



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:49 PM UTC

PDB ID : 3NOC / pdb_00003noc
Title : Designed ankyrin repeat protein (DARPin) binders to AcrB: Plasticity of the Interface
Authors : Monroe, N.; Briand, C.; Gruetter, M.G.
Deposited on : 2010-06-25
Resolution : 2.70 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

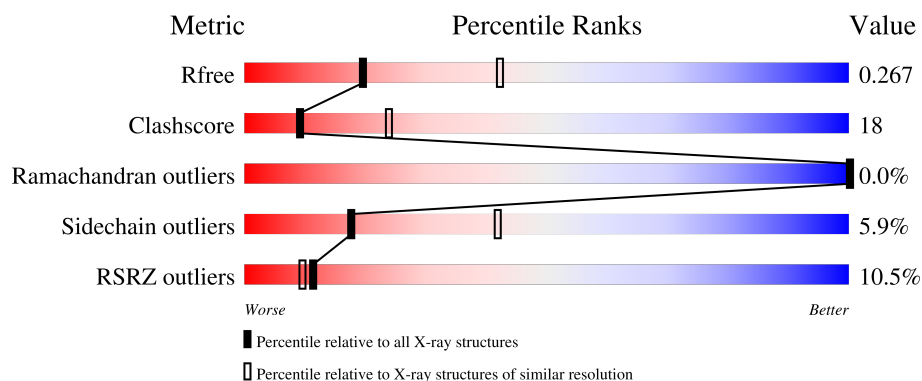
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	1049	12% 66% 29% ..
1	B	1049	9% 69% 27% ..
1	C	1049	8% 69% 26% ..
2	D	169	9% 60% 21% 9% 9%
2	E	169	26% 39% 38% 11% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25558 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 Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1028	Total	C	N	O	S	5	0	0
			7569	4878	1234	1417	40			
1	B	1026	Total	C	N	O	S	2	0	0
			7632	4916	1248	1426	42			
1	C	1034	Total	C	N	O	S	0	0	0
			7690	4957	1264	1426	43			

- Molecule 2 is a protein called Designed ankyrin repeat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	154	Total	C	N	O	S	0	0	0
			1128	708	208	211	1			
2	E	152	Total	C	N	O		11	0	0
			1101	691	205	205				

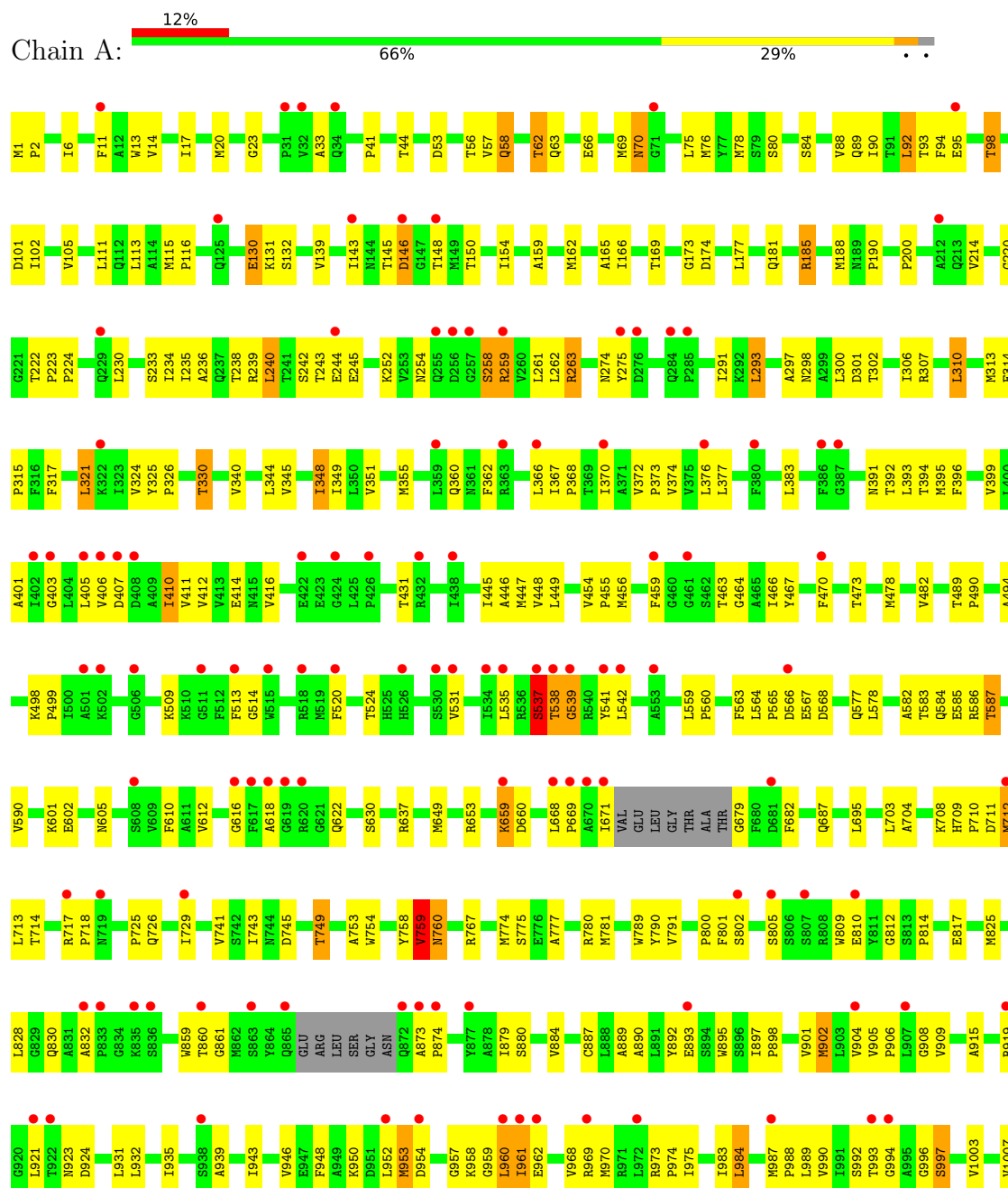
- Molecule 3 is water.

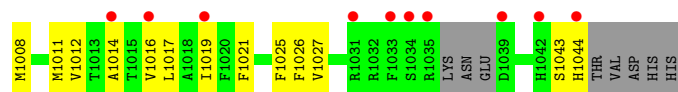
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	133	Total	O	0	0
			133	133		
3	B	132	Total	O	0	0
			132	132		
3	C	151	Total	O	0	0
			151	151		
3	D	17	Total	O	0	0
			17	17		
3	E	5	Total	O	0	0
			5	5		

3 Residue-property plots [i](#)

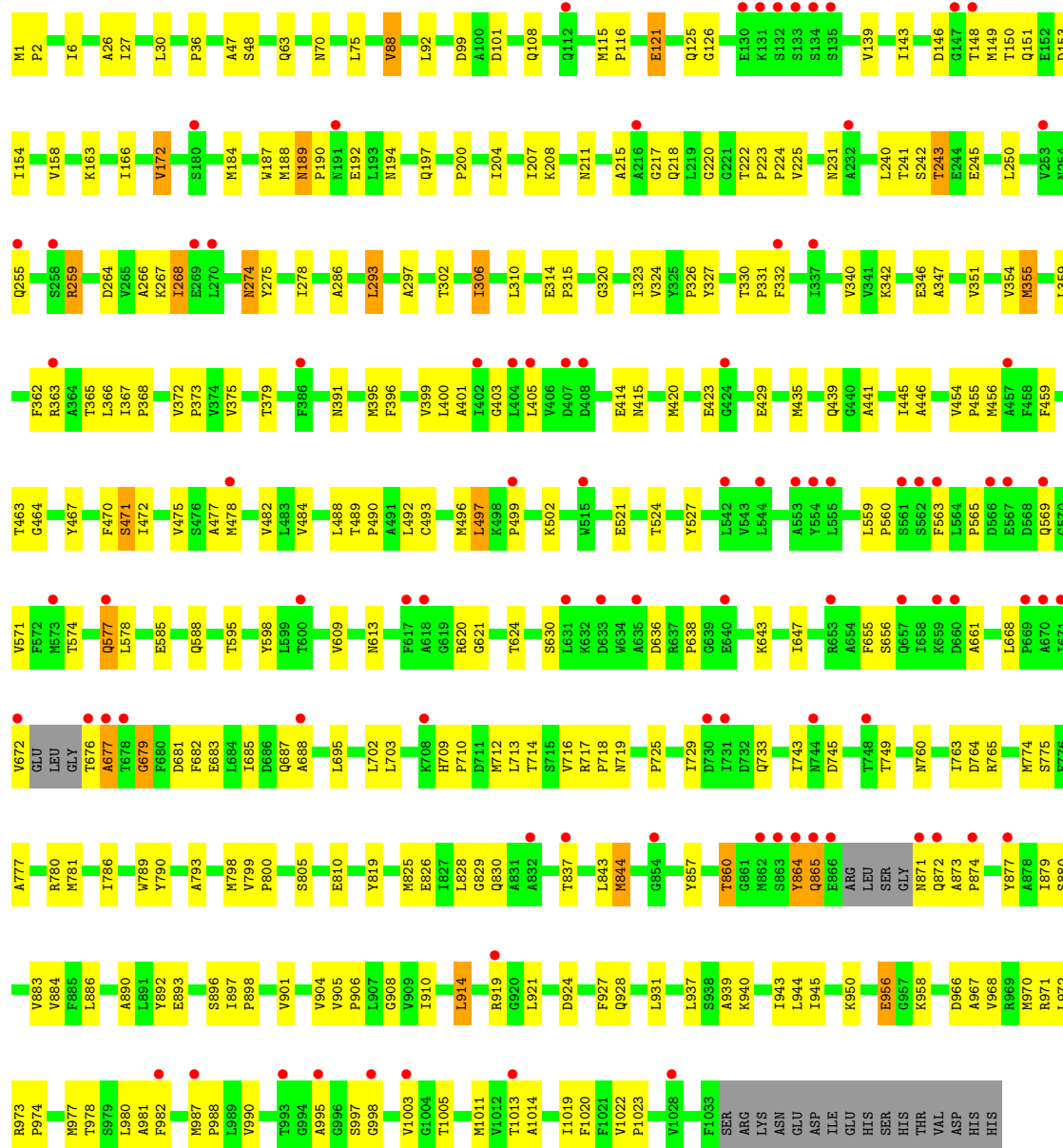
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

