N	2:E:115:PRO:CD	2.76	0.48
1:A:275:HIS:CD2	1:A:277:ARG:HE	2.32	0.48
1:A:530:LEU:HD22	1:A:558:GLN:HA	1.96	0.48
2:B:85:ASN:HA	2:B:107:GLY:O	2.14	0.48
1:D:416:TYR:H	1:D:416:TYR:HD1	1.60	0.48
1:A:148:HIS:HE1	3:C:11:ARG:NH1	2.12	0.48
1:A:331:ARG:CG	2:B:314:ARG:NH2	2.77	0.48
2:B:301:PRO:CA	2:B:310:ARG:HG2	2.44	0.48
1:D:592:ARG:NH1	2:E:170:TYR:HD2	2.11	0.48
2:E:96:TYR:C	2:E:98:PRO:HD3	2.39	0.48
1:A:329:LEU:O	1:A:333:ILE:HG13	2.14	0.48
1:D:140:THR:CG2	1:D:140:THR:O	2.62	0.48
1:D:503:LEU:HB3	1:D:510:ILE:HD11	1.95	0.48
2:E:235:LEU:HD12	2:E:236:GLU:N	2.27	0.48
1:D:92:HIS:ND1	1:D:94:ASP:HB2	2.28	0.47
1:D:329:LEU:O	1:D:333:ILE:HG13	2.14	0.47
1:D:655:VAL:CB	1:D:681:TYR:CD1	2.95	0.47
2:E:36:GLU:HG3	2:E:95:GLN:CB	2.44	0.47
1:A:431:MET:SD	2:B:310:ARG:CZ	3.01	0.47
1:A:599:LYS:CE	2:B:234:VAL:CG1	2.92	0.47
1:D:438:LEU:HB3	1:D:458:SER:OG	2.13	0.47
1:D:173:PRO:O	1:D:226:PHE:HB2	2.14	0.47
1:A:503:LEU:HB3	1:A:510:ILE:HD11	1.96	0.47
1:D:84:TYR:CD1	1:D:84:TYR:C	2.93	0.47
2:E:190:THR:HG22	2:E:191:LEU:N	2.29	0.47
2:B:96:TYR:C	2:B:98:PRO:HD3	2.39	0.47
1:A:140:THR:CG2	1:A:140:THR:O	2.62	0.47
1:A:191:ARG:NH2	3:C:108:LEU:CD1	2.77	0.47
1:A:431:MET:CE	1:A:472:PRO:HA	2.40	0.47
1:D:185:LEU:HD12	1:D:186:SER:N	2.30	0.47
1:A:185:LEU:HD12	1:A:186:SER:N	2.30	0.47
1:A:268:THR:O	1:A:271:ALA:HB3	2.15	0.47
1:A:431:MET:SD	1:A:472:PRO:HB3	2.55	0.47
1:A:614:LEU:CD1	2:B:233:ASP:OD2	2.61	0.47
1:D:275:HIS:CD2	1:D:277:ARG:HE	2.32	0.47
2:B:158:ASN:O	2:B:161:VAL:HG12	2.14	0.47
2:B:266:LEU:CD1	2:B:281:PRO:HB3	2.45	0.47
1:D:530:LEU:HD22	1:D:558:GLN:HA	1.96	0.47
2:E:158:ASN:O	2:E:161:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:239:SER:HA	2:E:312:HIS:ND1	2.30	0.47
1:A:269:LEU:HD23	1:A:269:LEU:N	2.27	0.47
1:A:271:ALA:O	1:A:273:THR:N	2.48	0.47
2:B:301:PRO:HG3	2:B:310:ARG:HD3	1.97	0.47
1:D:119:ALA:HB3	1:D:133:CYS:HB2	1.97	0.47
2:E:266:LEU:CD1	2:E:281:PRO:HB3	2.45	0.47
2:B:43:PRO:HA	2:B:68:ASP:O	2.16	0.46
1:D:271:ALA:O	1:D:273:THR:N	2.48	0.46
1:A:51:PRO:HA	1:A:508:LYS:HB3	1.95	0.46
1:A:243:ASP:O	1:A:244:SER:C	2.59	0.46
1:A:84:TYR:CD1	1:A:84:TYR:C	2.93	0.46
1:A:294:MET:HE3	1:A:424:LEU:HB2	1.97	0.46
1:A:604:LEU:CG	2:B:124:TRP:CZ2	2.97	0.46
1:A:735:ILE:HG12	1:D:719:GLU:HB2	1.97	0.46
1:D:580:ARG:HG2	1:D:625:THR:HG22	1.96	0.46
1:A:238:LEU:HD12	1:A:241:PHE:HE2	1.79	0.46
1:D:55:VAL:HG22	1:D:64:LEU:HD23	1.96	0.46
1:D:243:ASP:O	1:D:244:SER:C	2.59	0.46
1:D:600:LYS:HA	2:E:170:TYR:OH	2.15	0.46
2:E:43:PRO:HA	2:E:68:ASP:O	2.15	0.46
1:A:447:LYS:CD	1:A:535:PHE:HB3	2.32	0.46
1:D:64:LEU:HD12	1:D:71:TYR:HB2	1.98	0.46
1:A:600:LYS:HZ1	2:B:148:SER:HB2	1.79	0.46
2:E:157:ILE:HD13	2:E:157:ILE:N	2.31	0.46
1:A:64:LEU:HD12	1:A:71:TYR:HB2	1.98	0.46
1:A:119:ALA:HB3	1:A:133:CYS:HB2	1.97	0.46
