



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:51 pm BST

PDB ID : 5WQL
Title : Structure of a PDZ-protease bound to a substrate-binding adaptor
Authors : Su, M.Y.; Chang, C.I.
Deposited on : 2016-11-27
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

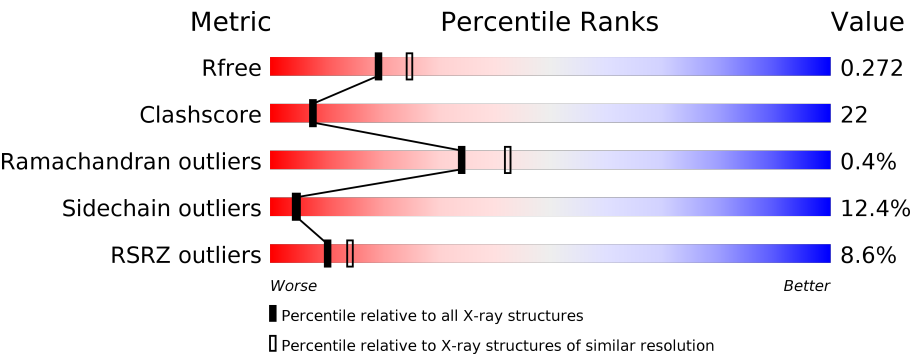
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	278	<div><div></div><div><div></div><div>81%</div><div>14%</div><div></div><div></div></div><div></div></div>
1	B	278	<div><div></div><div><div></div><div>77%</div><div>16%</div><div></div><div></div></div><div></div></div>
2	C	682	<div><div>11%</div><div><div></div><div>59%</div><div>28%</div><div>7%</div><div>5%</div></div><div></div></div>
2	D	682	<div><div>11%</div><div><div></div><div>56%</div><div>29%</div><div>10%</div><div>5%</div></div><div></div></div>
3	F	6	<div><div>17%</div><div><div></div><div>67%</div><div>33%</div></div><div></div></div>
3	H	6	<div><div>33%</div><div><div></div><div>67%</div><div>33%</div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
4	E	4	
5	G	4	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15704 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 Lipoprotein NlpI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	268	Total	C	N	O	S	0	0	0
			2176	1387	362	424	3			
1	A	270	Total	C	N	O	S	0	0	0
			2190	1395	364	427	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	GLY	-	expression tag	UNP P0AFB1
B	18	HIS	-	expression tag	UNP P0AFB1
B	19	MET	-	expression tag	UNP P0AFB1
A	17	GLY	-	expression tag	UNP P0AFB1
A	18	HIS	-	expression tag	UNP P0AFB1
A	19	MET	-	expression tag	UNP P0AFB1

- Molecule 2 is a protein called Tail-specific protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	648	Total	C	N	O	S	0	0	0
			5140	3233	897	998	12			
2	D	647	Total	C	N	O	S	0	0	0
			5139	3233	899	995	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	477	ALA	LYS	engineered mutation	UNP P23865
D	477	ALA	LYS	engineered mutation	UNP P23865

- Molecule 3 is a protein called ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	6	Total	C	N	O	0	0	0
			30	18	6	6			
3	H	6	Total	C	N	O	0	0	0
			30	18	6	6			

- Molecule 4 is a protein called ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	4	Total	C	N	O	0	0	0
			21	12	4	5			

- Molecule 5 is a protein called LEU-SER-ARG-SER.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	4	Total	C	N	O	0	0	0
			32	18	7	7			

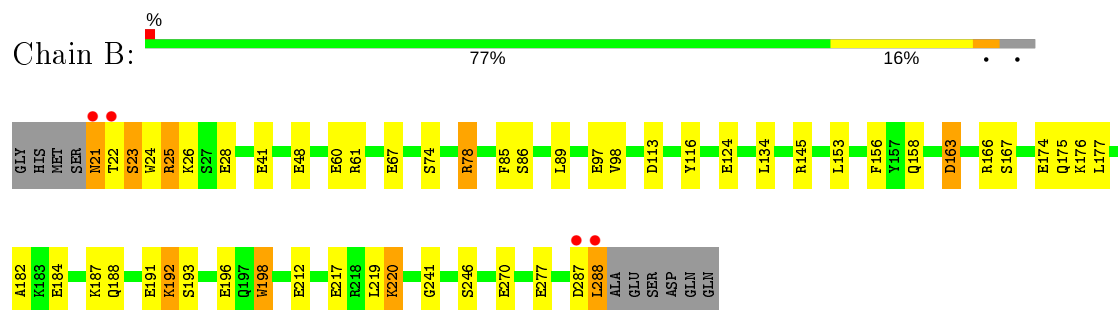
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	251	Total	O	0	0
			251	251		
6	A	250	Total	O	0	0
			250	250		
6	C	203	Total	O	0	0
			203	203		
6	D	241	Total	O	0	0
			241	241		
6	F	1	Total	O	0	0
			1	1		

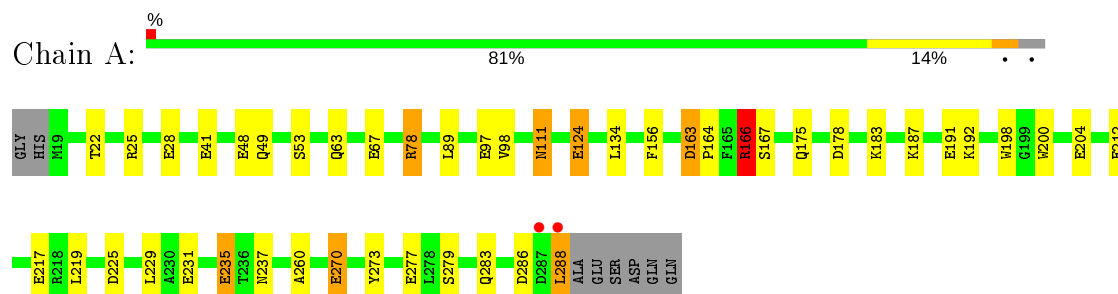
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