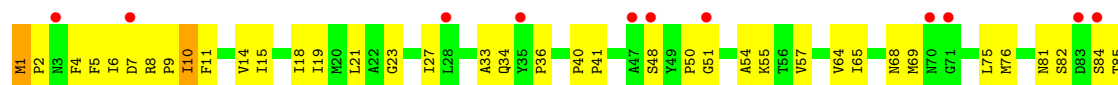


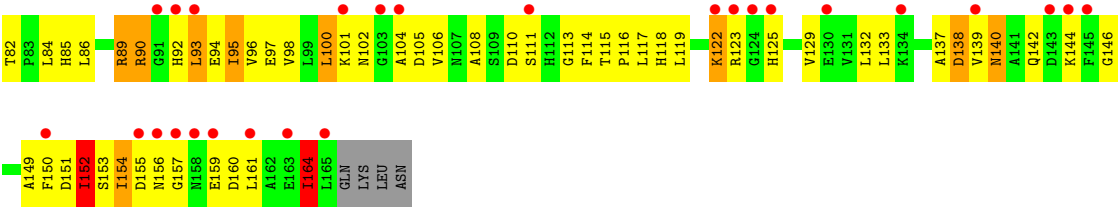


• Molecule 1: Acriflavine resistance protein B



• Molecule 1: Acriflavine resistance protein B





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.85Å 158.92Å 245.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 2.70 49.21 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.21-2.70) 99.0 (49.21-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.6.2_432	Depositor
R, R_{free}	0.242 , 0.268 0.240 , 0.267	Depositor DCC
R_{free} test set	1548 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25558	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FME

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	0.55	2/7702 (0.0%)	0.80	10/10496 (0.1%)
1	B	0.55	3/7768 (0.0%)	0.76	10/10581 (0.1%)
1	C	0.48	3/7828 (0.0%)	0.76	8/10661 (0.1%)
2	D	1.25	3/1145 (0.3%)	1.14	16/1554 (1.0%)
2	E	1.16	1/1117 (0.1%)	1.25	12/1519 (0.8%)
All	All	0.62	12/25560 (0.0%)	0.82	56/34811 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	236	ALA	CA-CB	-7.11	1.42	1.53
1	A	410	ILE	CA-CB	-6.33	1.46	1.54
2	D	139	VAL	CA-CB	-6.24	1.46	1.54
2	D	82	THR	C-O	-6.22	1.18	1.24
1	C	760	ASN	C-O	-6.00	1.18	1.24
1	C	235	ILE	C-O	-5.86	1.18	1.24
2	E	152	ILE	CA-CB	-5.80	1.47	1.54
1	B	470	PHE	C-O	-5.67	1.17	1.24
1	B	760	ASN	C-O	-5.58	1.19	1.24
2	D	65	VAL	CA-CB	-5.46	1.47	1.54
1	B	688	ALA	CA-CB	-5.07	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	SER	C-O	-5.06	1.17	1.23

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	15	GLY	N-CA-C	-17.97	91.16	112.73
1	C	506	GLY	N-CA-C	-9.48	97.44	112.61
2	D	90	ARG	N-CA-C	-9.46	97.30	110.35
1	B	865	GLN	N-CA-C	-8.55	99.55	111.52
1	B	864	TYR	N-CA-C	-8.17	96.94	109.85
2	E	157	GLY	N-CA-C	-8.15	103.94	115.43
1	A	759	VAL	N-CA-C	8.12	118.16	110.53
1	C	236	ALA	N-CA-C	-7.65	98.05	108.38
2	D	58	GLY	N-CA-C	7.62	127.47	113.76
2	D	60	LEU	N-CA-C	7.48	119.44	111.28
1	A	410	ILE	CB-CA-C	-7.25	102.21	112.22
1	A	235	ILE	CA-C-N	7.12	134.54	122.15
1	A	235	ILE	C-N-CA	7.12	134.54	122.15
1	A	539	GLY	N-CA-C	7.07	121.21	112.73
1	A	145	THR	N-CA-C	7.05	119.04	111.36
2	E	14	LEU	N-CA-C	-7.03	91.32	111.00
1	B	685	ILE	N-CA-C	6.83	117.68	108.11
1	B	679	GLY	N-CA-C	-6.71	103.33	112.52
2	D	58	GLY	CA-C-N	-6.63	113.76	123.05
2	D	58	GLY	C-N-CA	-6.63	113.76	123.05
1	B	995	ALA	N-CA-C	6.53	120.09	111.28
1	A	537	SER	N-CA-C	-6.49	104.13	111.07
2	E	14	LEU	CA-C-N	-6.39	112.89	119.98
2	E	14	LEU	C-N-CA	-6.39	112.89	119.98
1	C	326	PRO	N-CA-C	6.29	121.83	113.40
1	B	864	TYR	CA-C-N	-6.16	113.78	122.34
1	B	864	TYR	C-N-CA	-6.16	113.78	122.34
2	E	152	ILE	CB-CA-C	-6.09	103.81	112.22
2	E	16	LYS	N-CA-C	6.06	117.88	111.28
2	D	139	VAL	CA-C-N	6.05	128.38	120.28
2	D	139	VAL	C-N-CA	6.05	128.38	120.28
1	A	760	ASN	N-CA-C	6.04	117.42	108.60
2	E	155	ASP	N-CA-C	5.76	117.64	111.36
2	E	58	GLY	CA-C-N	-5.74	115.37	122.84
2	E	58	GLY	C-N-CA	-5.74	115.37	122.84
2	D	143	ASP	CA-C-N	5.69	127.91	120.28
2	D	143	ASP	C-N-CA	5.69	127.91	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	139	VAL	N-CA-C	5.65	116.38	110.62
1	A	325	TYR	CA-C-N	5.62	124.98	118.85
1	A	325	TYR	C-N-CA	5.62	124.98	118.85
2	D	138	ASP	CA-C-N	5.55	128.07	120.46
2	D	138	ASP	C-N-CA	5.55	128.07	120.46
2	D	142	GLN	CA-C-N	5.49	131.38	121.06
2	D	142	GLN	C-N-CA	5.49	131.38	121.06
2	E	78	SER	N-CA-C	-5.43	105.46	111.71
2	E	164	ILE	CB-CA-C	-5.34	104.93	112.14
1	C	235	ILE	CA-C-N	5.30	130.90	122.10
1	C	235	ILE	C-N-CA	5.30	130.90	122.10
1	C	325	TYR	CA-C-N	5.19	124.51	118.85
1	C	325	TYR	C-N-CA	5.19	124.51	118.85
1	C	362	PHE	N-CA-C	5.11	116.93	111.36
1	B	563	PHE	N-CA-C	5.10	116.65	111.14
1	B	189	ASN	CA-C-N	5.03	124.64	119.05
1	B	189	ASN	C-N-CA	5.03	124.64	119.05
2	D	144	LYS	CA-C-N	5.02	127.95	120.31
2	D	144	LYS	C-N-CA	5.02	127.95	120.31

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	759	VAL	Peptide
1	C	235	ILE	Peptide

5.2 Too-close contacts [i](#)

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	7569	0	7466	287	0
1	B	7632	0	7566	227	0
1	C	7690	0	7693	259	0
2	D	1128	0	1096	57	0
2	E	1101	0	1067	130	0
3	A	133	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	132	0	0	13	0
3	C	151	0	0	13	0
3	D	17	0	0	2	0
3	E	5	0	0	1	0
All	All	25558	0	24888	910	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 18.