2:B:215:LEU:HB2	2:B:237:LEU:HD23	1.98	0.46
1:D:268:THR:O	1:D:271:ALA:HB3	2.15	0.46
1:D:576:GLU:HG2	1:D:728:LEU:C	2.40	0.46
2:B:157:ILE:HD13	2:B:157:ILE:N	2.31	0.46
2:E:201:ILE:HB	2:E:204:LEU:HD12	1.97	0.46
2:E:215:LEU:HB2	2:E:237:LEU:HD23	1.98	0.46
2:E:267:VAL:HG13	2:E:300:GLN:HB2	1.98	0.46
1:A:41:TYR:HH	1:A:522:HIS:CD2	2.32	0.45
2:B:169:LEU:HD21	2:B:171:LEU:HD11	1.98	0.45
2:B:239:SER:HA	2:B:312:HIS:ND1	2.31	0.45
1:D:291:TYR:C	1:D:292:MET:HG3	2.41	0.45
2:E:169:LEU:HD21	2:E:171:LEU:HD11	1.98	0.45
1:D:294:MET:HA	1:D:295:PRO:HD2	1.76	0.45
2:E:38:ILE:HG12	2:E:72:GLN:OE1	2.17	0.45
1:A:335:ALA:O	1:A:336:SER:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:GLU:HG3	2:B:95:GLN:CB	2.44	0.45
2:B:38:ILE:HG12	2:B:72:GLN:OE1	2.17	0.45
2:B:267:VAL:HG22	2:B:300:GLN:HG2	1.99	0.45
1:D:124:THR:O	1:D:124:THR:CG2	2.65	0.45
2:E:48:PHE:CE2	2:E:57:ILE:HG13	2.52	0.45
1:A:139:GLY:O	1:A:176:VAL:N	2.46	0.45
2:B:48:PHE:CE2	2:B:57:ILE:HG13	2.52	0.45
2:B:267:VAL:HG13	2:B:300:GLN:HB2	1.98	0.45
1:D:294:MET:HE3	1:D:424:LEU:HB2	1.97	0.45
2:E:267:VAL:HG22	2:E:300:GLN:HG2	1.98	0.45
1:A:243:ASP:O	1:A:245:TYR:HA	2.17	0.45
1:A:291:TYR:C	1:A:292:MET:HG3	2.41	0.45
1:A:687:SER:HA	1:A:688:ARG:NH1	2.32	0.45
2:B:201:ILE:HB	2:B:204:LEU:HD12	1.98	0.45
1:A:432:GLY:C	1:A:434:PHE:N	2.74	0.45
2:B:286:HIS:O	2:B:288:PRO:HD3	2.17	0.45
1:D:469:ARG:CD	2:E:299:TYR:CD2	2.99	0.45
2:E:149:LEU:HB3	2:E:154:ILE:HD11	1.99	0.45
1:A:254:GLU:HG3	1:A:259:ILE:HD13	1.99	0.45
2:B:204:LEU:CA	2:B:207:LEU:HD22	2.45	0.45
1:A:491:ILE:O	1:A:502:THR:HA	2.17	0.45
1:A:574:PRO:HB3	1:A:729:ALA:HB2	1.96	0.45
1:A:719:GLU:CB	1:D:735:ILE:HG12	2.47	0.45
1:D:335:ALA:O	1:D:336:SER:HB3	2.16	0.45
1:A:496:LEU:O	1:A:497:ASN:HB2	2.17	0.45
1:A:604:LEU:CG	2:B:124:TRP:HZ2	2.30	0.45
2:B:202:VAL:N	2:B:203:PRO:CD	2.80	0.45
1:A:201:ILE:HD11	1:A:211:LEU:C	2.43	0.44
1:A:612:LEU:HD23	1:A:624:CYS:HB3	1.99	0.44
1:D:201:ILE:HD11	1:D:211:LEU:C	2.42	0.44
1:D:531:SER:OG	1:D:596:PHE:HE2	1.89	0.44
1:D:560:ILE:CG2	1:D:562:LEU:HG	2.45	0.44
2:E:61:LEU:HD21	2:E:78:ILE:HD11	1.99	0.44
2:B:202:VAL:HG11	2:E:224:ARG:NH1	2.32	0.44
1:D:130:LEU:HD12	1:D:130:LEU:HA	1.80	0.44
1:A:330:ALA:O	1:A:331:ARG:C	2.60	0.44
1:D:254:GLU:HG3	1:D:259:ILE:HD13	1.99	0.44
1:D:687:SER:HA	1:D:688:ARG:NH1	2.32	0.44
2:E:202:VAL:N	2:E:203:PRO:CD	2.80	0.44
2:E:286:HIS:O	2:E:288:PRO:HD3	2.16	0.44
2:E:297:ILE:HD11	2:E:314:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:PHE:HD1	1:A:362:MET:CE	2.31	0.44
1:D:148:HIS:CE1	3:F:12:ALA:CA	2.89	0.44
1:D:247:ILE:HG23	1:D:265:GLN:HG2	1.99	0.44
1:D:612:LEU:HD23	1:D:624:CYS:HB3	1.99	0.44
1:D:87:GLY:O	1:D:88:PRO:C	2.61	0.44
1:D:263:THR:HG21	1:D:265:GLN:HE21	1.82	0.44
1:D:496:LEU:O	1:D:497:ASN:HB2	2.17	0.44
1:D:655:VAL:HG11	1:D:681:TYR:CD1	2.52	0.44