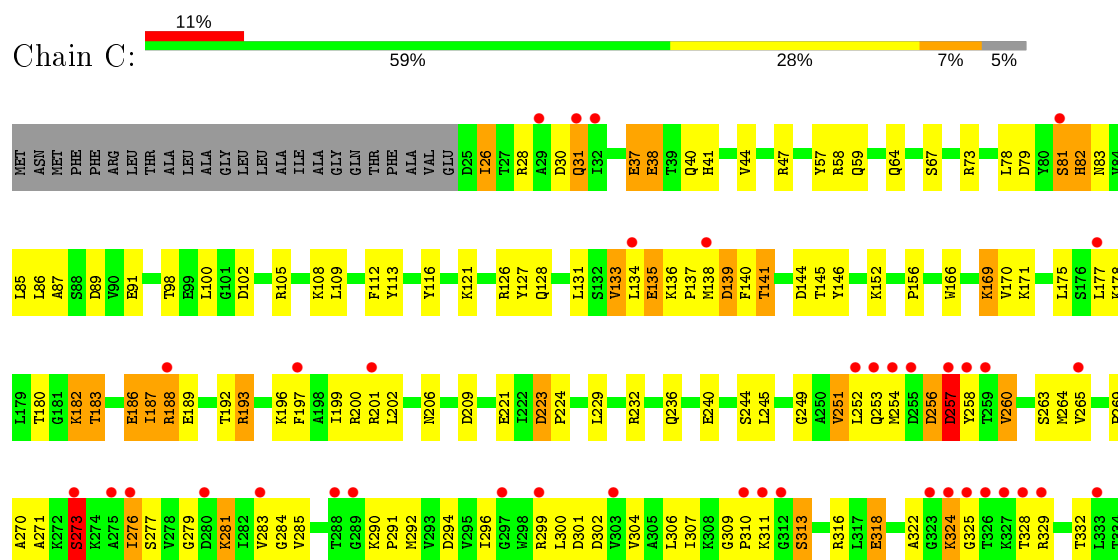
• Molecule 1: Lipoprotein NlpI

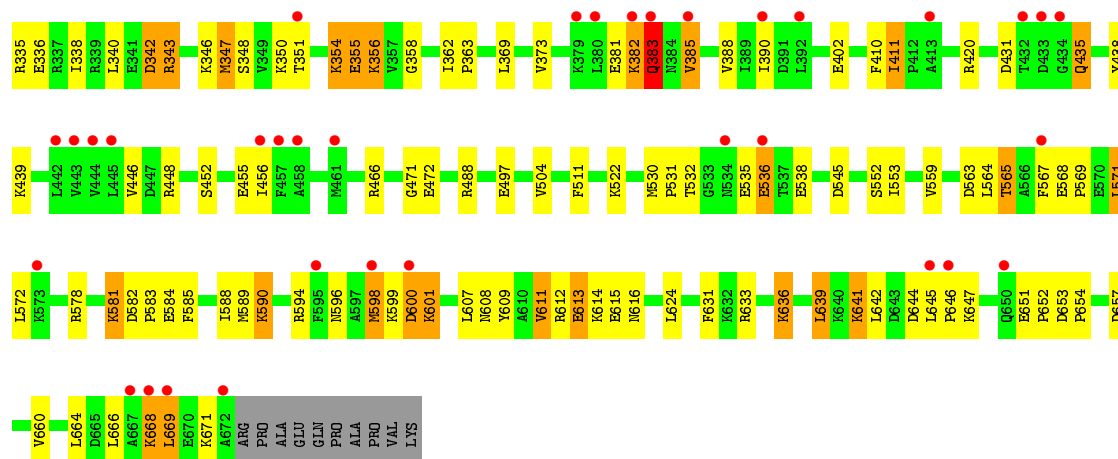


• Molecule 1: Lipoprotein NlpI

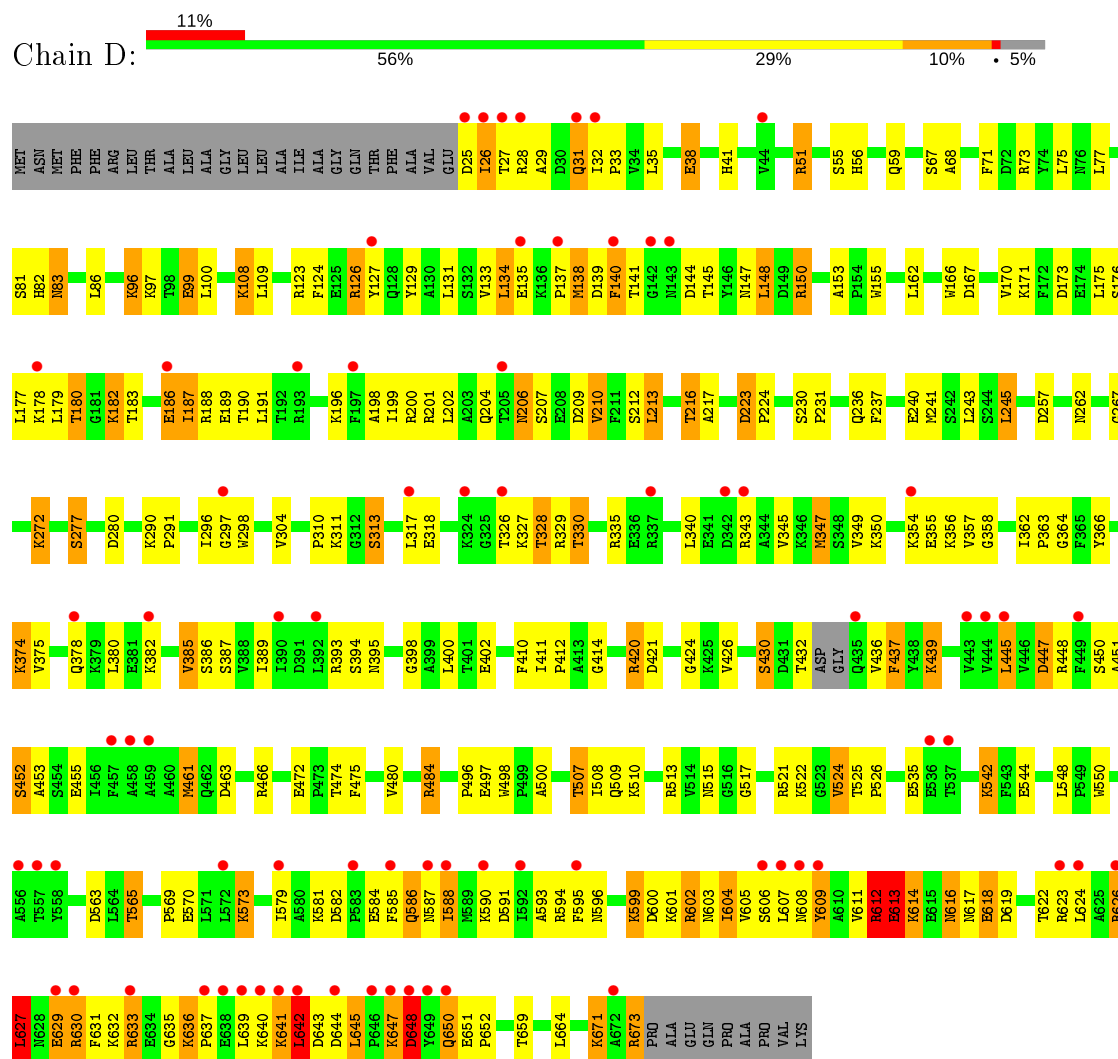


• Molecule 2: Tail-specific protease



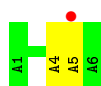


• Molecule 2: Tail-specific protease

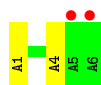


• Molecule 3: ALA-ALA-ALA-ALA-ALA-ALA

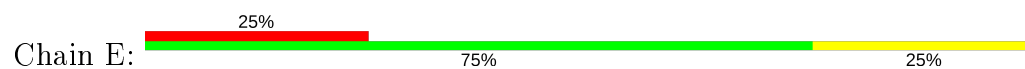




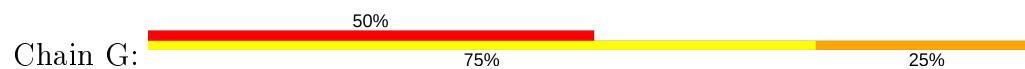
- Molecule 3: ALA-ALA-ALA-ALA-ALA-ALA



- Molecule 4: ALA-ALA-ALA-ALA



- Molecule 5: LEU-SER-ARG-SER



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.59Å 146.73Å 148.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	104.35 – 2.30 27.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.3 (104.35-2.30) 90.3 (27.93-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.217 , 0.271 0.222 , 0.272	Depositor DCC
R_{free} test set	5470 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15704	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2069e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	1.71	19/2236 (0.8%)	0.96	8/3034 (0.3%)
1	B	1.67	22/2222 (1.0%)	0.89	2/3016 (0.1%)
2	C	1.21	5/5227 (0.1%)	0.84	6/7059 (0.1%)
2	D	1.21	4/5225 (0.1%)	0.94	15/7054 (0.2%)
3	F	1.16	0/29	1.16	0/39
3	H	0.94	0/29	1.10	0/39
4	E	0.89	0/20	0.71	0/25
5	G	0.85	0/31	0.73	0/38
All	All	1.37	50/15019 (0.3%)	0.90	31/20304 (0.2%)

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	GLU	CD-OE1	-7.41	1.17	1.25
1	B	48	GLU	CD-OE1	-7.40	1.17	1.25
1	B	212	GLU	CD-OE2	-7.26	1.17	1.25
1	A	97	GLU	CD-OE1	-6.95	1.18	1.25
1	B	41	GLU	CD-OE1	-6.92	1.18	1.25
1	A	235	GLU	CD-OE2	-6.92	1.18	1.25
1	B	48	GLU	CD-OE2	-6.90	1.18	1.25
1	A	41	GLU	CD-OE1	-6.85	1.18	1.25
1	A	124	GLU	CD-OE1	-6.70	1.18	1.25
1	A	212	GLU	CD-OE1	-6.62	1.18	1.25
2	C	221	GLU	CD-OE1	-6.52	1.18	1.25
1	B	60	GLU	CD-OE2	-6.47	1.18	1.25
1	A	270	GLU	CD-OE2	-6.22	1.18	1.25
1	A	48	GLU	CD-OE1	-6.16	1.18	1.25
1	A	41	GLU	CD-OE2	-6.14	1.18	1.25
1	A	204	GLU	CD-OE1	-6.13	1.19	1.25
1	B	97	GLU	CD-OE2	-6.10	1.19	1.25
2	C	38	GLU	CD-OE1	-6.07	1.19	1.25
1	A	217	GLU	CD-OE2	-5.99	1.19	1.25
1	A	204	GLU	CD-OE2	-5.82	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	GLU	CD-OE1	-5.71	1.19	1.25
1	B	270	GLU	CD-OE2	-5.70	1.19	1.25
1	B	241	GLY	C-O	-5.69	1.14	1.23
1	B	167	SER	CB-OG	-5.64	1.34	1.42
1	B	277	GLU	CD-OE2	-5.57	1.19	1.25
1	A	231	GLU	CD-OE2	-5.53	1.19	1.25
1	A	277	GLU	CD-OE1	-5.50	1.19	1.25
1	A	48	GLU	CD-OE2	-5.47	1.19	1.25
1	B	60	GLU	CD-OE1	-5.46	1.19	1.25
1	B	67	GLU	CD-OE2	-5.42	1.19	1.25
1	B	86	SER	CB-OG	-5.40	1.35	1.42
1	B	124	GLU	CD-OE1	-5.39	1.19	1.25
1	B	41	GLU	CD-OE2	-5.37	1.19	1.25
2	C	38	GLU	CD-OE2	-5.37	1.19	1.25
1	B	78	ARG	CZ-NH2	-5.35	1.26	1.33
1	B	28	GLU	CD-OE2	-5.27	1.19	1.25
1	B	277	GLU	CD-OE1	-5.26	1.19	1.25
2	C	455	GLU	CD-OE1	-5.22	1.20	1.25
1	B	28	GLU	CD-OE1	-5.22	1.20	1.25
2	D	402	GLU	CD-OE1	-5.21	1.20	1.25
1	A	212	GLU	CD-OE2	-5.19	1.20	1.25
1	B	124	GLU	CD-OE2	-5.18	1.20	1.25
1	A	28	GLU	CD-OE2	-5.18	1.20	1.25
2	C	402	GLU	CD-OE2	-5.16	1.20	1.25
2	D	544	GLU	CD-OE1	-5.14	1.20	1.25
2	D	498	TRP	CB-CG	-5.09	1.41	1.50
1	A	97	GLU	CD-OE2	-5.08	1.20	1.25
1	B	198	TRP	CE3-CZ3	-5.06	1.29	1.38
2	D	55	SER	CB-OG	-5.02	1.35	1.42
1	A	167	SER	CB-OG	-5.01	1.35	1.42

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	51	ARG	NE-CZ-NH2	-8.01	116.29	120.30
2	D	51	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	166	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	163	ASP	CB-CG-OD1	7.29	124.86	118.30
2	D	645	LEU	CA-CB-CG	-7.07	99.04	115.30
2	D	140	PHE	N-CA-C	7.04	130.01	111.00
1	A	166	ARG	NE-CZ-NH2	-7.01	116.79	120.30
2	C	223	ASP	CB-CG-OD1	6.59	124.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	A	225	ASP	CB-CG-OD1	6.31	123.98	118.30
2	D	447	ASP	CB-CG-OD1	6.17	123.85	118.30
2	D	648	ASP	N-CA-C	-5.96	94.91	111.00
2	D	627	LEU	CB-CG-CD1	5.95	121.12	111.00
2	C	383	GLN	N-CA-C	-5.94	94.97	111.00
2	D	421	ASP	CB-CG-OD1	5.88	123.59	118.30
2	D	613	GLU	N-CA-CB	5.78	121.00	110.60
2	C	139	ASP	N-CA-C	5.67	126.30	111.00
2	C	273	SER	N-CA-C	-5.50	96.16	111.00
2	D	206	ASN	CB-CA-C	-5.48	99.44	110.40
2	D	83	ASN	N-CA-C	5.43	125.66	111.00
2	D	635	GLY	N-CA-C	5.31	126.38	113.10
2	D	642	LEU	CA-CB-CG	5.27	127.43	115.30
1	A	229	LEU	CB-CG-CD2	5.21	119.85	111.00
2	D	213	LEU	CB-CG-CD2	5.20	119.85	111.00
2	D	612	ARG	C-N-CA	5.20	134.70	121.70
1	A	273	TYR	CB-CA-C	5.18	120.76	110.40
1	B	163	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	61	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	178	ASP	CB-CG-OD1	5.14	122.93	118.30
2	C	58	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	C	653	ASP	CB-CG-OD1	5.05	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2190	0	2114	24	0
1	B	2176	0	2100	24	0
2	C	5140	0	5151	262	0
2	D	5139	0	5156	337	0
3	F	30	0	32	2	0
3	H	30	0	32	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	21	0	22	1	0
5	G	32	0	36	2	0
6	A	250	0	0	2	0
6	B	251	0	0	4	0
6	C	203	0	0	5	0
6	D	241	0	0	5	0
6	F	1	0	0	0	0
All	All	15704	0	14643	647	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 22.