All (910) 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:960:LEU:HD12	1:A:961:ILE:N	1.40	1.32
1:A:960:LEU:HD12	1:A:960:LEU:C	1.53	1.29
2:E:18:LEU:O	2:E:18:LEU:HD13	1.35	1.24
1:C:509:LYS:O	1:C:510:LYS:HE3	1.37	1.18
1:A:259:ARG:HD3	1:A:259:ARG:N	1.44	1.15
2:E:92:HIS:O	2:E:96:VAL:HG23	1.46	1.14
1:C:509:LYS:HG3	1:C:510:LYS:HG3	1.27	1.13
1:C:125:GLN:HA	1:C:125:GLN:NE2	1.64	1.10
2:D:138:ASP:HB3	2:D:140:ASN:ND2	1.68	1.09
2:E:82:THR:OG1	2:E:85:HIS:HD2	1.35	1.07
1:A:58:GLN:HA	1:A:62:THR:HG23	1.37	1.06
1:C:510:LYS:HD2	1:C:510:LYS:N	1.66	1.05
2:E:57:PHE:HB3	2:E:59:HIS:HE1	1.21	1.04
2:E:18:LEU:HD13	2:E:18:LEU:C	1.81	1.02
2:E:93:LEU:HD23	2:E:93:LEU:H	1.18	1.01
1:A:960:LEU:C	1:A:960:LEU:CD1	2.30	1.00
1:A:649:MET:HG3	3:A:1169:HOH:O	1.62	0.98
2:D:138:ASP:CB	2:D:140:ASN:ND2	2.29	0.96
1:B:146:ASP:HB2	1:B:320:GLY:HA3	1.47	0.96
2:E:93:LEU:HD23	2:E:93:LEU:N	1.75	0.95
2:E:82:THR:OG1	2:E:85:HIS:CD2	2.20	0.95
1:A:259:ARG:N	1:A:259:ARG:CD	2.30	0.94
1:A:259:ARG:HD3	1:A:259:ARG:H	1.21	0.94
1:A:960:LEU:HD12	1:A:961:ILE:CA	1.98	0.93
1:C:510:LYS:HD2	1:C:510:LYS:H	1.28	0.93
1:A:960:LEU:CD1	1:A:961:ILE:N	2.30	0.92
2:E:57:PHE:HB3	2:E:59:HIS:CE1	2.03	0.91
1:C:125:GLN:HE21	1:C:125:GLN:CA	1.81	0.90
2:E:93:LEU:H	2:E:93:LEU:CD2	1.83	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:SER:OG	1:A:245:GLU:HG3	1.71	0.90
1:B:456:MET:HE3	1:B:471:SER:HB2	1.51	0.90
1:C:125:GLN:NE2	1:C:125:GLN:CA	2.30	0.90
2:E:93:LEU:HA	2:E:96:VAL:CG2	2.00	0.90
1:B:717:ARG:HG2	1:B:717:ARG:HH11	1.37	0.89
1:C:509:LYS:CG	1:C:510:LYS:HG3	2.02	0.89
2:D:17:LYS:HB2	2:D:17:LYS:HZ3	1.39	0.88
2:D:140:ASN:ND2	2:D:140:ASN:H	1.61	0.88
2:E:152:ILE:HG22	2:E:153:SER:N	1.90	0.87
2:E:152:ILE:CG2	2:E:153:SER:N	2.38	0.86
2:D:138:ASP:HB3	2:D:140:ASN:HD22	1.33	0.86
2:E:161:LEU:HA	2:E:164:ILE:HG13	1.58	0.86
2:E:84:LEU:HD23	2:E:116:PRO:HG2	1.58	0.86
2:D:138:ASP:CB	2:D:140:ASN:HD21	1.88	0.85
2:D:60:LEU:HD12	2:D:95:ILE:HD13	1.58	0.85
2:E:57:PHE:O	2:E:59:HIS:CE1	2.29	0.84
2:E:18:LEU:C	2:E:18:LEU:CD1	2.50	0.84
1:A:20:MET:HE2	1:A:374:VAL:HG22	1.61	0.83
1:A:355:MET:HE2	1:A:368:PRO:HG2	1.61	0.83
1:C:185:ARG:HH12	1:C:774:MET:HE3	1.43	0.82
1:C:510:LYS:N	1:C:510:LYS:CD	2.30	0.82
2:E:48:TRP:CD1	2:E:77:ASP:OD1	2.34	0.81
2:E:93:LEU:HA	2:E:96:VAL:HG23	1.61	0.81
1:A:712:MET:HA	1:A:832:ALA:HB2	1.62	0.81
1:A:749:THR:HG21	1:A:791:VAL:HG12	1.63	0.81
1:B:420:MET:HB3	3:B:1156:HOH:O	1.81	0.80
2:D:150:PHE:CE1	2:D:154:ILE:HD11	2.15	0.80
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.64	0.80
1:C:573:MET:HE1	1:C:617:PHE:HE2	1.47	0.79
2:E:92:HIS:C	2:E:96:VAL:HG23	2.08	0.79
1:B:977:MET:HB3	3:B:1109:HOH:O	1.83	0.79
1:B:108:GLN:HG3	1:C:112:GLN:HG3	1.65	0.78
1:A:258:SER:C	1:A:259:ARG:HD3	2.09	0.78
2:D:140:ASN:ND2	2:D:140:ASN:N	2.29	0.77
1:A:44:THR:HG23	3:A:1116:HOH:O	1.84	0.77
2:E:122:LYS:HG3	2:E:152:ILE:HD11	1.65	0.77
1:A:890:ALA:HB2	1:C:14:VAL:HG21	1.65	0.77
1:C:139:VAL:O	1:C:326:PRO:HD2	1.83	0.77
1:C:937:LEU:HD13	1:C:1011:MET:HG2	1.67	0.77
2:E:92:HIS:O	2:E:96:VAL:CG2	2.30	0.77
1:C:587:THR:HG21	1:C:622:GLN:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:122:LYS:HA	2:E:152:ILE:HD11	1.68	0.76
1:A:537:SER:OG	1:A:538:THR:C	2.29	0.76
2:D:17:LYS:HB2	2:D:17:LYS:NZ	2.01	0.75
2:E:138:ASP:OD1	2:E:138:ASP:C	2.30	0.75
1:C:248:LYS:HE2	2:E:156:ASN:HA	1.69	0.74
2:E:79:LEU:O	2:E:111:SER:CB	2.35	0.74
1:A:181:GLN:HE22	1:A:767:ARG:HH11	1.32	0.74
1:B:966:ASP:HB2	3:B:1170:HOH:O	1.86	0.74
1:A:407:ASP:O	1:A:411:VAL:HG23	1.88	0.74
2:E:59:HIS:ND1	2:E:59:HIS:N	2.32	0.74
2:E:14:LEU:O	2:E:15:GLY:C	2.29	0.73
1:C:509:LYS:C	1:C:510:LYS:HE3	2.12	0.73
1:C:372:VAL:HG22	1:C:373:PRO:HD3	1.71	0.73
1:B:977:MET:SD	3:B:1109:HOH:O	2.46	0.73
2:D:143:ASP:OD1	2:D:143:ASP:C	2.30	0.73
1:A:132:SER:HB3	1:A:173:GLY:HA3	1.71	0.73
2:E:40:VAL:CG1	2:E:71:ALA:HB2	2.19	0.73
1:A:401:ALA:O	1:A:405:LEU:HG	1.87	0.73
1:B:150:THR:O	1:B:154:ILE:HD12	1.89	0.73
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.72	0.71
1:A:957:GLY:O	1:A:958:LYS:HG2	1.90	0.71
1:A:975:ILE:HG21	1:A:1019:ILE:HD11	1.71	0.71
1:B:445:ILE:HD13	1:B:940:LYS:HG3	1.70	0.71
1:A:953:MET:HG3	1:A:958:LYS:O	1.92	0.70
1:C:395:MET:HE2	1:C:395:MET:HA	1.73	0.70
1:A:300:LEU:HD23	1:A:330:THR:HG23	1.74	0.70
1:A:214:VAL:HG23	1:A:236:ALA:HB3	1.73	0.70
2:E:93:LEU:CA	2:E:96:VAL:HG23	2.20	0.70
1:C:876:LEU:HD11	1:C:932:LEU:HD11	1.72	0.70
2:E:161:LEU:H	2:E:161:LEU:HD23	1.55	0.70
1:B:492:LEU:HB3	1:B:496:MET:HE2	1.74	0.69
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.74	0.69
1:B:395:MET:HA	1:B:395:MET:HE2	1.73	0.69
1:A:76:MET:HE3	1:A:95:GLU:HA	1.74	0.69
1:C:447:MET:SD	1:C:887:CYS:HB3	2.33	0.69
1:C:509:LYS:O	1:C:510:LYS:CE	2.30	0.69
1:B:355:MET:HG2	1:B:365:THR:HA	1.75	0.68
1:A:983:ILE:HG23	1:A:1008:MET:HG3	1.74	0.68
1:A:767:ARG:HA	1:B:63:GLN:NE2	2.08	0.68
1:B:310:LEU:HD13	1:B:323:ILE:HD12	1.75	0.68
2:E:79:LEU:O	2:E:111:SER:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:VAL:HA	3:A:1171:HOH:O	1.92	0.68
1:A:414:GLU:HG2	1:A:974:PRO:HB3	1.76	0.68
1:A:162:MET:HG2	1:A:313:MET:HE3	1.75	0.68
1:A:539:GLY:HA2	1:A:542:LEU:HD23	1.74	0.68
1:A:275:TYR:CD1	1:C:223:PRO:HG3	2.29	0.68
1:B:668:LEU:HD23	1:B:668:LEU:H	1.58	0.68
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.76	0.68
1:B:220:GLY:HA2	1:C:781:MET:SD	2.34	0.68
1:B:403:GLY:HA3	1:B:982:PHE:CE2	2.30	0.67
1:C:459:PHE:CE1	1:C:876:LEU:HD23	2.29	0.67
1:A:1011:MET:HE3	1:A:1011:MET:HA	1.76	0.67
1:C:982:PHE:CD2	1:C:1011:MET:HG3	2.29	0.67
1:A:456:MET:HE2	1:A:467:TYR:HD1	1.57	0.67
2:D:49:THR:H	2:D:52:HIS:CD2	2.13	0.67
1:B:184:MET:HE2	1:B:268:ILE:HG22	1.76	0.67
1:B:877:TYR:HA	1:B:880:SER:HB3	1.76	0.67
1:C:703:LEU:HD11	1:C:718:PRO:HG3	1.76	0.67
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.77	0.67
1:A:909:VAL:HG22	1:A:931:LEU:HD21	1.77	0.67
2:E:40:VAL:HG12	2:E:71:ALA:HB2	1.76	0.66
2:E:150:PHE:O	2:E:154:ILE:CG1	2.42	0.66
1:C:415:ASN:HD21	1:C:437:GLN:HE21	1.41	0.66
1:C:901:VAL:O	1:C:904:VAL:HG12	1.95	0.66
1:B:354:VAL:HG21	1:B:981:ALA:HB2	1.78	0.66
1:B:717:ARG:HG2	1:B:717:ARG:NH1	2.11	0.66