1:A:130:LEU:HA	1:A:130:LEU:HD12	1.80	0.44
1:A:247:ILE:HG23	1:A:265:GLN:HG2	2.00	0.44
1:D:162:PHE:CD1	1:D:162:PHE:O	2.71	0.44
1:D:546:VAL:CG1	1:D:550:GLU:HG3	2.48	0.44
2:E:201:ILE:HD12	2:E:226:LEU:HD11	2.00	0.44
1:A:463:MET:HB2	1:A:477:VAL:O	2.18	0.44
1:D:343:PHE:HD1	1:D:362:MET:CE	2.31	0.44
1:D:463:MET:HB2	1:D:477:VAL:O	2.18	0.44
1:A:263:THR:HG21	1:A:265:GLN:HE21	1.82	0.44
1:D:243:ASP:O	1:D:245:TYR:HA	2.17	0.44
1:D:432:GLY:C	1:D:434:PHE:N	2.74	0.44
1:D:516:ASN:HB3	1:D:535:PHE:HE1	1.78	0.44
1:D:561:CYS:O	1:D:642:ASN:ND2	2.41	0.44
2:B:61:LEU:HD21	2:B:78:ILE:HD11	1.99	0.44
2:B:125:LEU:HD12	2:B:126:PHE:H	1.81	0.44
1:D:491:ILE:O	1:D:502:THR:HA	2.17	0.44
2:E:138:LEU:O	2:E:139:LYS:C	2.61	0.44
2:E:201:ILE:C	2:E:203:PRO:HD2	2.43	0.44
1:A:87:GLY:O	1:A:88:PRO:C	2.61	0.43
2:B:280:LYS:HA	2:B:281:PRO:HA	1.86	0.43
1:D:605:LEU:HD13	1:D:638:ILE:HG12	2.00	0.43
1:A:546:VAL:CG1	1:A:550:GLU:HG3	2.48	0.43
1:A:655:VAL:CG2	1:A:657:PRO:HD3	2.29	0.43
2:B:149:LEU:HB3	2:B:154:ILE:HD11	1.99	0.43
1:D:330:ALA:O	1:D:331:ARG:C	2.60	0.43
2:B:103:LEU:HD23	2:B:103:LEU:HA	1.87	0.43
2:B:138:LEU:O	2:B:139:LYS:C	2.61	0.43
1:D:343:PHE:CE2	1:D:444:THR:HG21	2.53	0.43
1:D:560:ILE:CG2	1:D:562:LEU:CG	2.86	0.43
2:E:204:LEU:CA	2:E:207:LEU:HD22	2.45	0.43
1:A:122:VAL:HG23	1:A:130:LEU:HD13	2.00	0.43
1:A:191:ARG:NH2	3:C:74:HIS:CA	2.81	0.43
2:B:254:VAL:HG13	2:B:282:ASN:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:ARG:HE	3:F:108:LEU:CD2	2.31	0.43
2:E:97:LEU:O	2:E:100:VAL:HG12	2.18	0.43
2:B:97:LEU:O	2:B:100:VAL:HG12	2.18	0.43
2:B:201:ILE:C	2:B:203:PRO:HD2	2.43	0.43
1:A:124:THR:O	1:A:124:THR:CG2	2.65	0.43
1:A:343:PHE:CE2	1:A:444:THR:HG21	2.53	0.43
1:D:191:ARG:NE	3:F:108:LEU:CD2	2.82	0.43
2:E:312:HIS:ND1	2:E:312:HIS:C	2.77	0.43
1:A:605:LEU:HD13	1:A:638:ILE:HG12	2.00	0.43
2:B:125:LEU:HD11	2:B:127:LEU:HG	2.01	0.43
1:D:191:ARG:HD3	3:F:78:SER:OG	2.19	0.43
1:D:217:ARG:HB3	1:D:228:PHE:CD1	2.54	0.43
1:D:432:GLY:C	1:D:434:PHE:H	2.26	0.43
2:E:254:VAL:HG13	2:E:282:ASN:HB3	2.00	0.43
2:E:257:ASN:HB3	2:E:266:LEU:HD22	2.01	0.43
1:D:53:GLN:HE22	1:D:67:THR:N	2.17	0.43
1:D:203:SER:O	1:D:205:TYR:N	2.52	0.43
1:D:321:TYR:CE2	1:D:323:SER:HB3	2.54	0.43
1:D:431:MET:CE	1:D:472:PRO:HA	2.49	0.43
2:E:101:THR:HG22	2:E:121:ASN:O	2.19	0.43
2:E:125:LEU:HD12	2:E:126:PHE:H	1.82	0.43
2:B:97:LEU:HD12	2:B:97:LEU:N	2.34	0.43
1:A:252:ALA:HB2	1:A:261:PHE:CE2	2.54	0.43
1:A:321:TYR:CE2	1:A:323:SER:HB3	2.54	0.43
1:A:600:LYS:HZ3	2:B:148:SER:HB2	1.81	0.43
2:B:195:ASP:H	2:B:217:LYS:HB2	1.84	0.43
2:B:231:ASN:HD22	2:B:231:ASN:HA	1.62	0.43
2:B:297:ILE:HD11	2:B:314:ARG:HD3	1.99	0.43
1:D:178:SER:HB3	1:D:199:ASN:OD1	2.19	0.43
1:A:604:LEU:HG	2:B:124:TRP:CZ2	2.48	0.42
1:D:47:THR:HG23	1:D:509:LYS:HG2	2.01	0.42
1:A:665:LYS:HB3	1:A:665:LYS:HE3	1.78	0.42