All (647) 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:D:640:LYS:HG3	2:D:643:ASP:CB	1.34	1.56
2:D:640:LYS:CG	2:D:643:ASP:HB2	1.29	1.53
2:D:393:ARG:HH11	2:D:445:LEU:CD1	1.55	1.19
2:D:175:LEU:CD2	2:D:179:LEU:HD11	1.73	1.17
2:C:608:ASN:HB3	2:C:611:VAL:CG1	1.76	1.14
2:D:455:GLU:HG2	2:D:474:THR:HG21	1.14	1.13
2:C:292:MET:CE	2:C:318:GLU:HB2	1.77	1.12
2:C:139:ASP:HB3	2:C:141:THR:HG22	1.16	1.12
2:D:175:LEU:HD23	2:D:179:LEU:CD1	1.78	1.12
2:D:175:LEU:HD21	2:D:179:LEU:HD11	1.19	1.11
2:D:175:LEU:CD2	2:D:179:LEU:CD1	2.28	1.11
2:D:175:LEU:HD23	2:D:179:LEU:HD12	1.24	1.11
2:C:264:MET:HE2	2:C:271:ALA:HA	1.19	1.10
2:D:26:ILE:HG23	2:D:31:GLN:HB3	1.32	1.09
2:D:28:ARG:HD3	2:D:31:GLN:HE22	1.18	1.09
2:D:393:ARG:HH11	2:D:445:LEU:HD11	1.04	1.08
2:C:567:PHE:CD1	2:C:669:LEU:HD13	1.87	1.08
2:D:126:ARG:HG2	2:D:166:TRP:CE2	1.88	1.07
2:D:182:LYS:HZ3	2:D:186:GLU:HG3	1.12	1.06
2:D:461:MET:CE	2:D:466:ARG:HG2	1.85	1.06
2:C:139:ASP:HB3	2:C:141:THR:CG2	1.85	1.06
2:C:563:ASP:OD1	2:C:565:THR:HG22	1.54	1.06
2:C:283:VAL:HG23	2:C:296:ILE:CG1	1.85	1.06
2:D:182:LYS:NZ	2:D:186:GLU:HG3	1.70	1.06
2:C:264:MET:CE	2:C:271:ALA:HA	1.85	1.06
2:C:139:ASP:CB	2:C:141:THR:HG22	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:633:ARG:HB2	2:D:633:ARG:HH21	1.15	1.05
2:C:283:VAL:HG23	2:C:296:ILE:HG13	1.33	1.04
2:D:614:LYS:O	2:D:618:GLU:HB3	1.59	1.03
2:C:292:MET:HE2	2:C:318:GLU:CB	1.89	1.03
2:C:290:LYS:HB3	2:C:291:PRO:HD2	1.41	1.02
2:D:177:LEU:HD21	2:D:190:THR:HG21	1.36	1.02
2:D:455:GLU:CG	2:D:474:THR:HG21	1.89	1.02
2:C:567:PHE:O	2:C:571:LEU:HD12	1.60	1.02
2:C:292:MET:CE	2:C:318:GLU:N	2.21	1.01
2:D:393:ARG:NH1	2:D:445:LEU:CD1	2.23	1.01
2:D:393:ARG:NH1	2:D:445:LEU:HD11	1.74	1.01
2:C:568:GLU:HB3	2:C:569:PRO:HD3	1.37	1.01
2:D:631:PHE:HA	2:D:637:PRO:CD	1.88	1.01
2:C:567:PHE:CD1	2:C:669:LEU:CD1	2.44	1.00
2:C:608:ASN:OD1	2:C:611:VAL:HG12	1.58	1.00
2:D:26:ILE:CG2	2:D:31:GLN:HB3	1.90	1.00
2:D:631:PHE:CD1	2:D:637:PRO:HG2	1.97	0.99
2:D:631:PHE:CB	2:D:637:PRO:HD2	1.93	0.98
2:D:631:PHE:CA	2:D:637:PRO:HD2	1.94	0.98
2:C:608:ASN:HB3	2:C:611:VAL:HG11	1.43	0.98
2:D:631:PHE:HA	2:D:637:PRO:HD2	1.46	0.98
2:C:299:ARG:HG2	2:C:302:ASP:OD2	1.64	0.97
2:C:292:MET:HE2	2:C:318:GLU:HB2	0.97	0.96
2:D:393:ARG:HD3	2:D:445:LEU:HD13	1.45	0.95
2:D:626:ARG:HH21	2:D:629:GLU:HG2	1.30	0.95
2:D:318:GLU:OE2	2:D:328:THR:HG23	1.66	0.95
1:A:22:THR:HB	1:A:25:ARG:NH1	1.81	0.94
2:D:126:ARG:HG2	2:D:166:TRP:NE1	1.83	0.94
2:D:642:LEU:HD13	2:D:644:ASP:HB2	1.50	0.93
2:C:26:ILE:H	2:C:26:ILE:HD12	1.29	0.93
2:C:197:PHE:CE2	2:C:256:ASP:HB3	2.04	0.93
2:C:197:PHE:CE1	2:C:200:ARG:NH2	2.37	0.92
2:D:134:LEU:HD23	2:D:188:ARG:HG2	1.49	0.92
2:D:474:THR:HG22	2:D:475:PHE:H	1.34	0.91
2:C:26:ILE:HG22	2:C:31:GLN:HB3	1.53	0.89
2:C:609:TYR:CE2	2:C:613:GLU:HG3	2.08	0.89
2:D:579:ILE:HG22	2:D:585:PHE:CD2	2.08	0.89
2:D:640:LYS:CB	2:D:643:ASP:HB2	2.01	0.89
2:C:188:ARG:HH11	2:C:188:ARG:HG2	1.34	0.89
2:C:563:ASP:O	2:C:564:LEU:HD23	1.72	0.89
2:D:177:LEU:CD2	2:D:190:THR:HG21	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:ILE:HG23	2:D:31:GLN:CB	2.03	0.88
2:C:264:MET:CE	2:C:271:ALA:CA	2.51	0.88
1:A:22:THR:HB	1:A:25:ARG:HH12	1.36	0.88
2:D:633:ARG:NH2	2:D:633:ARG:HB2	1.89	0.88
2:C:538:GLU:N	2:C:538:GLU:OE1	2.05	0.87
2:C:343:ARG:O	2:C:363:PRO:HG2	1.75	0.87
2:D:650:GLN:O	2:D:650:GLN:NE2	2.08	0.87
2:C:608:ASN:CB	2:C:611:VAL:HG12	2.05	0.86
2:C:292:MET:HE3	2:C:318:GLU:N	1.91	0.86
2:C:264:MET:HE2	2:C:271:ALA:CA	2.04	0.86
2:D:182:LYS:HZ3	2:D:186:GLU:CG	1.87	0.86
2:D:461:MET:HE3	2:D:466:ARG:HG2	1.58	0.86
2:D:602:ARG:HH11	2:D:602:ARG:HB3	1.41	0.86
2:C:608:ASN:CG	2:C:611:VAL:HG12	1.96	0.86
2:D:26:ILE:H	2:D:26:ILE:HD12	1.41	0.86
2:D:310:PRO:O	2:D:313:SER:HB2	1.76	0.85
2:C:382:LYS:HD2	2:C:383:GLN:HG2	1.59	0.85
2:D:587:ASN:O	2:D:591:ASP:HB2	1.78	0.84
2:D:521:ARG:O	2:D:542:LYS:HE2	1.77	0.84
2:D:126:ARG:CG	2:D:166:TRP:CE2	2.61	0.83
2:C:608:ASN:CB	2:C:611:VAL:CG1	2.56	0.83
2:C:608:ASN:HB3	2:C:611:VAL:HG12	1.58	0.83
2:C:175:LEU:O	2:C:175:LEU:HD12	1.79	0.82
2:D:570:GLU:HA	2:D:573:LYS:HE3	1.60	0.82
2:D:28:ARG:HD3	2:D:31:GLN:NE2	1.92	0.82
2:C:139:ASP:CB	2:C:141:THR:CG2	2.52	0.82
2:C:292:MET:HE3	2:C:318:GLU:H	1.44	0.82
2:D:579:ILE:CG2	2:D:585:PHE:CD2	2.61	0.82
2:D:140:PHE:O	2:D:609:TYR:CD1	2.32	0.82
2:D:631:PHE:HB3	2:D:636:LYS:HB2	1.62	0.81
2:C:139:ASP:CG	2:C:141:THR:CG2	2.48	0.81
2:C:354:LYS:H	2:C:354:LYS:HD2	1.44	0.81
2:C:299:ARG:CG	2:C:302:ASP:OD2	2.28	0.80
2:D:126:ARG:CG	2:D:166:TRP:NE1	2.44	0.80
2:C:563:ASP:C	2:C:564:LEU:HD23	2.01	0.80
2:D:585:PHE:O	2:D:586:GLN:NE2	2.14	0.80
2:C:336:GLU:O	2:C:338:ILE:HD12	1.81	0.80
2:D:134:LEU:CD2	2:D:188:ARG:HG2	2.10	0.80
2:C:223:ASP:HB2	2:C:224:PRO:HD2	1.65	0.79
2:D:626:ARG:NH2	2:D:629:GLU:HG2	1.96	0.79
2:C:567:PHE:HD1	2:C:669:LEU:CD1	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:669:LEU:O	2:C:669:LEU:HD22	1.83	0.79
2:D:474:THR:HG22	2:D:475:PHE:N	1.98	0.79
2:D:175:LEU:HD12	2:D:609:TYR:CE1	2.19	0.78
2:D:450:SER:O	2:D:474:THR:HG23	1.83	0.78
2:C:264:MET:HE1	2:C:270:ALA:O	1.84	0.78
2:C:292:MET:CE	2:C:318:GLU:H	1.96	0.78
2:D:484:ARG:HH21	2:D:484:ARG:HG3	1.47	0.78
2:C:166:TRP:O	2:C:170:VAL:HG13	1.83	0.78
2:D:318:GLU:OE2	2:D:328:THR:CG2	2.31	0.78
2:D:608:ASN:HB3	2:D:611:VAL:HG12	1.65	0.78
1:A:163:ASP:OD2	1:A:166:ARG:HD2	1.84	0.78
2:C:264:MET:CE	2:C:271:ALA:N	2.46	0.78
2:C:178:LYS:HE3	2:C:609:TYR:CE1	2.18	0.77
2:C:283:VAL:CG2	2:C:296:ILE:HG13	2.12	0.77
2:D:357:VAL:HG22	2:D:387:SER:HB2	1.66	0.77
2:D:627:LEU:H	2:D:627:LEU:HD12	1.50	0.77
2:D:177:LEU:HD13	2:D:191:LEU:CD1	2.15	0.77
2:D:29:ALA:O	2:D:32:ILE:HG22	1.84	0.77
2:D:563:ASP:OD1	2:D:565:THR:HG22	1.85	0.77
2:C:87:ALA:O	2:C:91:GLU:HG2	1.84	0.76
2:C:600:ASP:HB2	2:C:601:LYS:HD3	1.68	0.76
2:D:86:LEU:HD21	2:D:162:LEU:CD1	2.15	0.76
2:D:461:MET:CE	2:D:466:ARG:CG	2.64	0.76
2:D:614:LYS:O	2:D:618:GLU:CB	2.35	0.75
2:D:631:PHE:CG	2:D:637:PRO:HD2	2.22	0.75
2:C:283:VAL:HG21	2:C:296:ILE:HD11	1.68	0.75
2:C:264:MET:CE	2:C:270:ALA:C	2.54	0.75
2:D:627:LEU:H	2:D:627:LEU:CD1	1.96	0.75
2:C:128:GLN:HA	2:C:131:LEU:HD12	1.67	0.75
2:C:596:ASN:HA	2:C:599:LYS:HE3	1.69	0.75
2:C:292:MET:HE1	2:C:318:GLU:N	2.00	0.75
2:D:186:GLU:O	2:D:189:GLU:N	2.20	0.74
2:C:354:LYS:HD3	2:C:355:GLU:HG2	1.68	0.74
2:C:448:ARG:NH2	2:C:532:THR:CG2	2.50	0.74
2:C:292:MET:CE	2:C:318:GLU:CB	2.57	0.74
2:D:642:LEU:O	2:D:642:LEU:HD12	1.88	0.74
2:C:139:ASP:OD2	2:C:141:THR:CG2	2.36	0.74
2:D:461:MET:HE2	2:D:466:ARG:HG2	1.67	0.74
2:D:596:ASN:HA	2:D:599:LYS:HE2	1.70	0.74
2:D:134:LEU:HD21	2:D:188:ARG:HA	1.69	0.74
2:C:264:MET:HE3	2:C:271:ALA:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:283:VAL:CG2	2:C:296:ILE:HD11	2.17	0.73
2:C:651:GLU:HG3	2:C:652:PRO:HD2	1.70	0.73
6:C:803:HOH:O	3:H:1:ALA:HA	1.86	0.73
2:D:393:ARG:HH11	2:D:445:LEU:HD13	1.52	0.73
2:D:150:ARG:HG2	2:D:150:ARG:HH11	1.53	0.73
2:D:393:ARG:CD	2:D:445:LEU:HD13	2.18	0.73
2:D:639:LEU:O	2:D:640:LYS:HD3	1.89	0.73
2:D:175:LEU:O	2:D:179:LEU:HD12	1.89	0.72
2:C:608:ASN:O	2:C:611:VAL:HG13	1.88	0.72
2:C:290:LYS:HB3	2:C:291:PRO:CD	2.18	0.72
2:C:197:PHE:CZ	2:C:256:ASP:HB3	2.25	0.72
2:C:448:ARG:HH21	2:C:532:THR:HG22	1.53	0.72
2:D:26:ILE:HD12	2:D:26:ILE:N	2.03	0.72