2:E:45:PHE:CE1	2:E:46:THR:HG23	2.31	0.66
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.61	0.65
1:B:184:MET:CE	1:B:268:ILE:HG22	2.27	0.65
2:E:151:ASP:HA	2:E:154:ILE:CD1	2.26	0.65
1:B:454:VAL:HG12	1:B:455:PRO:HD3	1.79	0.65
1:C:505:HIS:O	1:C:505:HIS:ND1	2.30	0.65
2:E:150:PHE:O	2:E:154:ILE:HG12	1.97	0.65
2:D:138:ASP:CA	2:D:140:ASN:HD21	2.09	0.65
2:E:43:ARG:HG2	2:E:47:GLY:O	1.96	0.65
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.79	0.65
2:E:110:ASP:OD2	2:E:110:ASP:C	2.38	0.65
1:A:535:LEU:O	1:A:538:THR:HB	1.95	0.65
1:B:420:MET:HE2	3:B:1156:HOH:O	1.96	0.65
2:E:110:ASP:OD2	2:E:113:GLY:N	2.30	0.65
1:B:375:VAL:O	1:B:379:THR:HG23	1.97	0.65
1:A:960:LEU:HD12	1:A:961:ILE:HA	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:39:ASP:OD2	2:E:40:VAL:N	2.30	0.64
1:A:166:ILE:HD11	1:A:310:LEU:HD13	1.77	0.64
1:C:248:LYS:O	1:C:261:LEU:HD22	1.97	0.64
2:E:57:PHE:CB	2:E:59:HIS:HE1	2.05	0.64
1:A:994:GLY:N	1:A:997:SER:OG	2.29	0.64
1:A:957:GLY:O	1:A:958:LYS:CG	2.45	0.64
1:C:904:VAL:HG13	1:C:938:SER:HB3	1.78	0.64
1:A:223:PRO:HG3	1:B:275:TYR:CG	2.33	0.64
1:C:162:MET:HA	1:C:313:MET:HE1	1.79	0.64
2:E:20:GLU:OE1	2:E:23:ARG:NE	2.30	0.64
1:B:151:GLN:HE22	1:B:278:ILE:HA	1.63	0.64
1:A:531:VAL:O	1:A:535:LEU:HG	1.98	0.64
1:A:578:LEU:HD22	1:A:587:THR:HG23	1.80	0.64
2:E:79:LEU:O	2:E:111:SER:HB3	1.98	0.63
1:B:676:THR:HG22	1:B:676:THR:O	1.98	0.63
1:C:248:LYS:O	1:C:249:ILE:C	2.41	0.63
1:C:626:ILE:HD13	1:C:627:ALA:N	2.12	0.63
2:E:48:TRP:HD1	2:E:77:ASP:OD1	1.79	0.63
1:B:184:MET:HE1	1:B:243:THR:HB	1.81	0.63
1:C:505:HIS:O	1:C:505:HIS:CG	2.52	0.63
1:A:711:ASP:OD1	1:A:712:MET:N	2.30	0.63
1:C:527:TYR:CE2	1:C:968:VAL:HG13	2.33	0.63
2:D:44:ASP:OD1	2:D:44:ASP:C	2.39	0.63
2:E:63:VAL:HG21	2:E:95:ILE:HD13	1.81	0.63
1:A:711:ASP:OD1	1:A:711:ASP:N	2.30	0.63
1:A:448:VAL:HG23	1:A:449:LEU:HD12	1.79	0.63
1:A:456:MET:HE2	1:A:467:TYR:CD1	2.34	0.62
1:B:966:ASP:N	3:B:1170:HOH:O	2.32	0.62
2:D:140:ASN:HD22	2:D:140:ASN:N	1.96	0.62
1:C:370:ILE:O	1:C:373:PRO:HD2	1.99	0.62
1:B:340:VAL:HG21	1:B:395:MET:HB3	1.81	0.62
1:B:1022:VAL:HG22	1:B:1023:PRO:HD3	1.80	0.62
1:C:34:GLN:HB2	1:C:333:VAL:HG13	1.81	0.62
1:B:676:THR:O	1:B:677:ALA:HB2	1.99	0.62
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.82	0.62
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.80	0.62
1:B:204:ILE:O	1:B:208:LYS:HG3	1.99	0.62
1:C:193:LEU:HD12	1:C:265:VAL:HB	1.81	0.62
1:A:445:ILE:HG23	1:A:449:LEU:HD13	1.82	0.62
1:B:864:TYR:O	1:B:865:GLN:C	2.40	0.62
1:A:447:MET:HE2	1:A:447:MET:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:PHE:O	1:A:952:LEU:HG	2.00	0.62
2:E:44:ASP:OD2	2:E:47:GLY:N	2.31	0.62
2:D:150:PHE:CZ	2:D:154:ILE:HD11	2.35	0.62
2:D:112:HIS:O	2:D:144:LYS:HB2	2.00	0.62
2:D:17:LYS:NZ	2:D:17:LYS:CB	2.61	0.61
1:A:566:ASP:CA	3:A:1096:HOH:O	2.47	0.61
2:E:39:ASP:OD2	2:E:41:ASN:N	2.29	0.61
2:E:84:LEU:HD23	2:E:116:PRO:CG	2.30	0.61
1:C:68:ASN:HD22	1:C:114:ALA:HB2	1.65	0.61
1:C:125:GLN:HE21	1:C:125:GLN:N	1.99	0.61
1:A:659:LYS:HD3	1:A:659:LYS:H	1.66	0.61
2:D:77:ASP:HB3	2:D:79:LEU:H	1.64	0.61
1:A:431:THR:HG21	1:A:494:ALA:HB2	1.83	0.61
2:E:152:ILE:HG22	2:E:153:SER:H	1.65	0.61
1:A:214:VAL:CG2	1:A:236:ALA:CB	2.79	0.61
1:A:745:ASP:O	1:A:749:THR:HG22	2.01	0.61
2:E:60:LEU:HD13	2:E:95:ILE:HG12	1.83	0.61
1:A:214:VAL:HG23	1:A:236:ALA:CB	2.31	0.61
1:A:566:ASP:HA	3:A:1096:HOH:O	1.99	0.61
1:C:897:ILE:N	1:C:898:PRO:HD2	2.16	0.60
2:D:81:VAL:HG23	2:D:110:ASP:OD2	2.01	0.60
1:B:242:SER:OG	1:B:245:GLU:HG3	2.01	0.60
1:A:261:LEU:HD12	1:A:263:ARG:NH1	2.15	0.60
1:B:456:MET:HE3	1:B:471:SER:CB	2.28	0.60
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.83	0.60
1:A:326:PRO:O	1:A:630:SER:HB2	2.01	0.60
2:E:89:ARG:HB3	2:E:119:LEU:HB3	1.82	0.60
1:A:94:PHE:HB3	1:A:98:THR:HG21	1.83	0.60
1:A:449:LEU:HB2	1:A:478:MET:HE1	1.83	0.60
1:C:937:LEU:HB3	1:C:1011:MET:HE3	1.83	0.60
2:E:15:GLY:HA3	2:E:42:ALA:HB1	1.82	0.60
1:B:414:GLU:OE2	1:B:974:PRO:HG3	2.02	0.60
1:B:471:SER:O	1:B:475:VAL:HG23	2.00	0.60
1:A:902:MET:HE2	1:A:902:MET:HA	1.84	0.59
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.84	0.59
1:B:702:LEU:HD21	1:B:844:MET:HE1	1.82	0.59
2:E:115:THR:O	2:E:118:HIS:N	2.35	0.59
1:C:688:ALA:HB3	1:C:690:LEU:HD13	1.84	0.59
1:A:960:LEU:HD13	1:A:1027:VAL:HG12	1.82	0.59
1:C:790:TYR:CE1	1:C:800:PRO:HG3	2.38	0.59
1:B:362:PHE:O	1:B:365:THR:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:974:PRO:O	1:B:978:THR:HG22	2.02	0.59
2:E:39:ASP:OD2	2:E:39:ASP:C	2.43	0.59
1:C:57:VAL:HG13	1:C:82:SER:HB3	1.85	0.59
1:A:78:MET:HG3	1:A:92:LEU:HD22	1.85	0.59
2:D:82:THR:OG1	2:D:85:HIS:ND1	2.35	0.59
1:A:58:GLN:HA	1:A:62:THR:CG2	2.24	0.58
1:A:781:MET:HE1	1:C:224:PRO:HA	1.84	0.58
1:B:274:ASN:HD22	1:B:274:ASN:H	1.51	0.58
1:B:574:THR:HG21	1:B:598:TYR:OH	2.03	0.58
1:B:790:TYR:CE1	1:B:800:PRO:HG3	2.38	0.58
1:B:26:ALA:O	1:B:30:LEU:HB2	2.02	0.58
2:E:44:ASP:CG	2:E:46:THR:OG1	2.46	0.58
1:A:139:VAL:O	1:A:326:PRO:HD2	2.03	0.58
1:A:567:GLU:N	3:A:1096:HOH:O	2.36	0.58
1:A:190:PRO:HG3	1:A:789:TRP:CZ2	2.39	0.58
1:B:712:MET:HG2	1:B:843:LEU:HD22	1.86	0.58
2:D:110:ASP:HB3	2:D:112:HIS:H	1.69	0.58
1:A:66:GLU:HG2	1:A:78:MET:HE2	1.84	0.58
1:B:703:LEU:HD11	1:B:718:PRO:HG3	1.85	0.58
1:C:521:GLU:O	1:C:525:HIS:HD2	1.87	0.58
1:B:223:PRO:HG3	1:C:275:TYR:CG	2.39	0.58
1:C:509:LYS:C	1:C:510:LYS:CD	2.77	0.58
1:B:347:ALA:O	1:B:351:VAL:HG23	2.04	0.57
1:C:393:LEU:HD13	1:C:466:ILE:HG23	1.86	0.57
1:A:326:PRO:HB3	1:A:610:PHE:HB2	1.86	0.57
1:A:790:TYR:CE1	1:A:800:PRO:HG3	2.39	0.57
1:B:278:ILE:HD11	1:B:588:GLN:OE1	2.05	0.57
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.85	0.57
1:B:559:LEU:HD12	1:B:560:PRO:CD	2.34	0.57
2:D:150:PHE:CZ	2:D:154:ILE:CD1	2.87	0.57
1:A:362:PHE:O	1:A:366:LEU:HD13	2.05	0.57
1:C:75:LEU:HD21	1:C:92:LEU:HB3	1.86	0.57
1:A:102:ILE:HD13	1:C:101:ASP:HB3	1.86	0.57
1:A:537:SER:CB	1:A:538:THR:HA	2.35	0.57
1:B:423:GLU:HA	1:B:502:LYS:HE2	1.85	0.57
2:E:122:LYS:CA	2:E:152:ILE:HD11	2.33	0.57
2:E:18:LEU:O	2:E:18:LEU:CD1	2.30	0.56
2:E:151:ASP:HA	2:E:154:ILE:HG13	1.87	0.56
1:A:90:ILE:HG22	1:A:92:LEU:HD21	1.87	0.56