2:B:174:ASN:HB3	2:B:175:LYS:H	1.70	0.42
2:B:201:ILE:HD12	2:B:226:LEU:HD11	2.00	0.42
2:B:272:ILE:HG21	2:B:276:GLY:HA3	2.01	0.42
1:D:56:ILE:HD13	1:D:120:LEU:HG	2.00	0.42
1:A:162:PHE:CD1	1:A:162:PHE:O	2.71	0.42
1:A:217:ARG:HB3	1:A:228:PHE:CD1	2.54	0.42
1:A:432:GLY:C	1:A:434:PHE:H	2.27	0.42
2:B:202:VAL:CG1	2:E:224:ARG:HH12	2.30	0.42
1:D:238:LEU:HB2	1:D:241:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:LEU:HD23	1:D:262:LEU:HA	1.93	0.42
1:D:665:LYS:HB3	1:D:665:LYS:HE3	1.78	0.42
1:A:178:SER:HB3	1:A:199:ASN:OD1	2.19	0.42
2:B:147:LEU:HD11	2:B:149:LEU:CG	2.49	0.42
2:E:97:LEU:HD12	2:E:97:LEU:N	2.34	0.42
2:E:195:ASP:H	2:E:217:LYS:HB2	1.84	0.42
1:A:47:THR:HG23	1:A:509:LYS:HG2	2.01	0.42
1:A:239:PRO:HG3	1:A:242:ARG:NH1	2.35	0.42
1:A:416:TYR:H	1:A:416:TYR:HD1	1.60	0.42
1:D:92:HIS:HB3	1:D:95:CYS:H	1.85	0.42
1:D:252:ALA:HB2	1:D:261:PHE:CE2	2.54	0.42
1:D:602:ARG:NH2	2:E:170:TYR:CZ	2.76	0.42
2:E:125:LEU:HD11	2:E:127:LEU:HG	2.01	0.42
2:E:268:THR:HA	2:E:269:PRO:HD3	1.85	0.42
1:A:53:GLN:HE22	1:A:67:THR:N	2.17	0.42
1:D:122:VAL:HG23	1:D:130:LEU:HD13	2.01	0.42
1:D:331:ARG:O	2:E:314:ARG:NH1	2.53	0.42
1:A:191:ARG:NH2	3:C:108:LEU:HD13	2.34	0.42
1:A:203:SER:O	1:A:205:TYR:N	2.52	0.42
2:B:101:THR:HG22	2:B:121:ASN:O	2.19	0.42
1:D:430:PHE:O	1:D:431:MET:CG	2.58	0.42
1:A:56:ILE:HD13	1:A:120:LEU:HG	2.00	0.42
1:D:191:ARG:HD2	3:F:108:LEU:HD22	2.00	0.42
1:D:239:PRO:HG3	1:D:242:ARG:NH1	2.35	0.42
1:D:662:ILE:HG12	1:D:734:SER:HB2	2.02	0.42
1:A:238:LEU:HB2	1:A:241:PHE:CD2	2.55	0.42
2:B:312:HIS:ND1	2:B:312:HIS:C	2.77	0.42
1:D:245:TYR:O	1:D:266:ARG:NH1	2.53	0.42
1:D:469:ARG:HD3	2:E:299:TYR:CD2	2.51	0.42
2:B:147:LEU:HD12	2:B:148:SER:N	2.35	0.41
1:D:438:LEU:O	1:D:440:THR:HG23	2.20	0.41
1:A:191:ARG:HH22	3:C:74:HIS:CB	2.30	0.41
1:A:662:ILE:HG12	1:A:734:SER:HB2	2.02	0.41
2:E:147:LEU:HD12	2:E:148:SER:N	2.35	0.41
2:E:217:LYS:N	2:E:238:PHE:O	2.45	0.41
1:A:191:ARG:HE	3:C:108:LEU:HD11	1.85	0.41
2:B:180:THR:CG2	2:E:224:ARG:HD3	2.49	0.41
2:B:200:ASP:OD1	2:B:202:VAL:HG23	2.21	0.41
1:A:98:CYS:SG	1:A:162:PHE:CB	3.09	0.41
1:A:191:ARG:HD3	3:C:78:SER:HB2	2.01	0.41
2:B:257:ASN:HB3	2:B:266:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:THR:HA	2:B:269:PRO:HD3	1.85	0.41
1:D:447:LYS:HD2	1:D:535:PHE:CD2	2.55	0.41
1:A:92:HIS:HB3	1:A:95:CYS:H	1.85	0.41
1:A:191:ARG:HH21	3:C:108:LEU:HD11	1.85	0.41
1:A:252:ALA:HB2	1:A:261:PHE:CD2	2.55	0.41
1:D:516:ASN:OD1	1:D:535:PHE:CE1	2.73	0.41
1:D:516:ASN:CG	1:D:535:PHE:CE1	2.98	0.41
2:E:240:GLN:HG2	2:E:312:HIS:O	2.21	0.41
3:F:32:ASP:OD1	3:F:32:ASP:C	2.64	0.41
1:A:245:TYR:O	1:A:266:ARG:NH1	2.54	0.41
1:A:619:MET:HE3	1:A:619:MET:HB3	1.96	0.41
2:B:190:THR:HG22	2:B:191:LEU:H	1.85	0.41
3:C:32:ASP:C	3:C:32:ASP:OD1	2.63	0.41