2:D:631:PHE:HA	2:D:637:PRO:HD3	1.71	0.72
2:C:568:GLU:HB3	2:C:569:PRO:CD	2.18	0.71
1:B:163:ASP:HB3	1:B:166:ARG:HG3	1.71	0.71
2:D:647:LYS:HD3	2:D:647:LYS:H	1.55	0.71
2:D:582:ASP:HB3	2:D:585:PHE:HB2	1.72	0.71
2:D:626:ARG:HD2	2:D:629:GLU:HB3	1.72	0.71
2:C:281:LYS:HE2	2:C:322:ALA:HA	1.72	0.70
2:C:197:PHE:HE1	2:C:200:ARG:HH22	1.38	0.70
2:D:450:SER:O	2:D:474:THR:CG2	2.39	0.70
2:C:307:ILE:O	2:C:335:ARG:NH1	2.24	0.70
2:C:435:GLN:HA	2:C:435:GLN:OE1	1.90	0.70
1:A:63:GLN:NE2	1:A:67:GLU:OE2	2.22	0.70
2:C:144:ASP:OD2	2:C:171:LYS:NZ	2.23	0.70
2:D:177:LEU:CD1	2:D:191:LEU:HD11	2.20	0.70
2:C:26:ILE:HD12	2:C:26:ILE:N	2.04	0.70
2:C:448:ARG:NH2	2:C:532:THR:HG22	2.07	0.70
2:D:177:LEU:CD1	2:D:191:LEU:CD1	2.70	0.70
2:C:567:PHE:O	2:C:571:LEU:CD1	2.37	0.69
2:D:602:ARG:HB3	2:D:602:ARG:NH1	2.05	0.69
2:D:420:ARG:HD3	2:D:424:GLY:HA2	1.74	0.69
2:D:144:ASP:O	2:D:607:LEU:HB2	1.93	0.69
2:D:177:LEU:HD21	2:D:190:THR:CG2	2.17	0.69
2:C:578:ARG:HA	2:C:581:LYS:HE3	1.75	0.69
2:D:186:GLU:OE1	2:D:186:GLU:HA	1.92	0.69
2:D:586:GLN:NE2	2:D:586:GLN:HA	2.07	0.69
2:D:522:LYS:HD2	2:D:550:TRP:CD1	2.28	0.69
2:C:283:VAL:CG2	2:C:296:ILE:CD1	2.72	0.68
2:C:178:LYS:HE3	2:C:609:TYR:CD1	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:150:ARG:HG2	2:D:150:ARG:NH1	2.07	0.68
2:D:175:LEU:O	2:D:175:LEU:HD23	1.93	0.68
2:D:201:ARG:HH12	2:D:202:LEU:HD23	1.58	0.68
2:C:200:ARG:NH2	2:C:257:ASP:OD2	2.27	0.68
2:D:389:ILE:CD1	2:D:659:THR:HG22	2.24	0.68
2:D:86:LEU:HD21	2:D:162:LEU:HD12	1.74	0.68
2:C:600:ASP:HB2	2:C:601:LYS:CD	2.24	0.67
2:D:614:LYS:HD2	2:D:614:LYS:C	2.13	0.67
2:C:264:MET:HE1	2:C:270:ALA:C	2.12	0.67
1:B:24:TRP:O	1:B:26:LYS:N	2.28	0.67
2:C:283:VAL:HG23	2:C:296:ILE:CD1	2.24	0.67
2:D:137:PRO:C	2:D:138:MET:HG2	2.14	0.67
2:C:448:ARG:HH21	2:C:532:THR:CG2	2.07	0.67
2:D:631:PHE:CD1	2:D:637:PRO:CG	2.76	0.67
1:A:22:THR:CB	1:A:25:ARG:HH12	2.07	0.67
2:D:497:GLU:OE1	2:D:497:GLU:N	2.23	0.67
2:D:133:VAL:HG11	2:D:170:VAL:HG11	1.74	0.67
2:C:342:ASP:OD2	5:G:3:ARG:NH2	2.28	0.66
1:B:191:GLU:OE1	1:B:191:GLU:HA	1.94	0.66
2:C:567:PHE:HD1	2:C:669:LEU:HD11	1.60	0.66
2:D:640:LYS:HG3	2:D:643:ASP:CG	2.14	0.66
2:D:133:VAL:CG1	2:D:170:VAL:HG11	2.26	0.66
2:D:177:LEU:HD13	2:D:191:LEU:HD13	1.75	0.66
1:B:176:LYS:HE3	6:B:413:HOH:O	1.96	0.66
2:C:193:ARG:HH12	2:C:256:ASP:CG	1.97	0.66
2:D:631:PHE:O	2:D:636:LYS:HA	1.96	0.65
2:C:472:GLU:OE2	2:C:532:THR:CG2	2.44	0.65
2:D:420:ARG:HG3	2:D:426:VAL:HG22	1.78	0.65
2:D:389:ILE:HD13	2:D:659:THR:HG22	1.78	0.65
2:C:232:ARG:NH1	2:C:301:ASP:HB2	2.12	0.65
2:D:343:ARG:HE	2:D:363:PRO:HB2	1.61	0.65
1:A:78:ARG:NH2	6:A:303:HOH:O	2.29	0.65
2:C:139:ASP:OD2	2:C:141:THR:HG21	1.96	0.65
2:D:393:ARG:NH1	2:D:445:LEU:HD13	2.10	0.64
2:C:310:PRO:O	2:C:313:SER:HB2	1.97	0.64
2:C:81:SER:O	2:C:83:ASN:N	2.30	0.64
2:D:624:LEU:HD21	2:D:642:LEU:HB2	1.79	0.64
2:C:563:ASP:CG	2:C:565:THR:HG22	2.18	0.64
2:D:182:LYS:HB3	2:D:187:ILE:CD1	2.27	0.64
2:D:484:ARG:HG3	2:D:484:ARG:NH2	2.09	0.64
2:D:587:ASN:O	2:D:591:ASP:CB	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLN:NE2	1:A:49:GLN:HA	2.13	0.64
2:C:178:LYS:CE	2:C:609:TYR:CD1	2.81	0.64
2:D:175:LEU:C	2:D:175:LEU:HD23	2.18	0.64
2:D:631:PHE:HB3	2:D:637:PRO:HD2	1.80	0.64
2:D:474:THR:CG2	2:D:475:PHE:H	2.09	0.64
2:C:188:ARG:NH1	2:C:188:ARG:HG2	2.12	0.64
2:D:26:ILE:CG2	2:D:31:GLN:CB	2.68	0.63
2:D:563:ASP:OD1	2:D:565:THR:CG2	2.45	0.63
2:C:223:ASP:HB2	2:C:224:PRO:CD	2.27	0.63
2:D:223:ASP:OD2	2:D:507:THR:HG21	1.98	0.63
2:C:188:ARG:HH11	2:C:188:ARG:CG	2.10	0.63
2:D:207:SER:O	2:D:210:VAL:HG13	1.99	0.63
2:D:461:MET:HE3	2:D:466:ARG:CG	2.25	0.63
2:D:178:LYS:HD2	2:D:609:TYR:HE2	1.62	0.63
2:C:139:ASP:CG	2:C:141:THR:HG21	2.19	0.63
2:D:126:ARG:HD3	2:D:166:TRP:CD1	2.33	0.62
2:C:290:LYS:CB	2:C:291:PRO:HD2	2.23	0.62
2:C:584:GLU:O	2:C:588:ILE:HG13	1.98	0.62
2:D:223:ASP:HB2	2:D:224:PRO:HD3	1.80	0.62
2:D:267:GLY:O	2:D:272:LYS:HE2	2.00	0.62
2:D:126:ARG:HG2	2:D:166:TRP:CZ2	2.34	0.62
2:D:410:PHE:HB2	2:D:461:MET:HE1	1.82	0.62
2:D:606:SER:HB3	2:D:612:ARG:HD3	1.81	0.62
2:C:452:SER:HB2	3:H:4:ALA:O	1.99	0.61
2:D:223:ASP:HB2	2:D:224:PRO:CD	2.30	0.61
2:C:252:LEU:HD11	2:C:307:ILE:HD13	1.82	0.61
2:D:650:GLN:CD	2:D:650:GLN:H	2.03	0.61
2:D:212:SER:O	2:D:216:THR:HG23	2.01	0.61
2:D:623:ARG:O	2:D:627:LEU:HD11	2.01	0.61
2:D:452:SER:HB3	3:F:4:ALA:O	2.01	0.61
2:C:264:MET:HE3	2:C:270:ALA:C	2.20	0.61
1:B:22:THR:HA	1:B:24:TRP:CD1	2.36	0.60
2:C:292:MET:CE	2:C:318:GLU:CA	2.78	0.60
2:C:354:LYS:HD2	2:C:354:LYS:N	2.16	0.60
2:D:647:LYS:CD	2:D:647:LYS:H	2.12	0.60
2:D:182:LYS:HB3	2:D:187:ILE:HD11	1.83	0.60
2:D:627:LEU:HD12	2:D:627:LEU:N	2.16	0.60
2:C:81:SER:HB2	6:C:701:HOH:O	2.01	0.60
2:D:461:MET:HE2	2:D:466:ARG:CG	2.28	0.60
2:D:178:LYS:HD3	2:D:609:TYR:CD2	2.35	0.60
2:C:199:ILE:O	2:C:202:LEU:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:411:ILE:HD11	2:D:466:ARG:HB2	1.84	0.60
2:C:256:ASP:O	2:C:258:TYR:N	2.34	0.60
1:B:188:GLN:O	1:B:192:LYS:HB2	2.02	0.59
2:C:609:TYR:CZ	2:C:613:GLU:HG3	2.37	0.59
2:D:579:ILE:HG22	2:D:585:PHE:CG	2.37	0.59
2:D:631:PHE:HB3	2:D:636:LYS:CB	2.32	0.59
1:A:187:LYS:O	1:A:191:GLU:HG2	2.03	0.59
2:C:196:LYS:NZ	2:C:200:ARG:HE	2.01	0.59
2:C:472:GLU:OE2	2:C:532:THR:HG22	2.03	0.59
2:C:40:GLN:O	2:C:44:VAL:HG23	2.02	0.59
2:C:182:LYS:HG2	2:C:186:GLU:HG3	1.83	0.59
2:C:369:LEU:O	2:C:373:VAL:HG23	2.02	0.59
2:D:455:GLU:CD	2:D:474:THR:HG21	2.22	0.59
2:C:236:GLN:O	2:C:240:GLU:HG3	2.03	0.59
2:D:145:THR:OG1	2:D:604:ILE:HG23	2.03	0.59
2:D:137:PRO:HA	2:D:188:ARG:HH22	1.68	0.59
1:B:78:ARG:NH1	6:B:303:HOH:O	2.35	0.58
2:C:183:THR:O	2:C:187:ILE:HG13	2.03	0.58
2:C:206:ASN:OD1	2:C:209:ASP:OD2	2.21	0.58
1:B:184:GLU:OE2	1:B:187:LYS:HE2	2.04	0.58
2:C:73:ARG:NH2	2:C:545:ASP:OD2	2.36	0.58
2:D:187:ILE:HD13	2:D:187:ILE:H	1.68	0.58
2:D:600:ASP:OD1	2:D:601:LYS:HG2	2.03	0.58
2:C:452:SER:CB	3:H:4:ALA:O	2.51	0.58
2:C:608:ASN:O	2:C:611:VAL:CG1	2.52	0.58
2:D:474:THR:OG1	2:D:524:VAL:HG13	2.04	0.58
2:D:182:LYS:HG3	2:D:186:GLU:HG3	1.86	0.57
2:D:223:ASP:CB	2:D:224:PRO:CD	2.82	0.57
2:D:609:TYR:H	2:D:609:TYR:HD1	1.52	0.57
2:D:508:ILE:HG13	2:D:509:GLN:HG2	1.86	0.57
2:C:309:GLY:HA3	2:C:335:ARG:NE	2.20	0.57
2:D:148:LEU:HD12	2:D:603:ASN:O	2.04	0.57
2:C:64:GLN:HG2	2:C:98:THR:HB	1.87	0.56
2:D:513:ARG:HB2	2:D:515:ASN:HB2	1.86	0.56
2:C:283:VAL:CG2	2:C:296:ILE:CG1	2.70	0.56
2:C:645:LEU:HD12	2:C:646:PRO:HD2	1.86	0.56
2:D:178:LYS:HD2	2:D:609:TYR:CE2	2.41	0.56
1:B:198:TRP:CH2	1:B:219:LEU:HA	2.39	0.56
2:C:256:ASP:C	2:C:258:TYR:H	2.08	0.56
2:C:316:ARG:HG2	2:C:332:THR:OG1	2.06	0.56
2:D:144:ASP:O	2:D:607:LEU:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:290:LYS:CB	2:C:291:PRO:CD	2.82	0.56
2:C:328:THR:O	2:C:328:THR:HG23	2.05	0.56
2:D:313:SER:HB3	2:D:335:ARG:HD2	1.88	0.56
2:C:232:ARG:NH1	2:C:301:ASP:CB	2.69	0.56
2:D:177:LEU:HD13	2:D:191:LEU:HD11	1.84	0.56
2:D:206:ASN:HB2	2:D:209:ASP:OD2	2.06	0.56
2:D:347:MET:HE1	2:D:349:VAL:HG23	1.88	0.56
2:D:579:ILE:CG2	2:D:585:PHE:CE2	2.89	0.56
2:D:644:ASP:O	2:D:645:LEU:HD12	2.06	0.56
1:B:21:ASN:N	6:B:304:HOH:O	2.39	0.55
2:D:38:GLU:HB2	2:D:41:HIS:CE1	2.41	0.55
2:D:480:VAL:HB	2:D:509:GLN:HG3	1.86	0.55
2:D:579:ILE:HG21	2:D:585:PHE:CD2	2.41	0.55
2:C:342:ASP:N	2:C:342:ASP:OD1	2.30	0.55
2:D:626:ARG:NH2	2:D:629:GLU:CG	2.66	0.55