1:A:687:GLN:HG3	1:C:316:PHE:CZ	2.40	0.56
1:C:115:MET:N	1:C:116:PRO:HD2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:PRO:HA	1:A:810:GLU:O	2.06	0.56
1:B:274:ASN:HD22	1:B:274:ASN:N	2.02	0.56
1:B:745:ASP:O	1:B:749:THR:HG23	2.04	0.56
2:D:28:ASP:O	2:D:32:ILE:HG13	2.05	0.56
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.86	0.56
1:A:412:VAL:O	1:A:416:VAL:HG23	2.06	0.56
2:E:57:PHE:CB	2:E:59:HIS:CE1	2.84	0.56
1:C:361:ASN:OD1	1:C:361:ASN:C	2.46	0.56
2:D:138:ASP:CG	2:D:140:ASN:ND2	2.63	0.56
1:B:910:ILE:HG23	1:B:1013:THR:HG21	1.88	0.56
2:D:48:TRP:CD1	2:D:77:ASP:OD1	2.59	0.56
1:C:873:ALA:HB3	1:C:874:PRO:HD3	1.87	0.56
1:A:223:PRO:HD2	1:B:780:ARG:HH22	1.71	0.56
1:C:222:THR:HA	1:C:224:PRO:HD3	1.88	0.56
1:B:655:PHE:C	3:B:1112:HOH:O	2.48	0.55
2:D:150:PHE:CE1	2:D:154:ILE:CD1	2.87	0.55
1:A:317:PHE:HB3	1:A:321:LEU:HB3	1.88	0.55
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.87	0.55
1:A:923:ASN:C	1:A:923:ASN:HD22	2.14	0.55
1:C:569:GLN:NE2	3:C:1116:HOH:O	2.38	0.55
1:A:563:PHE:O	1:A:924:ASP:HB2	2.07	0.55
1:C:361:ASN:OD1	1:C:362:PHE:N	2.39	0.55
1:C:681:ASP:HB2	3:C:1143:HOH:O	2.07	0.55
2:E:84:LEU:CD2	2:E:116:PRO:HG2	2.35	0.55
1:B:403:GLY:HA3	1:B:982:PHE:HE2	1.70	0.55
1:B:679:GLY:HA3	1:B:829:GLY:O	2.07	0.55
1:B:656:SER:N	3:B:1112:HOH:O	2.40	0.55
1:B:679:GLY:HA2	1:B:830:GLN:HA	1.89	0.55
2:E:85:HIS:HE1	2:E:114:PHE:O	1.89	0.55
1:A:582:ALA:HA	1:A:586:ARG:NH2	2.22	0.54
1:B:36:PRO:HG3	1:B:391:ASN:ND2	2.22	0.54
1:B:302:THR:O	1:B:306:ILE:HG23	2.07	0.54
1:B:521:GLU:O	1:B:524:THR:HG22	2.07	0.54
1:B:351:VAL:O	1:B:355:MET:HB2	2.08	0.54
1:C:605:ASN:O	1:C:632:LYS:HG2	2.07	0.54
1:B:224:PRO:HA	1:C:781:MET:HE1	1.90	0.54
1:C:361:ASN:O	1:C:365:THR:HG22	2.08	0.54
2:D:138:ASP:CG	2:D:140:ASN:HD21	2.16	0.54
1:A:275:TYR:CG	1:C:223:PRO:HG3	2.43	0.54
1:A:1016:VAL:HG23	1:A:1017:LEU:HD13	1.89	0.54
2:E:161:LEU:HD23	2:E:161:LEU:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:LEU:HD13	1:B:843:LEU:HD23	1.88	0.54
2:E:149:ALA:O	2:E:152:ILE:HG22	2.08	0.54
2:E:151:ASP:HA	2:E:154:ILE:HD11	1.90	0.54
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.88	0.54
1:B:414:GLU:CD	1:B:974:PRO:HG3	2.33	0.54
1:A:403:GLY:O	1:A:406:VAL:HG12	2.08	0.54
1:B:908:GLY:HA2	1:B:1014:ALA:HB2	1.88	0.54
1:C:1011:MET:HE2	1:C:1011:MET:HA	1.90	0.54
1:B:647:ILE:HG23	3:B:1164:HOH:O	2.08	0.53
1:C:36:PRO:HG3	1:C:391:ASN:ND2	2.23	0.53
1:C:509:LYS:C	1:C:510:LYS:CE	2.79	0.53
2:E:14:LEU:N	2:E:17:LYS:H	2.06	0.53
1:A:679:GLY:N	3:A:1084:HOH:O	2.39	0.53
1:B:420:MET:HE1	1:B:499:PRO:HA	1.90	0.53
1:A:653:ARG:NH2	3:A:1169:HOH:O	2.37	0.53
1:A:668:LEU:HD23	1:A:668:LEU:H	1.74	0.53
1:B:717:ARG:HH11	1:B:717:ARG:CG	2.16	0.53
1:C:15:ILE:O	1:C:19:ILE:HG12	2.07	0.53
2:E:57:PHE:C	2:E:59:HIS:CE1	2.86	0.53
1:A:214:VAL:CG2	1:A:236:ALA:HB1	2.39	0.53
1:A:777:ALA:O	1:A:781:MET:HG2	2.08	0.53
1:C:4:PHE:O	1:C:8:ARG:HG2	2.09	0.53
1:A:973:ARG:N	1:A:974:PRO:HD2	2.23	0.53
1:C:509:LYS:HB2	1:C:510:LYS:HA	1.91	0.53
1:C:943:ILE:O	1:C:947:GLU:HB3	2.08	0.53
1:A:537:SER:CB	1:A:538:THR:CA	2.87	0.53
1:A:709:HIS:N	1:A:710:PRO:HD3	2.23	0.53
2:D:59:HIS:N	2:D:59:HIS:CD2	2.77	0.53
2:E:115:THR:O	2:E:117:LEU:N	2.42	0.53
1:B:966:ASP:CA	3:B:1170:HOH:O	2.57	0.52
1:C:971:ARG:C	1:C:974:PRO:HD2	2.34	0.52
1:A:889:ALA:O	1:C:10:ILE:HD11	2.09	0.52
1:C:336:SER:O	1:C:340:VAL:HG23	2.08	0.52
2:E:150:PHE:O	2:E:154:ILE:HG13	2.09	0.52
1:B:223:PRO:HD2	1:C:780:ARG:HH22	1.73	0.52
1:B:571:VAL:HG12	1:B:630:SER:HA	1.92	0.52
1:C:162:MET:HG2	1:C:313:MET:HE2	1.91	0.52
1:C:509:LYS:HB2	1:C:510:LYS:CA	2.39	0.52
1:C:897:ILE:O	1:C:901:VAL:HG12	2.08	0.52
1:A:584:GLN:HG3	3:A:1055:HOH:O	2.10	0.52
1:B:924:ASP:O	1:B:928:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41:ASN:N	2:E:41:ASN:HD22	2.06	0.52
2:D:49:THR:H	2:D:52:HIS:HD2	1.56	0.52
2:E:123:ARG:HB3	2:E:125:HIS:NE2	2.24	0.52
1:A:383:LEU:HD21	1:A:473:THR:HG22	1.92	0.52
1:B:47:ALA:HB3	1:B:88:VAL:CG1	2.38	0.52
2:D:142:GLN:HB3	2:D:146:GLY:HA2	1.92	0.52
1:B:585:GLU:HB2	3:B:1071:HOH:O	2.08	0.52
1:C:164:ASP:HB2	3:C:1117:HOH:O	2.09	0.52
2:D:148:THR:H	2:D:151:ASP:HB2	1.74	0.52
1:A:586:ARG:NH1	3:A:1131:HOH:O	2.43	0.52
1:C:509:LYS:CB	1:C:510:LYS:HG3	2.38	0.52
1:A:69:MET:HE2	1:A:92:LEU:HD11	1.92	0.52
1:C:1015:THR:O	1:C:1019:ILE:HB	2.10	0.52
1:A:58:GLN:NE2	3:A:1127:HOH:O	2.31	0.52
1:A:961:ILE:CG2	1:A:962:GLU:N	2.72	0.52
1:B:126:GLY:HA3	1:C:116:PRO:CB	2.39	0.52
1:B:379:THR:HG21	1:B:477:ALA:HA	1.92	0.52
1:C:48:SER:O	1:C:50:PRO:HD3	2.10	0.52
1:C:973:ARG:HB3	1:C:974:PRO:HD3	1.92	0.52
1:A:407:ASP:OD1	1:A:411:VAL:HG23	2.10	0.51
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.91	0.51
1:C:332:PHE:HA	1:C:335:ILE:HG22	1.92	0.51
1:A:780:ARG:HH22	1:C:223:PRO:HD2	1.74	0.51
1:B:805:SER:O	2:D:144:LYS:NZ	2.43	0.51
1:C:69:MET:HE1	1:C:107:VAL:HG13	1.91	0.51
1:C:302:THR:O	1:C:306:ILE:HG13	2.10	0.51
2:E:57:PHE:O	2:E:59:HIS:ND1	2.43	0.51
1:A:780:ARG:NH2	1:C:223:PRO:HD2	2.25	0.51
1:B:973:ARG:HB3	1:B:974:PRO:HD3	1.92	0.51
1:C:150:THR:O	1:C:154:ILE:HG13	2.11	0.51
1:B:719:ASN:HB2	1:B:828:LEU:HG	1.93	0.51
1:C:84:SER:OG	1:C:814:PRO:HA	2.10	0.51
1:C:756:GLY:HA3	1:C:774:MET:HE2	1.92	0.51
2:E:40:VAL:C	2:E:41:ASN:HD22	2.18	0.51
2:E:52:HIS:HD2	2:E:86:LEU:HD11	1.76	0.51
2:E:140:ASN:OD1	2:E:140:ASN:N	2.43	0.51
1:B:215:ALA:HB1	1:C:51:GLY:HA3	1.92	0.51
1:A:781:MET:HB3	1:C:228:GLN:OE1	2.11	0.51
1:B:864:TYR:O	1:B:865:GLN:CB	2.55	0.51
1:B:944:LEU:HD13	1:B:971:ARG:NH1	2.25	0.51
2:E:101:LYS:HG2	2:E:102:ASN:HD22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:MET:O	1:B:439:GLN:HG3	2.11	0.51
1:B:679:GLY:CA	1:B:829:GLY:O	2.59	0.51
2:D:150:PHE:HB2	3:D:181:HOH:O	2.11	0.51
2:E:122:LYS:HA	2:E:152:ILE:CD1	2.37	0.51
1:C:185:ARG:HG3	1:C:271:GLY:HA3	1.93	0.51
1:A:393:LEU:HD22	1:A:470:PHE:HE1	1.76	0.50
1:B:47:ALA:HB3	1:B:88:VAL:HG13	1.94	0.50
1:A:150:THR:O	1:A:154:ILE:HG13	2.11	0.50
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.45	0.50
1:B:121:GLU:H	1:B:121:GLU:CD	2.17	0.50
1:C:489:THR:HB	1:C:490:PRO:HD3	1.92	0.50
1:C:819:TYR:OH	1:C:860:THR:HG23	2.11	0.50