1:D:41:TYR:CE1	1:D:522:HIS:NE2	2.80	0.41
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.93	0.41
1:D:506:THR:O	1:D:506:THR:HG22	2.20	0.41
2:E:147:LEU:HD11	2:E:149:LEU:CG	2.50	0.41
1:A:294:MET:HA	1:A:295:PRO:HD2	1.76	0.41
1:A:462:PHE:CE2	1:A:513:ILE:HG21	2.56	0.41
2:B:229:LEU:HB3	2:B:232:LEU:HG	2.03	0.41
1:D:252:ALA:HB2	1:D:261:PHE:CD2	2.55	0.41
1:D:447:LYS:HE3	1:D:535:PHE:CB	2.50	0.41
1:D:600:LYS:NZ	2:E:148:SER:HB2	2.36	0.41
2:E:35:MET:O	2:E:35:MET:HG3	2.21	0.41
2:E:318:PRO:O	2:E:319:LEU:HD23	2.21	0.41
1:A:593:ASN:ND2	2:B:194:GLU:CD	2.79	0.41
1:D:59:GLU:O	1:D:61:HIS:HD2	2.04	0.41
2:E:103:LEU:HD23	2:E:103:LEU:HA	1.87	0.41
2:E:190:THR:HG22	2:E:191:LEU:H	1.85	0.41
1:A:561:CYS:O	1:A:642:ASN:ND2	2.41	0.40
1:A:668:PRO:HD2	1:A:673:THR:OG1	2.21	0.40
1:D:92:HIS:CE1	1:D:94:ASP:HB2	2.56	0.40
1:D:668:PRO:HD2	1:D:673:THR:OG1	2.21	0.40
2:E:272:ILE:HG21	2:E:276:GLY:HA3	2.03	0.40
1:A:77:ASP:OD1	1:A:79:GLN:HB2	2.22	0.40
1:A:438:LEU:O	1:A:440:THR:HG23	2.20	0.40
2:B:113:ILE:CG1	2:B:137:SER:HB2	2.43	0.40
2:B:255:VAL:HA	2:B:256:PRO:HD3	1.91	0.40
2:E:113:ILE:CG1	2:E:137:SER:HB2	2.43	0.40
2:E:200:ASP:OD1	2:E:202:VAL:HG23	2.20	0.40
1:A:395:GLU:H	1:A:395:GLU:HG2	1.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:THR:O	1:A:506:THR:HG22	2.20	0.40
2:B:35:MET:O	2:B:35:MET:HG3	2.21	0.40
1:D:185:LEU:HD12	1:D:185:LEU:C	2.47	0.40
1:D:345:VAL:HG11	1:D:439:LEU:HB3	2.04	0.40
1:D:462:PHE:CE2	1:D:513:ILE:HG21	2.56	0.40
1:D:539:GLY:HA3	1:D:556:TRP:CE2	2.57	0.40
2:E:197:GLN:HA	2:E:219:HIS:CD2	2.56	0.40
2:E:201:ILE:CD1	2:E:226:LEU:HD11	2.52	0.40
1:A:201:ILE:HD11	1:A:211:LEU:HB2	2.04	0.40
1:A:533:PRO:HA	1:A:534:PRO:HD3	1.89	0.40
2:B:229:LEU:C	2:B:231:ASN:H	2.30	0.40
1:D:90:LEU:HB2	1:D:112:TRP:HD1	1.86	0.40

All (44) 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:D:459:GLU:OE2	1:D:635:ASN:ND2[2_455]	0.86	1.34
1:D:459:GLU:OE2	1:D:635:ASN:CG[2_455]	1.00	1.20
1:A:155:GLN:OE1	2:B:71:THR:CG2[2_554]	1.06	1.14
1:A:155:GLN:CD	2:B:71:THR:CG2[2_554]	1.06	1.14
1:A:398:PHE:CE1	1:A:739:ARG:NH2[3_444]	1.09	1.11
3:C:123:LYS:NZ	2:E:175:LYS:CB[3_544]	1.09	1.11
1:A:497:ASN:OD1	3:F:26:ALA:O[3_544]	1.40	0.80
2:B:175:LYS:CG	3:F:123:LYS:NZ[3_544]	1.44	0.76
1:A:497:ASN:ND2	3:F:22:MET:CE[3_544]	1.45	0.75
3:C:26:ALA:O	1:D:497:ASN:ND2[3_544]	1.46	0.74
1:A:155:GLN:CG	2:B:71:THR:CG2[2_554]	1.48	0.72
1:A:150:HIS:ND1	2:B:39:THR:CB[2_554]	1.51	0.69
3:C:26:ALA:O	1:D:497:ASN:CG[3_544]	1.53	0.67
1:D:459:GLU:OE2	1:D:635:ASN:OD1[2_455]	1.53	0.67
3:C:26:ALA:O	1:D:497:ASN:OD1[3_544]	1.55	0.65
1:A:696:THR:OG1	1:D:207:PRO:CG[2_454]	1.59	0.61
2:B:175:LYS:CB	3:F:123:LYS:NZ[3_544]	1.59	0.61
1:D:459:GLU:CD	1:D:635:ASN:ND2[2_455]	1.64	0.56
3:C:123:LYS:NZ	2:E:175:LYS:CG[3_544]	1.65	0.55
1:A:398:PHE:CZ	1:A:739:ARG:NH2[3_444]	1.66	0.54