2:D:81:SER:O	2:D:83:ASN:N	2.35	0.55
2:D:212:SER:O	2:D:216:THR:CG2	2.55	0.55
1:B:24:TRP:C	1:B:26:LYS:N	2.60	0.55
2:D:73:ARG:HD2	2:D:217:ALA:O	2.06	0.55
2:D:631:PHE:CA	2:D:637:PRO:CD	2.63	0.55
2:C:652:PRO:O	2:C:654:PRO:HD3	2.05	0.55
2:D:178:LYS:HD3	2:D:609:TYR:HD2	1.72	0.55
2:D:640:LYS:HG3	2:D:643:ASP:CA	2.28	0.55
1:A:22:THR:CG2	1:A:25:ARG:HH12	2.19	0.54
2:D:318:GLU:OE1	2:D:330:THR:HB	2.08	0.54
2:D:613:GLU:O	2:D:617:ASN:N	2.28	0.54
2:D:71:PHE:CE2	2:D:75:LEU:HD11	2.43	0.54
1:A:191:GLU:HA	1:A:191:GLU:OE1	2.07	0.54
2:C:188:ARG:O	2:C:192:THR:OG1	2.22	0.54
2:C:102:ASP:OD1	2:C:105:ARG:NH2	2.37	0.54
2:D:579:ILE:HG21	2:D:585:PHE:CE2	2.43	0.54
2:C:38:GLU:HB2	2:C:41:HIS:ND1	2.23	0.54
2:D:343:ARG:O	2:D:343:ARG:HG3	2.07	0.54
2:D:496:PRO:HD2	2:D:497:GLU:OE1	2.07	0.54
2:D:455:GLU:HG2	2:D:474:THR:CG2	2.09	0.54
2:D:374:LYS:HG2	2:D:437:PHE:CZ	2.43	0.53
2:D:599:LYS:HB3	2:D:602:ARG:NH2	2.22	0.53
2:D:614:LYS:HD2	2:D:614:LYS:O	2.09	0.53
2:C:279:GLY:O	2:C:281:LYS:HD3	2.08	0.53
2:D:126:ARG:CG	2:D:166:TRP:CD1	2.91	0.53
2:D:631:PHE:CE1	2:D:637:PRO:HG2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:624:LEU:O	2:D:624:LEU:HG	2.08	0.53
2:C:146:TYR:CE1	2:C:169:LYS:HA	2.44	0.53
2:C:590:LYS:HE2	2:C:590:LYS:O	2.09	0.53
2:D:585:PHE:C	2:D:586:GLN:HE21	2.12	0.53
2:D:173:ASP:O	2:D:177:LEU:HD12	2.09	0.53
2:D:38:GLU:HB2	2:D:41:HIS:ND1	2.24	0.52
1:A:49:GLN:HE21	1:A:49:GLN:HA	1.73	0.52
2:C:28:ARG:HG2	2:C:30:ASP:HB2	1.92	0.52
2:D:455:GLU:CG	2:D:474:THR:CG2	2.78	0.52
2:D:374:LYS:O	2:D:378:GLN:HG3	2.09	0.52
1:A:89:LEU:HG	1:A:98:VAL:HG11	1.91	0.52
2:D:182:LYS:HZ2	2:D:186:GLU:HG3	1.68	0.52
2:C:631:PHE:CD1	2:C:636:LYS:HD3	2.44	0.52
2:D:82:HIS:ND1	2:D:153:ALA:O	2.39	0.52
2:C:336:GLU:O	2:C:338:ILE:CD1	2.55	0.52
2:D:187:ILE:N	2:D:187:ILE:CD1	2.72	0.52
1:B:24:TRP:C	1:B:26:LYS:H	2.13	0.52
2:C:420:ARG:NH1	2:C:553:ILE:HG22	2.25	0.52
2:C:601:LYS:N	2:C:601:LYS:HD3	2.25	0.52
2:C:456:ILE:HG13	2:C:511:PHE:CE1	2.45	0.52
2:C:530:MET:HB3	2:C:531:PRO:HD2	1.92	0.52
2:C:600:ASP:OD1	2:C:600:ASP:N	2.42	0.52
2:C:411:ILE:HD11	2:C:466:ARG:HB2	1.92	0.51
2:D:134:LEU:HD21	2:D:188:ARG:CA	2.40	0.51
2:D:245:LEU:HD23	2:D:340:LEU:HD21	1.92	0.51
2:D:297:GLY:C	2:D:298:TRP:HD1	2.13	0.51
2:D:651:GLU:HB3	2:D:652:PRO:HD2	1.91	0.51
2:D:177:LEU:O	2:D:180:THR:HB	2.09	0.51
1:A:156:PHE:CD2	1:A:166:ARG:HG2	2.46	0.51
2:C:177:LEU:O	2:C:180:THR:OG1	2.29	0.51
2:C:641:LYS:HG2	2:C:644:ASP:OD2	2.11	0.51
2:D:619:ASP:HA	2:D:622:THR:OG1	2.11	0.51
2:C:351:THR:HG23	2:C:356:LYS:HE3	1.93	0.51
2:C:37:GLU:HB2	2:C:113:TYR:CE1	2.45	0.51
2:D:134:LEU:CD2	2:D:188:ARG:CG	2.84	0.51
2:C:126:ARG:NE	2:C:126:ARG:HA	2.26	0.51
2:C:362:ILE:HD12	2:C:390:ILE:CG2	2.41	0.51
2:C:497:GLU:N	2:C:497:GLU:OE2	2.41	0.51
1:B:22:THR:HA	1:B:24:TRP:NE1	2.26	0.51
2:C:292:MET:HE1	2:C:318:GLU:CA	2.40	0.50
2:D:374:LYS:HG2	2:D:437:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:HIS:CE1	2:D:507:THR:HG23	2.46	0.50
2:D:624:LEU:HD13	2:D:644:ASP:HA	1.92	0.50
2:C:269:PRO:HG3	2:C:336:GLU:HG2	1.93	0.50
2:C:585:PHE:O	2:C:589:MET:HG2	2.11	0.50
2:C:145:THR:CA	2:C:607:LEU:HD12	2.41	0.50
2:D:631:PHE:CD1	2:D:637:PRO:HD2	2.46	0.50
2:C:609:TYR:CD2	2:C:609:TYR:C	2.85	0.50
2:D:602:ARG:CB	2:D:602:ARG:NH1	2.72	0.50
2:D:673:ARG:O	6:D:701:HOH:O	2.20	0.50
2:D:304:VAL:HG22	4:E:4:ALA:HB2	1.92	0.50
2:C:188:ARG:NH1	2:C:188:ARG:CG	2.73	0.50
2:C:251:VAL:CG1	2:C:263:SER:OG	2.60	0.50
2:C:249:GLY:O	2:C:265:VAL:HG23	2.12	0.50
2:D:148:LEU:HD12	2:D:603:ASN:C	2.32	0.50
2:D:200:ARG:O	2:D:204:GLN:HG3	2.12	0.50
1:A:134:LEU:HB2	1:A:156:PHE:CD2	2.47	0.50
2:D:510:LYS:HD3	2:D:548:LEU:HD23	1.94	0.50
1:B:198:TRP:CH2	1:B:219:LEU:CA	2.95	0.50
2:D:277:SER:O	2:D:280:ASP:HB2	2.12	0.50
2:D:647:LYS:HD3	2:D:647:LYS:N	2.25	0.50
2:D:86:LEU:HD21	2:D:162:LEU:HD11	1.91	0.49
2:D:178:LYS:CD	2:D:609:TYR:CE2	2.94	0.49
2:D:201:ARG:NH1	2:D:202:LEU:HD23	2.24	0.49
2:D:26:ILE:HA	2:D:31:GLN:OE1	2.12	0.49
2:D:595:PHE:C	2:D:595:PHE:CD1	2.85	0.49
2:D:631:PHE:O	2:D:636:LYS:HB3	2.12	0.49
1:A:164:PRO:HB3	1:A:200:TRP:CD2	2.46	0.49
2:C:59:GLN:NE2	6:C:707:HOH:O	2.38	0.49
2:D:347:MET:HE2	2:D:380:LEU:HD21	1.94	0.49
2:D:626:ARG:HG3	2:D:626:ARG:O	2.12	0.49
2:D:183:THR:HG23	2:D:186:GLU:HG2	1.93	0.49
2:D:455:GLU:CD	2:D:474:THR:CG2	2.81	0.49
2:D:398:GLY:N	3:F:5:ALA:HB2	2.28	0.49
1:B:85:PHE:HB3	1:B:98:VAL:HG13	1.95	0.49
2:D:343:ARG:O	2:D:363:PRO:HG2	2.12	0.49
2:D:347:MET:CE	2:D:380:LEU:HD21	2.43	0.49
2:D:177:LEU:CD2	2:D:190:THR:CG2	2.83	0.49
2:D:586:GLN:NE2	6:D:704:HOH:O	2.30	0.49
2:D:133:VAL:HG11	2:D:170:VAL:CG1	2.42	0.48
2:D:420:ARG:CG	2:D:426:VAL:HG22	2.41	0.48
2:D:439:LYS:HE2	2:D:439:LYS:CA	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:593:ALA:O	2:D:596:ASN:HB2	2.13	0.48
2:C:356:LYS:HB2	2:C:385:VAL:HG23	1.96	0.48
2:D:223:ASP:OD2	2:D:507:THR:CG2	2.62	0.48
2:C:254:MET:HA	2:C:258:TYR:O	2.14	0.48
2:D:67:SER:OG	2:D:100:LEU:HB2	2.13	0.48
2:D:237:PHE:CZ	2:D:241:MET:CE	2.96	0.48
2:D:290:LYS:HB3	2:D:291:PRO:HD2	1.96	0.48
2:D:447:ASP:HA	2:D:472:GLU:HB2	1.94	0.48
2:D:231:PRO:HG3	2:D:500:ALA:O	2.13	0.48
2:D:515:ASN:HB3	2:D:517:GLY:H	1.77	0.48
2:D:141:THR:OG1	2:D:141:THR:O	2.27	0.48
2:C:81:SER:O	2:C:82:HIS:C	2.51	0.48
2:D:187:ILE:H	2:D:187:ILE:CD1	2.25	0.48
2:D:177:LEU:HD11	2:D:191:LEU:HD11	1.94	0.48
2:D:345:VAL:HG23	2:D:362:ILE:HG12	1.95	0.48
2:D:599:LYS:O	2:D:602:ARG:HB2	2.13	0.48
2:C:466:ARG:HD2	2:C:466:ARG:O	2.14	0.48
2:D:26:ILE:HG23	2:D:31:GLN:CG	2.43	0.48
2:D:412:PRO:HA	2:D:436:VAL:HG23	1.95	0.48
2:C:133:VAL:HG23	2:C:136:LYS:HE3	1.95	0.48
2:C:139:ASP:HB3	2:C:141:THR:H	1.79	0.48
2:C:223:ASP:CB	2:C:224:PRO:CD	2.91	0.48
2:C:283:VAL:O	2:C:283:VAL:HG22	2.13	0.48
2:D:311:LYS:O	2:D:311:LYS:HG3	2.13	0.48
2:D:347:MET:CE	2:D:349:VAL:HG23	2.43	0.48
2:C:223:ASP:CB	2:C:224:PRO:HD2	2.41	0.48
2:D:177:LEU:HD11	2:D:191:LEU:CD1	2.42	0.48
2:D:389:ILE:HD13	2:D:659:THR:CG2	2.42	0.48
2:D:631:PHE:C	2:D:636:LYS:HB3	2.34	0.48
2:C:410:PHE:O	2:C:411:ILE:HD13	2.14	0.47
2:C:178:LYS:HE2	2:C:609:TYR:CD1	2.49	0.47
2:D:631:PHE:HD1	2:D:637:PRO:HG2	1.71	0.47
2:C:109:LEU:HB3	2:C:112:PHE:HD2	1.79	0.47
2:C:598:MET:HE3	2:C:598:MET:HB2	1.78	0.47
2:D:127:TYR:CZ	2:D:198:ALA:HB1	2.50	0.47
2:D:640:LYS:CB	2:D:643:ASP:CB	2.84	0.47
1:B:89:LEU:HG	1:B:98:VAL:HG11	1.96	0.47
2:C:85:LEU:O	2:C:156:PRO:HD2	2.15	0.47
2:D:640:LYS:CG	2:D:643:ASP:CB	2.25	0.47
2:D:237:PHE:CZ	2:D:241:MET:HE3	2.50	0.47
2:C:657:ASP:O	2:C:660:VAL:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:79:ASP:O	2:C:82:HIS:HD2	1.98	0.47
2:D:236:GLN:O	2:D:240:GLU:HG3	2.14	0.47
2:D:461:MET:HE3	2:D:466:ARG:CB	2.45	0.47
2:C:146:TYR:HE1	2:C:169:LYS:HA	1.81	0.46
2:D:613:GLU:O	2:D:614:LYS:C	2.49	0.46
2:C:431:ASP:N	6:C:704:HOH:O	2.36	0.46
2:C:601:LYS:N	2:C:601:LYS:CD	2.79	0.46
2:D:129:TYR:OH	2:D:167:ASP:OD1	2.28	0.46
2:D:542:LYS:HB3	2:D:542:LYS:HE3	1.40	0.46
2:D:586:GLN:CA	2:D:586:GLN:NE2	2.77	0.46
2:C:567:PHE:HB3	2:C:669:LEU:HD12	1.97	0.46
2:D:148:LEU:HD12	2:D:603:ASN:HA	1.98	0.46
2:D:147:ASN:HA	2:D:603:ASN:O	2.16	0.46
1:B:24:TRP:O	1:B:25:ARG:C	2.54	0.46
2:C:144:ASP:N	2:C:144:ASP:OD1	2.36	0.46
2:C:252:LEU:HD11	2:C:307:ILE:CD1	2.46	0.46
2:C:189:GLU:HG2	2:C:189:GLU:O	2.16	0.46
2:D:521:ARG:O	2:D:542:LYS:CE	2.57	0.46