1:C:7:ASP:C	1:C:9:PRO:HD3	2.36	0.50
1:A:360:GLN:HG2	1:A:513:PHE:CD2	2.47	0.50
1:A:393:LEU:HD11	1:A:466:ILE:HG13	1.94	0.50
1:A:11:PHE:CD2	1:B:890:ALA:HB1	2.47	0.50
1:A:56:THR:HG22	1:C:213:GLN:NE2	2.26	0.50
1:A:463:THR:O	1:A:467:TYR:HD2	1.94	0.50
1:A:541:TYR:O	1:A:542:LEU:C	2.52	0.50
2:E:105:ASP:HB3	2:E:108:ALA:HB2	1.93	0.50
1:A:351:VAL:O	1:A:355:MET:HG2	2.11	0.50
1:C:242:SER:OG	1:C:244:GLU:HG2	2.11	0.50
2:E:15:GLY:HA2	2:E:42:ALA:CB	2.42	0.50
1:A:407:ASP:O	1:A:407:ASP:OD1	2.30	0.50
1:B:559:LEU:HD12	1:B:560:PRO:HD2	1.93	0.50
1:C:372:VAL:CG2	1:C:373:PRO:HD3	2.40	0.50
2:D:92:HIS:O	2:D:96:VAL:HG23	2.12	0.50
1:C:356:TYR:O	1:C:360:GLN:HA	2.11	0.50
1:C:572:PHE:HE2	1:C:631:LEU:HD21	1.75	0.50
1:C:904:VAL:HG23	1:C:907:LEU:HD12	1.92	0.50
2:E:44:ASP:OD2	2:E:46:THR:OG1	2.30	0.50
2:E:93:LEU:O	2:E:96:VAL:N	2.44	0.50
1:B:871:ASN:HD22	1:B:872:GLN:HG3	1.77	0.50
1:C:362:PHE:HA	1:C:365:THR:HG22	1.94	0.50
2:E:44:ASP:OD2	2:E:48:TRP:N	2.44	0.50
1:A:743:ILE:HD12	1:A:743:ILE:H	1.77	0.49
1:B:224:PRO:HA	1:C:781:MET:CE	2.41	0.49
1:A:537:SER:OG	1:A:539:GLY:N	2.45	0.49
1:C:167:SER:HB3	3:C:1079:HOH:O	2.11	0.49
1:C:888:LEU:HD13	1:C:901:VAL:HG11	1.94	0.49
2:D:77:ASP:HB2	2:D:81:VAL:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLY:HA2	1:B:781:MET:SD	2.52	0.49
1:A:412:VAL:HG11	1:A:489:THR:HG22	1.93	0.49
1:B:781:MET:HE2	1:B:781:MET:HA	1.93	0.49
2:D:77:ASP:HB2	2:D:81:VAL:H	1.76	0.49
1:B:126:GLY:CA	1:C:116:PRO:HB3	2.39	0.49
1:B:709:HIS:N	1:B:710:PRO:HD3	2.27	0.49
1:B:793:ALA:HA	3:B:1095:HOH:O	2.11	0.49
1:A:809:TRP:CE2	2:E:46:THR:HG22	2.47	0.49
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.94	0.49
1:A:489:THR:HB	1:A:490:PRO:HD3	1.94	0.49
1:A:893:GLU:OE2	1:C:8:ARG:HB3	2.12	0.49
1:C:691:GLY:O	1:C:695:LEU:HB2	2.13	0.49
2:E:151:ASP:HA	2:E:154:ILE:CG1	2.43	0.49
1:B:355:MET:HE2	1:B:359:LEU:HD11	1.94	0.49
2:E:77:ASP:HB2	2:E:81:VAL:H	1.78	0.49
1:B:255:GLN:H	1:B:255:GLN:CD	2.21	0.49
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.95	0.49
2:E:15:GLY:CA	2:E:42:ALA:HB1	2.42	0.49
1:A:391:ASN:H	1:A:394:THR:HB	1.78	0.49
2:E:90:ARG:HB3	2:E:92:HIS:CD2	2.48	0.49
2:E:133:LEU:HD23	2:E:137:ALA:HB3	1.93	0.49
1:A:660:ASP:CB	3:A:1173:HOH:O	2.61	0.48
1:A:860:THR:HG22	1:A:861:GLY:H	1.77	0.48
1:B:2:PRO:O	1:B:6:ILE:HG13	2.12	0.48
1:B:250:LEU:HD21	1:B:259:ARG:HB3	1.94	0.48
1:C:531:VAL:O	1:C:534:ILE:HG12	2.12	0.48
1:A:78:MET:HG3	1:A:92:LEU:CD2	2.42	0.48
1:A:130:GLU:HG2	1:A:174:ASP:HB2	1.96	0.48
1:B:987:MET:HB2	1:B:988:PRO:HD3	1.95	0.48
1:A:370:ILE:O	1:A:374:VAL:HG23	2.14	0.48
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.48	0.48
1:B:463:THR:HG22	1:B:467:TYR:HE1	1.79	0.48
1:C:65:ILE:O	1:C:69:MET:HG2	2.13	0.48
1:C:586:ARG:NH2	3:C:1091:HOH:O	2.46	0.48
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.95	0.48
2:D:51:LEU:HD11	2:D:67:LEU:HD21	1.95	0.48
1:A:13:TRP:O	1:A:17:ILE:HG13	2.14	0.48
1:A:445:ILE:HA	1:A:448:VAL:HG22	1.96	0.48
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.95	0.48
1:C:281:PHE:CE2	1:C:324:VAL:HG21	2.49	0.48
1:C:1008:MET:O	1:C:1012:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:44:ASP:OD1	2:E:46:THR:OG1	2.30	0.48
2:E:159:GLU:O	2:E:160:ASP:C	2.56	0.48
1:A:63:GLN:HE22	1:C:767:ARG:HA	1.79	0.48
1:A:578:LEU:HD13	1:A:587:THR:HG22	1.96	0.48
1:A:758:TYR:HE1	1:A:760:ASN:O	1.96	0.48
1:A:992:SER:C	1:A:993:THR:CG2	2.86	0.48
1:C:1:FME:HB2	1:C:2:PRO:HD3	1.95	0.48
1:C:76:MET:CG	1:C:95:GLU:HG3	2.44	0.48
1:C:351:VAL:HG21	1:C:402:ILE:HG22	1.95	0.48
2:D:52:HIS:CE1	2:D:83:PRO:HD3	2.49	0.48
2:E:60:LEU:HD11	2:E:98:VAL:HG21	1.94	0.48
1:B:455:PRO:HG2	1:B:880:SER:HB2	1.96	0.48
1:A:214:VAL:CG2	1:A:236:ALA:HB3	2.39	0.48
1:A:537:SER:HB3	1:A:538:THR:HA	1.95	0.48
1:A:960:LEU:CD1	1:A:961:ILE:CA	2.81	0.48
1:B:241:THR:HA	1:B:763:ILE:O	2.14	0.48
1:B:681:ASP:HB3	1:B:860:THR:O	2.12	0.48
1:C:167:SER:CB	3:C:1079:HOH:O	2.62	0.48
1:C:350:LEU:O	1:C:354:VAL:HG23	2.13	0.48
1:C:1032:ARG:C	1:C:1033:PHE:HD1	2.21	0.48
1:B:463:THR:HG22	1:B:467:TYR:CE1	2.48	0.48
1:B:729:ILE:HD11	1:B:786:ILE:HD13	1.95	0.48
1:A:146:ASP:N	1:A:146:ASP:OD1	2.43	0.47
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.96	0.47
1:A:960:LEU:CD1	1:A:961:ILE:HA	2.42	0.47
1:A:993:THR:HA	1:A:997:SER:HB3	1.94	0.47
1:B:944:LEU:HD13	1:B:971:ARG:HH11	1.79	0.47
1:B:997:SER:O	1:B:998:GLY:C	2.56	0.47
1:A:781:MET:SD	1:C:220:GLY:HA2	2.54	0.47
1:B:420:MET:CE	1:B:499:PRO:HA	2.44	0.47
1:B:893:GLU:O	1:B:893:GLU:HG3	2.14	0.47
1:B:223:PRO:HD2	1:C:780:ARG:NH2	2.29	0.47
2:D:17:LYS:HZ3	2:D:17:LYS:CB	2.15	0.47
1:A:105:VAL:HG13	3:A:1057:HOH:O	2.13	0.47
1:C:637:ARG:N	1:C:638:PRO:HD3	2.30	0.47
1:C:733:GLN:HG2	3:C:1178:HOH:O	2.13	0.47
1:A:2:PRO:O	1:A:6:ILE:HG13	2.14	0.47
1:A:703:LEU:HD11	1:A:718:PRO:HG3	1.97	0.47
1:C:33:ALA:O	1:C:391:ASN:HA	2.15	0.47
1:C:649:MET:HE1	1:C:653:ARG:HH21	1.80	0.47
2:E:110:ASP:OD2	2:E:114:PHE:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:LYS:NZ	3:A:1106:HOH:O	2.39	0.47
1:A:915:ALA:O	1:A:919:ARG:HB2	2.15	0.47
1:A:1043:SER:HA	1:A:1044:HIS:HA	1.50	0.47
1:B:362:PHE:HA	1:B:365:THR:HG22	1.96	0.47
1:B:901:VAL:O	1:B:904:VAL:HG22	2.15	0.47
1:C:578:LEU:HD13	1:C:587:THR:HB	1.95	0.47
1:A:33:ALA:O	1:A:391:ASN:HA	2.15	0.47
1:A:407:ASP:OD1	1:A:407:ASP:C	2.56	0.47
1:B:527:TYR:OH	1:B:1019:ILE:HB	2.15	0.47
1:B:595:THR:HG23	1:B:609:VAL:HB	1.96	0.47
1:B:777:ALA:O	1:B:781:MET:HG2	2.15	0.47
1:C:2:PRO:HB3	1:C:435:MET:HE2	1.96	0.47
1:C:166:ILE:HD11	1:C:310:LEU:HD13	1.96	0.47
1:C:902:MET:HE2	1:C:902:MET:HA	1.96	0.47
2:E:14:LEU:C	2:E:16:LYS:N	2.63	0.47
2:E:161:LEU:H	2:E:161:LEU:CD2	2.27	0.47
1:A:568:ASP:CG	1:A:637:ARG:HH22	2.23	0.47
1:A:669:PRO:O	1:A:671:ILE:HA	2.14	0.47
1:B:379:THR:CG2	1:B:477:ALA:HA	2.45	0.47
1:C:138:MET:HE2	1:C:306:ILE:HG21	1.96	0.47
1:C:600:THR:O	1:C:603:LYS:HE3	2.15	0.47
2:E:40:VAL:HG11	2:E:71:ALA:HB2	1.95	0.47
1:B:363:ARG:HB3	1:B:496:MET:O	2.15	0.47
1:C:326:PRO:O	1:C:630:SER:HB2	2.14	0.47
2:E:123:ARG:NH2	3:E:170:HOH:O	2.48	0.47
1:A:101:ASP:OD1	1:A:131:LYS:HE2	2.15	0.46
1:A:222:THR:HA	1:A:224:PRO:HD3	1.97	0.46