3:C:91:ALA:O	1:D:449:ASP:OD2[3_544]	1.71	0.49
3:C:123:LYS:CG	2:E:197:GLN:NE2[3_544]	1.75	0.45
1:A:350:LYS:NZ	1:D:80:LYS:O[2_454]	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:THR:CB	1:D:207:PRO:CG[2_454]	1.79	0.41
1:A:156:SER:O	2:B:73:ASN:CB[2_554]	1.81	0.39
1:A:155:GLN:CG	2:B:71:THR:CB[2_554]	1.82	0.38
2:B:197:GLN:NE2	3:F:123:LYS:CG[3_544]	1.85	0.35
1:A:616:GLU:OE1	1:D:103:SER:OG[2_454]	1.86	0.34
1:A:696:THR:CG2	1:D:207:PRO:CB[2_454]	1.89	0.31
1:A:150:HIS:ND1	2:B:39:THR:OG1[2_554]	1.90	0.30
3:C:22:MET:CE	1:D:497:ASN:ND2[3_544]	1.90	0.30
2:B:175:LYS:CD	3:F:123:LYS:NZ[3_544]	1.91	0.29
3:C:123:LYS:CB	2:E:197:GLN:NE2[3_544]	1.92	0.28
1:A:449:ASP:OD2	3:F:91:ALA:O[3_544]	1.96	0.24
1:A:497:ASN:CG	3:F:26:ALA:O[3_544]	2.05	0.15
1:A:150:HIS:CE1	2:B:39:THR:OG1[2_554]	2.08	0.12
1:A:156:SER:O	2:B:73:ASN:CA[2_554]	2.11	0.09
1:A:398:PHE:CE2	1:A:666:TYR:CE2[3_444]	2.11	0.09
3:C:57:THR:O	1:D:447:LYS:NZ[3_544]	2.11	0.09
3:C:123:LYS:NZ	2:E:175:LYS:CD[3_544]	2.12	0.08
1:A:357:MET:CE	1:D:83:GLU:OE2[2_454]	2.13	0.07
1:D:459:GLU:OE1	1:D:635:ASN:ND2[2_455]	2.13	0.07
1:A:398:PHE:CZ	1:A:666:TYR:CE2[3_444]	2.16	0.04
2:B:197:GLN:NE2	3:F:123:LYS:CD[3_544]	2.18	0.02

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	663/727 (91%)	589 (89%)	58 (9%)	16 (2%)	4	27
1	D	663/727 (91%)	588 (89%)	60 (9%)	15 (2%)	5	28
2	B	284/289 (98%)	228 (80%)	52 (18%)	4 (1%)	9	40
2	E	284/289 (98%)	227 (80%)	53 (19%)	4 (1%)	9	40
3	C	153/173 (88%)	149 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	153/173 (88%)	149 (97%)	4 (3%)	0	100	100
All	All	2200/2378 (92%)	1930 (88%)	231 (10%)	39 (2%)	6	34

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	GLY
1	A	270	ASP
1	A	272	GLN
1	A	483	SER
2	B	193	LEU
1	D	87	GLY
1	D	270	ASP
1	D	272	GLN
1	D	483	SER
2	E	193	LEU
1	A	107	LEU
1	A	204	SER
1	A	205	TYR
1	A	266	ARG
2	B	211	GLN
1	D	107	LEU
1	D	204	SER
1	D	205	TYR
1	D	266	ARG
1	D	433	GLN
2	E	211	GLN
1	A	244	SER
1	A	395	GLU
1	A	433	GLN
1	D	244	SER
1	D	395	GLU
1	A	448	GLY
1	A	507	GLY
1	D	448	GLY
1	D	507	GLY
1	A	242	ARG
2	B	191	LEU
2	E	191	LEU
1	A	246	PRO
2	B	305	GLY
1	D	246	PRO

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Mol	Chain	Res	Type
2	E	305	GLY
1	A	472	PRO
1	D	472	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	605/654 (92%)	486 (80%)	119 (20%)	1	7
1	D	605/654 (92%)	486 (80%)	119 (20%)	1	7
2	B	264/265 (100%)	251 (95%)	13 (5%)	22	43
2	E	264/265 (100%)	251 (95%)	13 (5%)	22	43
3	C	118/132 (89%)	118 (100%)	0	100	100
3	F	118/132 (89%)	118 (100%)	0	100	100
All	All	1974/2102 (94%)	1710 (87%)	264 (13%)	4	14

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	42	GLN
1	A	45	ASN
1	A	55	VAL
1	A	56	ILE
1	A	72	VAL
1	A	78	LEU
1	A	83	GLU
1	A	85	LYS
1	A	86	THR