2:D:630:ARG:HE	2:D:630:ARG:HB3	1.45	0.46
2:C:568:GLU:CB	2:C:569:PRO:CD	2.88	0.46
2:C:300:LEU:HD12	2:C:300:LEU:O	2.16	0.45
1:B:23:SER:O	1:B:26:LYS:HB3	2.16	0.45
2:C:196:LYS:HZ1	2:C:200:ARG:HE	1.64	0.45
2:C:253:GLN:O	2:C:260:VAL:N	2.49	0.45
2:D:257:ASP:O	2:D:296:ILE:O	2.33	0.45
2:D:497:GLU:HG3	6:D:871:HOH:O	2.16	0.45
2:D:525:THR:HA	2:D:526:PRO:HD3	1.80	0.45
2:D:609:TYR:CD1	2:D:609:TYR:N	2.83	0.45
2:C:350:LYS:HD2	2:C:660:VAL:HG21	1.97	0.45
2:C:564:LEU:HD23	2:C:564:LEU:N	2.31	0.45
2:D:32:ILE:HG23	2:D:32:ILE:O	2.16	0.45
2:C:256:ASP:C	2:C:258:TYR:N	2.70	0.45
2:C:411:ILE:HD12	2:C:411:ILE:HA	1.67	0.45
2:C:446:VAL:O	2:C:471:GLY:HA3	2.17	0.45
2:C:609:TYR:CE2	2:C:613:GLU:CG	2.92	0.45
2:D:642:LEU:HD13	2:D:644:ASP:CB	2.33	0.45
2:C:309:GLY:CA	2:C:335:ARG:HD2	2.47	0.45
2:C:358:GLY:O	2:C:388:VAL:HA	2.16	0.45
2:D:272:LYS:HE3	2:D:272:LYS:HB2	1.60	0.45
2:C:347:MET:C	2:C:347:MET:CE	2.85	0.45
2:D:144:ASP:OD1	2:D:144:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27:THR:OG1	2:D:28:ARG:HG3	2.17	0.45
2:D:608:ASN:HB3	2:D:611:VAL:CG1	2.40	0.45
2:C:271:ALA:C	2:C:273:SER:H	2.18	0.45
2:C:284:GLY:HA3	2:C:292:MET:HE2	1.98	0.45
2:C:67:SER:OG	2:C:100:LEU:HB2	2.16	0.45
2:C:452:SER:HB3	3:H:4:ALA:HB1	1.99	0.45
2:C:57:TYR:CD1	2:C:57:TYR:C	2.90	0.45
1:B:22:THR:O	1:B:22:THR:HG22	2.17	0.44
2:C:177:LEU:HB3	2:C:182:LYS:HD2	2.00	0.44
2:D:614:LYS:CD	2:D:614:LYS:C	2.85	0.44
2:C:100:LEU:HD23	2:C:100:LEU:HA	1.82	0.44
2:C:197:PHE:CZ	2:C:256:ASP:CB	2.99	0.44
2:D:411:ILE:HG12	2:D:461:MET:HE1	1.99	0.44
2:D:642:LEU:HD12	2:D:644:ASP:H	1.83	0.44
2:C:564:LEU:HD13	2:C:666:LEU:HD11	1.98	0.44
2:C:624:LEU:HD11	2:C:639:LEU:HD12	1.98	0.44
2:D:627:LEU:HA	2:D:630:ARG:HH21	1.83	0.44
1:A:198:TRP:CH2	1:A:219:LEU:HA	2.53	0.44
1:B:220:LYS:HE3	6:B:472:HOH:O	2.18	0.44
2:D:82:HIS:CD2	2:D:155:TRP:CH2	3.05	0.44
2:C:269:PRO:CG	2:C:336:GLU:HG2	2.48	0.44
1:B:288:LEU:HD22	1:B:288:LEU:HA	1.79	0.44
2:C:229:LEU:HD12	2:C:229:LEU:N	2.32	0.44
2:C:582:ASP:HA	2:C:583:PRO:HD3	1.74	0.44
2:D:245:LEU:CD2	2:D:340:LEU:HD21	2.47	0.44
2:C:388:VAL:HG23	2:C:438:TYR:OH	2.17	0.43
2:D:496:PRO:CD	2:D:497:GLU:OE1	2.66	0.43
2:C:134:LEU:HA	2:C:134:LEU:HD23	1.70	0.43
2:D:358:GLY:N	2:D:385:VAL:HG21	2.33	0.43
2:C:304:VAL:HG21	5:G:2:SER:OG	2.18	0.43
2:C:362:ILE:HD12	2:C:390:ILE:HG23	1.99	0.43
2:D:126:ARG:HG3	2:D:166:TRP:CE2	2.50	0.43
2:C:568:GLU:CB	2:C:569:PRO:HD3	2.23	0.43
2:D:124:PHE:CD1	2:D:199:ILE:HD13	2.53	0.43
2:D:59:GLN:NE2	6:D:710:HOH:O	2.32	0.43
2:C:26:ILE:CG2	2:C:31:GLN:HB3	2.37	0.43
2:D:178:LYS:CD	2:D:609:TYR:CD2	3.02	0.43
1:A:124:GLU:OE1	2:C:47:ARG:NH2	2.48	0.43
2:C:126:ARG:HB3	2:C:166:TRP:CE2	2.53	0.43
2:D:243:LEU:HD22	2:D:366:TYR:CD1	2.54	0.43
2:D:96:LYS:O	2:D:99:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:186:GLU:O	2:C:187:ILE:C	2.57	0.43
2:C:81:SER:HB3	2:C:83:ASN:ND2	2.33	0.43
2:C:285:VAL:HG11	2:C:306:LEU:HB3	2.01	0.43
2:C:536:GLU:H	2:C:536:GLU:HG2	1.60	0.43
2:C:664:LEU:O	2:C:668:LYS:HB2	2.19	0.43
2:D:108:LYS:HD3	2:D:108:LYS:HA	1.64	0.43
2:D:183:THR:CG2	2:D:186:GLU:HG2	2.49	0.43
2:D:355:GLU:CD	2:D:664:LEU:HD22	2.39	0.43
2:D:640:LYS:HG3	2:D:643:ASP:HB2	0.51	0.42
1:A:286:ASP:C	1:A:288:LEU:H	2.22	0.42
2:C:140:PHE:HB3	2:C:609:TYR:HB2	1.99	0.42
2:D:68:ALA:HB1	2:D:97:LYS:HE2	2.00	0.42
2:C:47:ARG:CZ	2:C:488:ARG:HG3	2.49	0.42
2:D:606:SER:O	2:D:607:LEU:HB2	2.18	0.42
2:D:99:GLU:OE1	6:D:702:HOH:O	2.21	0.42
2:C:270:ALA:HA	2:C:276:ILE:HD11	2.02	0.42
2:C:563:ASP:OD1	2:C:564:LEU:N	2.53	0.42
2:C:197:PHE:CD1	2:C:200:ARG:NH2	2.83	0.42
2:D:31:GLN:O	2:D:33:PRO:HD3	2.19	0.42
2:D:631:PHE:CD1	2:D:637:PRO:CD	3.02	0.42
2:C:310:PRO:O	2:C:313:SER:CB	2.66	0.42
2:C:78:LEU:HD21	2:C:116:TYR:CD2	2.54	0.42
2:C:86:LEU:O	2:C:89:ASP:HB2	2.19	0.42
2:D:35:LEU:HA	2:D:35:LEU:HD23	1.89	0.42
1:B:174:GLU:HB3	1:B:182:ALA:HB2	2.02	0.42
2:C:138:MET:HB2	6:C:793:HOH:O	2.19	0.42
2:C:127:TYR:HB3	2:C:199:ILE:HD11	2.02	0.42
2:C:197:PHE:CZ	2:C:257:ASP:OD2	2.72	0.42
2:D:647:LYS:HB2	2:D:648:ASP:H	1.67	0.42
1:B:134:LEU:HB2	1:B:156:PHE:CD2	2.55	0.42
2:C:362:ILE:HA	2:C:363:PRO:HD3	1.85	0.42
2:D:175:LEU:HD21	2:D:179:LEU:CD1	2.05	0.42
1:A:237:ASN:HB2	1:A:260:ALA:HB2	2.01	0.42
2:D:126:ARG:CD	2:D:166:TRP:NE1	2.82	0.42
1:B:113:ASP:HA	1:B:116:TYR:CD2	2.55	0.42
2:C:26:ILE:CD1	2:C:26:ILE:H	2.09	0.42
2:D:148:LEU:CD1	2:D:603:ASN:HA	2.50	0.42
2:D:201:ARG:HH22	2:D:202:LEU:HD21	1.85	0.42
2:C:382:LYS:HB3	2:C:382:LYS:HE3	1.57	0.41
1:A:163:ASP:HB3	1:A:166:ARG:HD3	2.02	0.41
2:C:38:GLU:HB2	2:C:41:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:452:SER:HB3	2:D:453:ALA:H	1.60	0.41
2:D:569:PRO:O	2:D:573:LYS:HG2	2.20	0.41
2:D:175:LEU:HD12	2:D:609:TYR:CD1	2.55	0.41
1:A:111:ASN:ND2	6:A:314:HOH:O	2.49	0.41
2:C:306:LEU:HA	2:C:306:LEU:HD23	1.60	0.41
2:C:347:MET:HE2	2:C:347:MET:HB3	1.28	0.41
2:C:642:LEU:O	2:C:642:LEU:HD12	2.20	0.41
2:D:230:SER:HB2	2:D:231:PRO:HD2	2.02	0.41
2:D:448:ARG:HB3	2:D:448:ARG:HE	1.66	0.41
2:C:590:LYS:HD2	2:C:590:LYS:HA	1.84	0.41
2:D:329:ARG:HD2	2:D:329:ARG:HH11	1.68	0.41
1:A:183:LYS:HB2	1:A:183:LYS:HE3	1.90	0.41
2:C:135:GLU:OE2	2:C:135:GLU:N	2.53	0.41
2:C:166:TRP:O	2:C:170:VAL:CG1	2.62	0.41
2:C:340:LEU:HA	2:C:340:LEU:HD23	1.81	0.41
2:D:613:GLU:H	2:D:616:ASN:H	1.68	0.41
2:C:324:LYS:HB3	2:C:325:GLY:H	1.59	0.41
2:C:354:LYS:HD3	2:C:355:GLU:CG	2.45	0.41
2:D:86:LEU:CD2	2:D:162:LEU:HD11	2.50	0.41
2:D:206:ASN:HB2	2:D:209:ASP:CG	2.40	0.41
2:D:414:GLY:O	2:D:430:SER:HB3	2.21	0.41
2:D:436:VAL:HG11	2:D:439:LYS:HG2	2.01	0.41
2:D:612:ARG:H	2:D:612:ARG:HG2	1.71	0.41
2:C:578:ARG:HA	2:C:581:LYS:CE	2.48	0.41
2:D:175:LEU:CD2	2:D:175:LEU:C	2.85	0.41
2:D:455:GLU:OE1	2:D:474:THR:CG2	2.69	0.41
2:D:463:ASP:OD1	2:D:513:ARG:NH2	2.51	0.41
2:D:631:PHE:O	2:D:636:LYS:CA	2.65	0.41
2:D:82:HIS:CD2	2:D:155:TRP:CZ3	3.09	0.41
2:D:364:GLY:HA2	2:D:395:ASN:OD1	2.21	0.40
2:C:175:LEU:C	2:C:175:LEU:HD12	2.34	0.40
2:D:135:GLU:H	2:D:135:GLU:HG2	1.75	0.40
2:D:671:LYS:HD2	2:D:671:LYS:HA	1.51	0.40
2:D:126:ARG:NE	2:D:126:ARG:HA	2.36	0.40
2:D:176:SER:HA	2:D:179:LEU:HD12	2.02	0.40
2:D:451:ALA:HA	2:D:455:GLU:HG3	2.02	0.40
2:D:584:GLU:O	2:D:588:ILE:HD12	2.20	0.40
2:D:641:LYS:HE3	2:D:641:LYS:HB2	1.49	0.40
2:C:452:SER:HB3	3:H:4:ALA:O	2.22	0.40
2:C:356:LYS:HB3	2:C:356:LYS:HE2	1.28	0.40
2:C:388:VAL:HG23	2:C:438:TYR:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:609:TYR:CZ	2:C:613:GLU:CG	3.04	0.40
2:D:410:PHE:HB2	2:D:461:MET:CE	2.49	0.40
1:A:198:TRP:CH2	1:A:219:LEU:CA	3.04	0.40
1:A:235:GLU:HA	1:A:270:GLU:HG2	2.03	0.40
2:C:177:LEU:O	2:C:182:LYS:HB2	2.21	0.40
2:C:351:THR:CG2	2:C:356:LYS:HE3	2.51	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	268/278 (96%)	264 (98%)	4 (2%)	0	100	100
1	B	266/278 (96%)	261 (98%)	3 (1%)	2 (1%)	19	23
2	C	646/682 (95%)	631 (98%)	11 (2%)	4 (1%)	25	31
2	D	643/682 (94%)	621 (97%)	21 (3%)	1 (0%)	47	58
3	F	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
3	H	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
4	E	2/4 (50%)	2 (100%)	0	0	100	100
5	G	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1835/1940 (95%)	1787 (97%)	41 (2%)	7 (0%)	34	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	82	HIS
2	C	257	ASP
1	B	25	ARG
2	D	613	GLU