1:A:243:THR:HG23	3:A:1135:HOH:O	2.14	0.46
1:A:520:PHE:O	1:A:524:THR:HG23	2.14	0.46
1:A:726:GLN:CD	1:A:812:GLY:HA3	2.40	0.46
1:C:741:VAL:HG11	1:C:799:VAL:HG11	1.96	0.46
1:C:880:SER:O	1:C:884:VAL:HG23	2.15	0.46
1:A:70:ASN:C	1:A:70:ASN:HD22	2.23	0.46
1:A:259:ARG:CD	1:A:259:ARG:H	2.08	0.46
1:C:131:LYS:NZ	3:C:1170:HOH:O	2.47	0.46
1:C:452:VAL:HG23	1:C:453:PHE:CD1	2.50	0.46
1:C:743:ILE:HG12	1:C:743:ILE:O	2.15	0.46
1:A:396:PHE:CD2	1:A:1003:VAL:HG21	2.50	0.46
1:B:149:MET:HB2	1:B:153:ASP:CB	2.45	0.46
1:B:719:ASN:HD22	1:B:826:GLU:CD	2.24	0.46
1:B:880:SER:O	1:B:884:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.51	0.46
1:C:799:VAL:HA	1:C:800:PRO:HD3	1.78	0.46
1:A:252:LYS:HE3	1:A:254:ASN:OD1	2.15	0.46
1:A:704:ALA:O	1:A:708:LYS:HG3	2.14	0.46
1:B:330:THR:HB	1:B:331:PRO:HD3	1.95	0.46
1:B:1022:VAL:N	1:B:1023:PRO:CD	2.79	0.46
1:A:880:SER:O	1:A:884:VAL:HG23	2.16	0.46
1:B:714:THR:HG23	1:B:830:GLN:HG3	1.97	0.46
1:B:775:SER:HB2	1:B:789:TRP:CZ2	2.51	0.46
1:C:184:MET:HB3	1:C:771:VAL:HG22	1.98	0.46
2:D:65:VAL:O	2:D:69:ASN:ND2	2.47	0.46
2:E:77:ASP:O	2:E:78:SER:C	2.58	0.46
2:E:93:LEU:O	2:E:97:GLU:N	2.32	0.46
2:E:122:LYS:CG	2:E:152:ILE:HD11	2.40	0.46
1:A:817:GLU:OE1	1:A:825:MET:HA	2.15	0.46
1:B:621:GLY:O	1:B:624:THR:HG22	2.16	0.46
2:D:89:ARG:C	2:D:90:ARG:O	2.55	0.46
1:A:802:SER:O	2:E:144:LYS:NZ	2.38	0.46
1:B:676:THR:O	1:B:677:ALA:CB	2.64	0.46
2:E:77:ASP:C	2:E:79:LEU:N	2.68	0.46
1:A:53:ASP:OD1	1:A:56:THR:HG23	2.16	0.46
1:C:40:PRO:HB3	1:C:94:PHE:O	2.15	0.46
2:D:143:ASP:O	2:D:146:GLY:N	2.39	0.46
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.96	0.46
1:A:622:GLN:NE2	1:C:222:THR:HG23	2.31	0.46
1:A:987:MET:HB3	1:A:988:PRO:HD3	1.98	0.46
1:B:620:ARG:HA	1:B:624:THR:HG21	1.98	0.46
1:C:5:PHE:CG	1:C:487:ILE:HG23	2.51	0.46
2:E:100:LEU:HD11	2:E:106:VAL:HG22	1.97	0.46
1:B:146:ASP:HB3	1:B:148:THR:HG22	1.97	0.46
1:B:342:LYS:O	1:B:346:GLU:HG2	2.16	0.46
1:B:400:LEU:HD21	1:B:1003:VAL:HB	1.98	0.46
2:E:115:THR:O	2:E:116:PRO:C	2.57	0.46
1:B:115:MET:N	1:B:116:PRO:CD	2.79	0.45
1:B:314:GLU:N	1:B:315:PRO:CD	2.79	0.45
1:C:530:SER:O	1:C:534:ILE:HG23	2.16	0.45
1:C:54:ALA:HA	1:C:57:VAL:HG12	1.98	0.45
2:E:60:LEU:C	2:E:62:ILE:N	2.72	0.45
1:A:115:MET:HB2	1:A:116:PRO:HD3	1.98	0.45
1:C:509:LYS:C	1:C:510:LYS:CG	2.88	0.45
2:E:161:LEU:O	2:E:164:ILE:HB	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:MET:HE1	1:A:200:PRO:HA	1.99	0.45
1:A:895:TRP:CZ2	1:C:10:ILE:HB	2.52	0.45
1:B:192:GLU:HG2	1:B:264:ASP:O	2.16	0.45
1:B:565:PRO:HG3	1:B:924:ASP:OD1	2.15	0.45
1:B:937:LEU:HD13	1:B:1011:MET:HE1	1.98	0.45
1:C:314:GLU:HA	1:C:317:PHE:CE2	2.52	0.45
1:C:404:LEU:HD13	1:C:982:PHE:HD1	1.82	0.45
1:C:431:THR:O	1:C:435:MET:HG2	2.15	0.45
1:B:293:LEU:CD2	1:B:297:ALA:HB3	2.46	0.45
1:C:563:PHE:O	1:C:924:ASP:HB2	2.15	0.45
1:C:1033:PHE:N	1:C:1033:PHE:CD1	2.84	0.45
2:E:94:GLU:O	2:E:98:VAL:HG23	2.17	0.45
1:A:240:LEU:N	1:A:240:LEU:CD1	2.79	0.45
1:A:679:GLY:HA2	1:A:830:GLN:HA	1.98	0.45
1:A:790:TYR:HE1	1:A:800:PRO:HG3	1.79	0.45
1:A:860:THR:HG22	1:A:861:GLY:N	2.31	0.45
1:B:139:VAL:HG22	1:B:327:TYR:HB3	1.98	0.45
1:C:181:GLN:OE1	1:C:767:ARG:HD3	2.16	0.45
2:D:138:ASP:CA	2:D:140:ASN:ND2	2.75	0.45
1:A:93:THR:HG23	3:A:1058:HOH:O	2.17	0.45
1:A:392:THR:O	1:A:396:PHE:HD1	2.00	0.45
1:A:537:SER:N	1:A:538:THR:HA	2.32	0.45
1:B:166:ILE:O	1:B:172:VAL:HG11	2.17	0.45
1:B:879:ILE:O	1:B:883:VAL:HG23	2.16	0.45
1:C:2:PRO:O	1:C:6:ILE:HG13	2.16	0.45
1:C:152:GLU:HG2	1:C:182:TYR:HE1	1.82	0.45
2:E:15:GLY:CA	2:E:42:ALA:CB	2.95	0.45
1:A:743:ILE:HD12	1:A:743:ILE:N	2.32	0.45
1:C:57:VAL:CG1	1:C:82:SER:HB3	2.46	0.45
2:E:81:VAL:HG11	2:E:86:LEU:HD21	1.99	0.45
1:A:84:SER:OG	1:A:814:PRO:HA	2.17	0.45
1:B:484:VAL:HG13	1:B:488:LEU:HB3	1.98	0.45
1:B:733:GLN:HE22	1:B:743:ILE:HG13	1.82	0.45
2:E:40:VAL:HG12	2:E:71:ALA:CB	2.46	0.45
1:A:200:PRO:HD2	1:A:749:THR:HB	1.99	0.45
1:A:302:THR:O	1:A:306:ILE:HG13	2.17	0.45
1:A:345:VAL:O	1:A:349:ILE:HG13	2.16	0.45
1:A:879:ILE:HD12	1:A:880:SER:N	2.32	0.45
1:A:959:GLY:O	1:A:960:LEU:C	2.57	0.45
1:B:278:ILE:HG12	1:B:613:ASN:HB3	1.99	0.45
2:D:122:LYS:NZ	2:D:122:LYS:HB2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ILE:O	1:B:278:ILE:HG13	2.17	0.44
1:B:1022:VAL:CG2	1:B:1023:PRO:HD3	2.46	0.44
1:C:777:ALA:O	1:C:781:MET:HG2	2.17	0.44
1:C:898:PRO:O	1:C:902:MET:HG2	2.17	0.44
1:B:441:ALA:O	1:B:445:ILE:HG13	2.17	0.44
1:B:914:LEU:HD13	1:B:914:LEU:HA	1.88	0.44
1:B:973:ARG:O	1:B:977:MET:HG3	2.16	0.44
1:C:504:ASP:O	1:C:506:GLY:O	2.34	0.44
1:A:969:ARG:HG3	1:A:970:MET:N	2.31	0.44
1:B:75:LEU:HD21	1:B:92:LEU:HB3	1.99	0.44
1:B:956:GLU:HG3	1:B:958:LYS:HE2	1.98	0.44
1:C:36:PRO:HG2	1:C:469:GLN:HG3	1.98	0.44
1:C:527:TYR:HE2	1:C:968:VAL:HG13	1.80	0.44
2:E:90:ARG:CB	2:E:92:HIS:CD2	3.00	0.44
1:B:717:ARG:NH1	1:B:717:ARG:CG	2.75	0.44
1:C:11:PHE:O	1:C:14:VAL:HG22	2.16	0.44
1:C:239:ARG:CG	1:C:762:PHE:HA	2.47	0.44
1:C:944:LEU:O	1:C:971:ARG:HG3	2.17	0.44
2:E:57:PHE:O	2:E:59:HIS:HE1	1.94	0.44
2:E:132:LEU:O	2:E:137:ALA:HB2	2.17	0.44
1:B:189:ASN:HA	1:B:190:PRO:HD2	1.81	0.44
1:B:217:GLY:HA3	1:C:754:TRP:C	2.43	0.44
2:D:61:GLU:O	2:D:65:VAL:HG23	2.17	0.44
2:E:60:LEU:HD12	2:E:63:VAL:HB	1.99	0.44
1:A:370:ILE:O	1:A:373:PRO:HD2	2.18	0.44
1:A:586:ARG:O	1:A:590:VAL:HG23	2.16	0.44
1:A:961:ILE:HG23	1:A:962:GLU:N	2.33	0.44
1:B:990:VAL:HG13	1:B:1005:THR:HG22	1.99	0.44
1:C:193:LEU:CD1	1:C:265:VAL:HB	2.46	0.44
1:C:404:LEU:HD13	1:C:982:PHE:CD1	2.52	0.44
1:A:159:ALA:HB2	1:A:177:LEU:HD22	1.99	0.44
1:A:344:LEU:O	1:A:348:ILE:HG22	2.18	0.44
1:A:412:VAL:HG11	1:A:489:THR:CG2	2.47	0.44
1:A:908:GLY:HA2	1:A:1014:ALA:HB2	2.00	0.44
1:B:188:MET:HA	1:B:266:ALA:HB2	2.00	0.44
1:B:240:LEU:CD1	1:B:240:LEU:N	2.80	0.44
1:B:919:ARG:HB3	1:B:921:LEU:HD13	1.99	0.44
1:C:166:ILE:HD11	1:C:310:LEU:CD1	2.47	0.44
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.78	0.44
1:A:307:ARG:HH22	1:A:330:THR:HG21	1.83	0.44
1:A:758:TYR:CD1	1:A:758:TYR:C	2.92	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:LYS:O	1:A:954:ASP:CB	2.65	0.44
1:B:725:PRO:HA	1:B:810:GLU:O	2.17	0.44
1:B:968:VAL:HG21	1:B:1023:PRO:HG3	1.99	0.44