1	A	89	VAL
1	A	90	LEU
1	A	98	CYS
1	A	99	GLN
1	A	100	ASP

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Mol	Chain	Res	Type
1	A	102	SER
1	A	103	SER
1	A	104	LYS
1	A	108	SER
1	A	112	TRP
1	A	113	LYS
1	A	118	MET
1	A	122	VAL
1	A	123	ASP
1	A	124	THR
1	A	136	VAL
1	A	138	ARG
1	A	140	THR
1	A	149	ASN
1	A	162	PHE
1	A	166	ILE
1	A	170	SER
1	A	177	VAL
1	A	178	SER
1	A	180	LEU
1	A	185	LEU
1	A	186	SER
1	A	188	VAL
1	A	189	LYS
1	A	200	THR
1	A	201	ILE
1	A	202	ASN
1	A	203	SER
1	A	204	SER
1	A	205	TYR
1	A	206	PHE
1	A	213	SER
1	A	214	ILE
1	A	219	LEU
1	A	229	LEU
1	A	240	GLU
1	A	242	ARG
1	A	245	TYR
1	A	248	LYS
1	A	255	SER
1	A	265	GLN
1	A	268	THR

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Mol	Chain	Res	Type
1	A	269	LEU
1	A	273	THR
1	A	278	ILE
1	A	279	ILE
1	A	280	ARG
1	A	282	CYS
1	A	284	ILE
1	A	294	MET
1	A	296	LEU
1	A	301	THR
1	A	312	GLU
1	A	313	VAL
1	A	324	LYS
1	A	329	LEU
1	A	333	ILE
1	A	337	LEU
1	A	339	ASP
1	A	345	VAL
1	A	353	SER
1	A	355	GLU
1	A	362	MET
1	A	367	ILE
1	A	368	LYS
1	A	385	CYS
1	A	386	LEU
1	A	387	GLN
1	A	394	HIS
1	A	395	GLU
1	A	397	CYS
1	A	398	PHE
1	A	414	ASP
1	A	416	TYR
1	A	417	ARG
1	A	418	THR
1	A	421	THR
1	A	424	LEU
1	A	427	VAL
1	A	429	LEU
1	A	433	GLN
1	A	438	LEU
1	A	443	SER
1	A	444	THR

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Mol	Chain	Res	Type
1	A	447	LYS
1	A	458	SER
1	A	461	ARG
1	A	470	SER
1	A	480	LEU
1	A	483	SER
1	A	491	ILE
1	A	493	GLU
1	A	495	THR
1	A	496	LEU
1	A	506	THR
1	A	508	LYS
1	A	510	ILE
1	A	511	THR
1	A	518	LEU
1	A	536	VAL
1	A	544	LYS
1	A	633	HIS
1	A	651	THR
1	A	695	LYS
2	B	37	THR
2	B	109	LYS
2	B	135	LEU
2	B	157	ILE
2	B	180	THR
2	B	181	VAL
2	B	207	LEU
2	B	217	LYS
2	B	226	LEU
2	B	247	ILE
2	B	287	LEU
2	B	302	VAL
2	B	312	HIS
1	D	40	LYS
1	D	42	GLN
1	D	45	ASN
1	D	55	VAL
1	D	56	ILE
1	D	72	VAL
1	D	78	LEU
1	D	83	GLU
1	D	85	LYS

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Mol	Chain	Res	Type
1	D	86	THR
1	D	89	VAL
1	D	90	LEU
1	D	98	CYS
1	D	99	GLN
1	D	100	ASP
1	D	102	SER
1	D	103	SER
1	D	104	LYS
1	D	108	SER
1	D	112	TRP
1	D	113	LYS
1	D	118	MET
1	D	122	VAL
1	D	123	ASP
1	D	124	THR
1	D	136	VAL
1	D	138	ARG
1	D	140	THR
1	D	149	ASN
1	D	162	PHE
1	D	166	ILE
1	D	170	SER
1	D	177	VAL
1	D	178	SER
1	D	180	LEU
1	D	185	LEU
1	D	186	SER
1	D	188	VAL
1	D	189	LYS
1	D	200	THR
1	D	201	ILE
1	D	202	ASN
1	D	203	SER
1	D	204	SER
1	D	205	TYR
1	D	206	PHE
1	D	213	SER
1	D	214	ILE
1	D	219	LEU
1	D	229	LEU
1	D	240	GLU

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Mol	Chain	Res	Type
1	D	242	ARG
1	D	245	TYR
1	D	248	LYS
1	D	255	SER
1	D	265	GLN
1	D	268	THR
1	D	269	LEU
1	D	273	THR
1	D	278	ILE
1	D	279	ILE
1	D	280	ARG
1	D	282	CYS
1	D	284	ILE
1	D	294	MET
1	D	296	LEU
1	D	301	THR
1	D	312	GLU
1	D	313	VAL
1	D	324	LYS
1	D	329	LEU
1	D	333	ILE