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Mol	Chain	Res	Type
1	B	287	ASP
2	C	187	ILE
2	C	137	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	231/237 (98%)	223 (96%)	8 (4%)	36	50
1	B	229/237 (97%)	214 (93%)	15 (7%)	16	22
2	C	558/583 (96%)	481 (86%)	77 (14%)	3	3
2	D	558/583 (96%)	465 (83%)	93 (17%)	2	2
5	G	4/4 (100%)	1 (25%)	3 (75%)	0	0
All	All	1580/1644 (96%)	1384 (88%)	196 (12%)	4	5

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	21	ASN
1	B	23	SER
1	B	74	SER
1	B	145	ARG
1	B	153	LEU
1	B	158	GLN
1	B	175	GLN
1	B	177	LEU
1	B	192	LYS
1	B	193	SER
1	B	196	GLU
1	B	217	GLU
1	B	220	LYS
1	B	246	SER
1	B	288	LEU
1	A	53	SER

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Mol	Chain	Res	Type
1	A	111	ASN
1	A	166	ARG
1	A	175	GLN
1	A	192	LYS
1	A	279	SER
1	A	283	GLN
1	A	288	LEU
2	C	26	ILE
2	C	31	GLN
2	C	37	GLU
2	C	81	SER
2	C	108	LYS
2	C	121	LYS
2	C	133	VAL
2	C	135	GLU
2	C	141	THR
2	C	152	LYS
2	C	169	LYS
2	C	182	LYS
2	C	183	THR
2	C	186	GLU
2	C	188	ARG
2	C	193	ARG
2	C	201	ARG
2	C	244	SER
2	C	245	LEU
2	C	251	VAL
2	C	256	ASP
2	C	257	ASP
2	C	260	VAL
2	C	273	SER
2	C	276	ILE
2	C	277	SER
2	C	281	LYS
2	C	294	ASP
2	C	311	LYS
2	C	313	SER
2	C	318	GLU
2	C	324	LYS
2	C	329	ARG
2	C	342	ASP
2	C	343	ARG

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Mol	Chain	Res	Type
2	C	346	LYS
2	C	347	MET
2	C	348	SER
2	C	354	LYS
2	C	355	GLU
2	C	356	LYS
2	C	381	GLU
2	C	382	LYS
2	C	383	GLN
2	C	385	VAL
2	C	411	ILE
2	C	435	GLN
2	C	439	LYS
2	C	504	VAL
2	C	522	LYS
2	C	535	GLU
2	C	536	GLU
2	C	552	SER
2	C	559	VAL
2	C	565	THR
2	C	571	LEU
2	C	572	LEU
2	C	581	LYS
2	C	590	LYS
2	C	594	ARG
2	C	598	MET
2	C	600	ASP
2	C	601	LYS
2	C	611	VAL
2	C	612	ARG
2	C	613	GLU
2	C	614	LYS
2	C	615	GLU
2	C	616	ASN
2	C	633	ARG
2	C	636	LYS
2	C	639	LEU
2	C	641	LYS
2	C	647	LYS
2	C	668	LYS
2	C	669	LEU
2	C	671	LYS

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Mol	Chain	Res	Type
2	D	25	ASP
2	D	26	ILE
2	D	31	GLN
2	D	38	GLU
2	D	51	ARG
2	D	77	LEU
2	D	96	LYS
2	D	99	GLU
2	D	108	LYS
2	D	109	LEU
2	D	123	ARG
2	D	126	ARG
2	D	131	LEU
2	D	134	LEU
2	D	138	MET
2	D	139	ASP
2	D	148	LEU
2	D	150	ARG
2	D	171	LYS
2	D	180	THR
2	D	182	LYS
2	D	186	GLU
2	D	187	ILE
2	D	196	LYS
2	D	210	VAL
2	D	213	LEU
2	D	216	THR
2	D	223	ASP
2	D	245	LEU
2	D	262	ASN
2	D	272	LYS
2	D	277	SER
2	D	313	SER
2	D	317	LEU
2	D	326	THR
2	D	327	LYS
2	D	328	THR
2	D	330	THR
2	D	347	MET
2	D	350	LYS
2	D	354	LYS
2	D	356	LYS

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Mol	Chain	Res	Type
2	D	374	LYS
2	D	375	VAL
2	D	382	LYS
2	D	385	VAL
2	D	386	SER
2	D	394	SER
2	D	400	LEU
2	D	420	ARG
2	D	430	SER
2	D	432	THR
2	D	437	PHE
2	D	439	LYS
2	D	445	LEU
2	D	452	SER
2	D	461	MET
2	D	484	ARG
2	D	507	THR
2	D	524	VAL
2	D	535	GLU
2	D	542	LYS
2	D	565	THR
2	D	573	LYS
2	D	581	LYS
2	D	586	GLN
2	D	588	ILE
2	D	590	LYS
2	D	594	ARG
2	D	599	LYS
2	D	602	ARG
2	D	604	ILE
2	D	605	VAL
2	D	609	TYR
2	D	612	ARG
2	D	613	GLU
2	D	614	LYS
2	D	616	ASN
2	D	618	GLU
2	D	626	ARG
2	D	627	LEU
2	D	629	GLU
2	D	630	ARG
2	D	632	LYS

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Mol	Chain	Res	Type
2	D	633	ARG
2	D	636	LYS
2	D	641	LYS
2	D	642	LEU
2	D	647	LYS
2	D	648	ASP
2	D	650	GLN
2	D	671	LYS
2	D	673	ARG
5	G	1	LEU
5	G	3	ARG
5	G	4	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	63	GLN
1	B	150	GLN
1	A	49	GLN
1	A	232	HIS
2	D	120	GLN
2	D	435	GLN
2	D	586	GLN
2	D	628	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	270/278 (97%)	-0.29	2 (0%) 87 91	10, 20, 41, 90	0
1	B	268/278 (96%)	-0.16	4 (1%) 73 79	11, 21, 47, 113	0
2	C	648/682 (95%)	0.49	73 (11%) 5 7	18, 52, 96, 132	0
2	D	647/682 (94%)	0.50	75 (11%) 4 6	19, 45, 92, 117	0
3	F	6/6 (100%)	0.65	1 (16%) 1 2	35, 40, 59, 64	0
3	H	6/6 (100%)	1.53	2 (33%) 0 0	38, 42, 61, 70	0
4	E	4/4 (100%)	1.26	1 (25%) 0 0	38, 51, 59, 70	0
5	G	4/4 (100%)	2.39	2 (50%) 0 0	56, 64, 65, 69	0
All	All	1853/1940 (95%)	0.30	160 (8%) 10 14	10, 40, 91, 132	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	G	1	LEU	6.2
2	D	648	ASP	6.1
2	D	641	LYS	6.0
2	C	326	THR	6.0
2	D	646	PRO	5.7
2	C	324	LYS	5.3
2	D	649	TYR	5.3
2	C	433	ASP	5.2
2	D	639	LEU	5.2
2	C	382	LYS	5.2
2	D	624	LEU	5.0
2	C	325	GLY	5.0
1	B	22	THR	4.8
2	C	288	THR	4.7
2	C	283	VAL	4.7
2	D	297	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
2	D	626	ARG	4.7
2	D	638	GLU	4.5
2	C	385	VAL	4.5
2	C	383	GLN	4.4
2	D	178	LYS	4.4
2	D	606	SER	4.4
2	D	590	LYS	4.3
2	C	432	THR	4.2
2	C	275	ALA	4.2
2	C	254	MET	4.2
2	C	600	ASP	4.1
2	D	536	GLU	4.1
2	C	434	GLY	4.0
2	D	137	PRO	4.0
2	C	258	TYR	4.0
2	D	572	LEU	4.0
2	C	444	VAL	3.9
2	D	609	TYR	3.8
2	D	444	VAL	3.7
2	C	31	GLN	3.7
2	D	629	GLU	3.7
2	C	567	PHE	3.7
2	C	289	GLY	3.6
2	D	140	PHE	3.6
2	D	457	PHE	3.6
2	D	127	TYR	3.6
2	D	142	GLY	3.6
2	C	380	LEU	3.6
2	C	197	PHE	3.5
2	C	328	THR	3.5
2	C	457	PHE	3.5
2	D	390	ILE	3.5
2	C	188	ARG	3.4
2	C	667	ALA	3.4
2	C	257	ASP	3.3
2	C	392	LEU	3.3
2	D	449	PHE	3.3
2	D	324	LYS	3.2
2	D	637	PRO	3.2
2	D	650	GLN	3.2
2	C	297	GLY	3.1
2	D	378	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	379	LYS	3.1
2	D	197	PHE	3.0
2	D	443	VAL	3.0
2	D	392	LEU	3.0
2	C	672	ALA	3.0
2	D	537	THR	3.0
2	C	252	LEU	3.0
1	A	288	LEU	2.9
2	D	630	ARG	2.9
2	C	458	ALA	2.9
2	D	642	LEU	2.9
2	D	644	ASP	2.9
3	H	6	ALA	2.8
2	C	351	THR	2.8
2	D	458	ALA	2.8
2	D	607	LEU	2.8
2	C	299	ARG	2.8
2	D	557	THR	2.8
2	C	650	GLN	2.8
2	C	598	MET	2.8
2	D	623	ARG	2.8
1	B	21	ASN	2.7
2	C	413	ALA	2.7
2	C	303	VAL	2.7
2	C	312	GLY	2.7
2	D	193	ARG	2.7
2	C	32	ILE	2.6
2	D	633	ARG	2.6
2	C	276	ILE	2.6
2	C	280	ASP	2.6
2	C	443	VAL	2.6
2	D	672	ALA	2.6
2	C	536	GLU	2.5
2	C	81	SER	2.5
2	D	640	LYS	2.5
2	C	273	SER	2.5
2	C	456	ILE	2.5
2	D	143	ASN	2.5
2	C	327	LYS	2.5
2	C	461	MET	2.5
2	D	31	GLN	2.5
2	C	329	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	579	ILE	2.4
2	C	445	LEU	2.4
2	C	645	LEU	2.4
2	D	556	ALA	2.4
2	D	608	ASN	2.4
1	B	287	ASP	2.4
2	D	592	ILE	2.4
2	C	255	ASP	2.4
2	D	28	ARG	2.4
2	C	534	ASN	2.4
2	C	310	PRO	2.4
2	D	583	PRO	2.4
2	D	354	LYS	2.4
2	C	259	THR	2.4
2	D	44	VAL	2.4
2	C	177	LEU	2.3
2	C	390	ILE	2.3
1	B	288	LEU	2.3
2	D	337	ARG	2.3
1	A	287	ASP	2.3
2	C	323	GLY	2.3
2	D	595	PHE	2.3
2	D	588	ILE	2.3
2	D	326	THR	2.2
2	D	25	ASP	2.2
2	D	135	GLU	2.2
2	D	186	GLU	2.2
2	D	343	ARG	2.2
2	D	585	PHE	2.2
2	C	29	ALA	2.2
2	D	459	ALA	2.2
2	C	333	LEU	2.2
2	C	442	LEU	2.2
2	D	205	THR	2.2
2	C	253	GLN	2.2
2	C	134	LEU	2.1
2	C	669	LEU	2.1
2	C	201	ARG	2.1
2	C	573	LYS	2.1
2	D	27	THR	2.1
2	D	342	ASP	2.1
2	C	265	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	595	PHE	2.1
2	D	587	ASN	2.1
2	C	646	PRO	2.1
2	D	32	ILE	2.1
5	G	2	SER	2.1
2	D	317	LEU	2.1
2	D	435	GLN	2.1
2	D	445	LEU	2.1
2	D	382	LYS	2.1
4	E	1	ALA	2.1
2	D	558	TYR	2.1
2	C	138	MET	2.0
3	F	5	ALA	2.0
3	H	5	ALA	2.0
2	D	26	ILE	2.0
2	C	311	LYS	2.0
2	C	668	LYS	2.0
2	D	647	LYS	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 carbohydrates 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.