1	D	337	LEU
1	D	339	ASP
1	D	345	VAL
1	D	353	SER
1	D	355	GLU
1	D	362	MET
1	D	367	ILE
1	D	368	LYS
1	D	385	CYS
1	D	386	LEU
1	D	387	GLN
1	D	394	HIS
1	D	395	GLU
1	D	397	CYS
1	D	398	PHE
1	D	414	ASP
1	D	416	TYR
1	D	417	ARG
1	D	418	THR
1	D	421	THR
1	D	424	LEU

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Mol	Chain	Res	Type
1	D	427	VAL
1	D	429	LEU
1	D	433	GLN
1	D	438	LEU
1	D	443	SER
1	D	444	THR
1	D	447	LYS
1	D	458	SER
1	D	461	ARG
1	D	470	SER
1	D	480	LEU
1	D	483	SER
1	D	491	ILE
1	D	493	GLU
1	D	495	THR
1	D	496	LEU
1	D	506	THR
1	D	508	LYS
1	D	510	ILE
1	D	511	THR
1	D	518	LEU
1	D	536	VAL
1	D	544	LYS
1	D	633	HIS
1	D	651	THR
1	D	695	LYS
2	E	37	THR
2	E	109	LYS
2	E	135	LEU
2	E	157	ILE
2	E	180	THR
2	E	181	VAL
2	E	207	LEU
2	E	217	LYS
2	E	226	LEU
2	E	247	ILE
2	E	287	LEU
2	E	302	VAL
2	E	312	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	61	HIS
1	A	129	GLN
1	A	142	GLN
1	A	148	HIS
1	A	256	ASN
1	A	275	HIS
1	A	332	GLN
1	A	387	GLN
1	A	425	GLN
1	A	497	ASN
1	A	522	HIS
1	A	633	HIS
1	A	686	ASN
1	A	704	ASN
2	B	60	ASN
2	B	76	ASN
2	B	121	ASN
2	B	158	ASN
2	B	211	GLN
2	B	231	ASN
2	B	257	ASN
2	B	282	ASN
3	C	81	HIS
1	D	53	GLN
1	D	61	HIS
1	D	129	GLN
1	D	142	GLN
1	D	256	ASN
1	D	275	HIS
1	D	332	GLN
1	D	387	GLN
1	D	425	GLN
1	D	497	ASN
1	D	593	ASN
1	D	633	HIS
1	D	704	ASN
2	E	60	ASN
2	E	76	ASN
2	E	80	GLN
2	E	121	ASN
2	E	158	ASN
2	E	173	ASN

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Mol	Chain	Res	Type
2	E	211	GLN
2	E	231	ASN
2	E	257	ASN
2	E	282	ASN
3	F	81	HIS

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	3
1	A	2
3	C	2
3	F	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	518:LEU	C	519:GLY	N	6.49
1	A	518:LEU	C	519:GLY	N	5.09
1	D	560:ILE	C	561:CYS	N	4.19
1	A	560:ILE	C	561:CYS	N	3.62
1	D	655:VAL	C	656:ASP	N	1.62
1	C	97:ALA	C	98:MET	N	1.11
1	F	97:ALA	C	98:MET	N	1.11
1	C	63:ALA	C	64:LYS	N	0.92
1	F	63:ALA	C	64:LYS	N	0.92

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	675/727 (92%)	-0.20	5 (0%) 84 73	240, 323, 360, 408	0
1	D	675/727 (92%)	-0.23	6 (0%) 81 70	253, 323, 376, 431	0
2	B	286/289 (98%)	-0.25	2 (0%) 84 73	223, 275, 324, 358	0
2	E	286/289 (98%)	-0.14	3 (1%) 79 68	252, 297, 365, 378	0
3	C	155/173 (89%)	-0.29	0 100 100	290, 335, 363, 370	0
3	F	155/173 (89%)	-0.14	2 (1%) 75 63	302, 336, 372, 384	0
All	All	2232/2378 (93%)	-0.21	18 (0%) 82 72	223, 321, 366, 431	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	538	CYS	3.9
1	D	70	ILE	3.2
1	D	176	VAL	2.9
2	B	160	LEU	2.8
2	E	182	LEU	2.8
2	E	185	LEU	2.8
1	D	467	VAL	2.7
3	F	128	VAL	2.6
1	A	283	SER	2.5
1	A	176	VAL	2.5
1	A	206	PHE	2.4
1	D	130	LEU	2.4
1	D	283	SER	2.1
1	D	613	THR	2.1
3	F	54	LEU	2.1
2	E	215	LEU	2.1
1	A	64	LEU	2.0
2	B	135	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.