1:C:1:FME:H	1:C:2:PRO:CD	2.31	0.44
1:C:538:THR:O	1:C:542:LEU:HD13	2.18	0.44
1:C:586:ARG:O	1:C:589:LYS:HB3	2.16	0.44
1:C:1033:PHE:HD1	1:C:1033:PHE:N	2.16	0.44
2:D:30:VAL:HG21	2:D:62:ILE:CD1	2.47	0.44
2:E:16:LYS:O	2:E:17:LYS:C	2.56	0.44
1:A:509:LYS:CB	1:A:514:GLY:CA	2.96	0.44
1:A:542:LEU:H	1:A:542:LEU:HD22	1.83	0.44
1:B:99:ASP:OD1	1:B:101:ASP:HB2	2.18	0.44
1:B:636:ASP:C	1:B:638:PRO:HD3	2.43	0.44
1:B:905:VAL:N	1:B:906:PRO:HD2	2.32	0.44
1:C:727:PHE:CE1	1:C:807:SER:HB2	2.53	0.44
2:E:142:GLN:HB3	2:E:146:GLY:HA2	2.00	0.44
1:A:230:LEU:C	1:A:230:LEU:HD12	2.42	0.43
1:A:602:GLU:HG3	1:A:605:ASN:HB2	1.99	0.43
1:B:154:ILE:O	1:B:158:VAL:HG23	2.17	0.43
1:B:324:VAL:HG23	1:B:326:PRO:HD3	1.99	0.43
1:C:1:FME:H	1:C:2:PRO:HD2	1.84	0.43
1:A:957:GLY:C	1:A:958:LYS:CG	2.92	0.43
1:C:545:TYR:O	1:C:549:VAL:HG23	2.17	0.43
1:A:41:PRO:HD2	1:A:95:GLU:O	2.18	0.43
1:C:1016:VAL:HG23	1:C:1017:LEU:HD13	1.99	0.43
2:E:93:LEU:HA	2:E:96:VAL:HG21	1.91	0.43
1:A:984:LEU:HD13	1:A:984:LEU:O	2.18	0.43
1:B:945:ILE:HD12	1:B:1022:VAL:HG21	2.00	0.43
1:C:480:LEU:O	1:C:484:VAL:HG23	2.18	0.43
1:C:717:ARG:HA	1:C:718:PRO:HD3	1.90	0.43
1:A:324:VAL:O	1:A:326:PRO:HD3	2.19	0.43
1:A:456:MET:HG2	1:A:467:TYR:HB3	2.00	0.43
1:A:616:GLY:C	1:A:618:ALA:H	2.27	0.43
1:A:809:TRP:CD2	2:E:46:THR:HG22	2.53	0.43
1:C:23:GLY:O	1:C:27:ILE:HG12	2.19	0.43
1:C:298:ASN:HB3	1:C:301:ASP:HB2	2.00	0.43
1:C:534:ILE:HB	1:C:541:TYR:CE2	2.54	0.43
2:D:62:ILE:HD13	2:D:62:ILE:HG23	1.78	0.43
1:A:939:ALA:O	1:A:943:ILE:HG13	2.18	0.43
1:B:240:LEU:N	1:B:240:LEU:HD12	2.32	0.43
1:B:454:VAL:N	1:B:455:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:THR:HB	1:B:490:PRO:HD3	1.99	0.43
1:C:76:MET:HG2	1:C:95:GLU:HG3	2.01	0.43
1:C:509:LYS:HB2	1:C:510:LYS:CB	2.49	0.43
2:D:31:ARG:O	2:D:34:MET:HB2	2.19	0.43
2:E:41:ASN:N	2:E:41:ASN:ND2	2.62	0.43
2:E:60:LEU:HD12	2:E:60:LEU:HA	1.70	0.43
1:B:48:SER:HB3	1:B:125:GLN:HG2	2.00	0.43
1:B:577:GLN:O	1:B:661:ALA:HB1	2.18	0.43
1:C:505:HIS:C	1:C:506:GLY:O	2.60	0.43
1:A:239:ARG:NE	3:A:1113:HOH:O	2.33	0.43
1:A:767:ARG:HA	1:B:63:GLN:HE22	1.82	0.43
1:B:149:MET:HB2	1:B:153:ASP:HB2	2.01	0.43
1:B:223:PRO:HG3	1:C:275:TYR:CD1	2.53	0.43
1:B:683:GLU:HG2	1:B:819:TYR:CG	2.54	0.43
1:C:876:LEU:HD13	1:C:932:LEU:HD21	2.01	0.43
1:A:166:ILE:HD11	1:A:310:LEU:CD1	2.46	0.43
1:A:919:ARG:HD2	1:A:921:LEU:HD13	2.01	0.43
1:B:401:ALA:O	1:B:405:LEU:HG	2.19	0.43
1:B:559:LEU:HD12	1:B:560:PRO:HD3	2.01	0.43
1:B:897:ILE:N	1:B:898:PRO:HD2	2.34	0.43
1:C:189:ASN:O	1:C:193:LEU:HD13	2.19	0.43
1:C:314:GLU:N	1:C:315:PRO:CD	2.81	0.43
1:C:605:ASN:C	1:C:632:LYS:HG2	2.43	0.43
2:E:117:LEU:HD21	2:E:129:VAL:HG13	2.00	0.43
2:E:151:ASP:CA	2:E:154:ILE:HG13	2.47	0.43
1:A:181:GLN:HE22	1:A:767:ARG:NH1	2.07	0.43
1:A:741:VAL:HA	3:A:1150:HOH:O	2.18	0.43
1:A:901:VAL:O	1:A:904:VAL:HG12	2.18	0.43
1:A:992:SER:C	1:A:993:THR:HG23	2.42	0.43
1:C:878:ALA:O	1:C:882:ILE:HG12	2.19	0.43
2:D:134:LYS:HG3	2:D:135:ASN:HD22	1.83	0.43
1:A:314:GLU:HB2	1:A:315:PRO:HD3	2.00	0.42
1:A:712:MET:HA	1:A:832:ALA:CB	2.42	0.42
1:A:892:TYR:O	1:A:950:LYS:HE3	2.19	0.42
1:C:358:PHE:CG	1:C:977:MET:HG2	2.54	0.42
1:A:537:SER:OG	1:A:538:THR:CA	2.67	0.42
1:B:774:MET:HE2	1:B:780:ARG:NE	2.34	0.42
1:C:696:THR:OG1	1:C:825:MET:HE1	2.19	0.42
1:C:735:LYS:O	1:C:739:LEU:HD13	2.19	0.42
1:A:767:ARG:HA	1:B:63:GLN:HE21	1.80	0.42
1:A:774:MET:HE2	1:A:780:ARG:CZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:PHE:O	1:A:805:SER:OG	2.34	0.42
1:B:194:ASN:ND2	1:B:798:MET:HG3	2.34	0.42
1:B:332:PHE:CZ	1:B:569:GLN:HA	2.53	0.42
1:B:897:ILE:N	1:B:898:PRO:CD	2.82	0.42
1:C:69:MET:CE	1:C:107:VAL:HG13	2.50	0.42
1:C:194:ASN:ND2	1:C:798:MET:HG3	2.34	0.42
1:C:235:ILE:HG22	1:C:236:ALA:H	1.84	0.42
1:C:505:HIS:CD2	1:C:505:HIS:H	2.35	0.42
2:E:18:LEU:HD22	2:E:18:LEU:HA	1.77	0.42
2:E:82:THR:O	2:E:85:HIS:N	2.49	0.42
1:A:293:LEU:CD2	1:A:297:ALA:HB3	2.49	0.42
1:A:753:ALA:O	1:A:775:SER:HB3	2.20	0.42
1:C:933:THR:O	1:C:937:LEU:HG	2.19	0.42
2:D:134:LYS:C	2:D:135:ASN:HD22	2.28	0.42
2:E:43:ARG:HB3	2:E:47:GLY:HA2	2.01	0.42
2:E:58:GLY:HA3	2:E:92:HIS:CE1	2.55	0.42
1:A:300:LEU:CD2	1:A:330:THR:HG23	2.45	0.42
1:A:314:GLU:HA	1:A:317:PHE:CD2	2.55	0.42
1:A:682:PHE:HD1	1:A:859:TRP:CH2	2.37	0.42
1:C:21:LEU:HD12	1:C:21:LEU:C	2.45	0.42
1:C:239:ARG:HG2	1:C:762:PHE:HA	2.01	0.42
1:C:413:VAL:O	1:C:417:GLU:HG2	2.19	0.42
1:A:234:ILE:HG21	1:A:234:ILE:HD13	1.70	0.42
1:A:263:ARG:H	1:A:263:ARG:HG3	1.62	0.42
1:A:459:PHE:O	1:A:464:GLY:HA3	2.19	0.42
1:A:585:GLU:HB2	3:C:1123:HOH:O	2.20	0.42
1:B:355:MET:HE2	1:B:359:LEU:CD1	2.49	0.42
1:B:892:TYR:O	1:B:950:LYS:HE3	2.19	0.42
1:C:14:VAL:O	1:C:18:ILE:HG13	2.19	0.42
1:C:40:PRO:HA	1:C:41:PRO:HD3	1.85	0.42
1:C:736:ALA:O	1:C:741:VAL:HG22	2.19	0.42
1:A:23:GLY:HA3	1:A:377:LEU:O	2.19	0.42
1:A:509:LYS:CB	1:A:514:GLY:HA2	2.49	0.42
1:A:1021:PHE:HB3	1:A:1025:PHE:CE1	2.55	0.42
1:B:27:ILE:O	1:B:27:ILE:HG12	2.19	0.42
1:C:583:THR:HB	3:C:1072:HOH:O	2.19	0.42
1:C:950:LYS:HA	1:C:953:MET:HE2	2.02	0.42
1:C:355:MET:SD	1:C:368:PRO:HB2	2.60	0.42
2:E:138:ASP:OD1	2:E:140:ASN:N	2.53	0.42
1:A:80:SER:HA	1:A:89:GLN:O	2.20	0.42
1:A:111:LEU:HD23	1:A:111:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ASN:HB3	1:A:301:ASP:HB2	2.01	0.42
1:A:564:LEU:HA	1:A:565:PRO:HD2	1.89	0.42
1:A:892:TYR:O	1:A:893:GLU:HB2	2.20	0.42
1:A:932:LEU:HA	1:A:935:ILE:HG22	2.01	0.42
1:C:573:MET:HE1	1:C:617:PHE:CE2	2.39	0.42
1:A:717:ARG:HA	1:A:718:PRO:HD3	1.93	0.42
1:B:222:THR:HG23	1:C:622:GLN:NE2	2.35	0.42
1:C:189:ASN:CG	1:C:192:GLU:HG2	2.44	0.42
1:C:370:ILE:C	1:C:373:PRO:HD2	2.45	0.42
1:C:893:GLU:HG3	1:C:893:GLU:O	2.20	0.42
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.20	0.42
2:D:89:ARG:HB2	2:D:119:LEU:HB3	2.01	0.42
1:A:62:THR:HB	1:A:88:VAL:HG11	2.02	0.41
1:A:1019:ILE:HD13	1:A:1019:ILE:HA	1.87	0.41
1:C:314:GLU:HA	1:C:317:PHE:CD2	2.55	0.41
2:E:100:LEU:HA	2:E:104:ALA:HB3	2.02	0.41
1:A:759:VAL:H	1:A:759:VAL:HG23	1.63	0.41
1:B:143:ILE:HG22	1:B:286:ALA:HB2	2.01	0.41
2:D:139:VAL:HG12	2:D:140:ASN:N	2.33	0.41
1:A:238:THR:HG22	1:A:239:ARG:N	2.36	0.41
1:A:583:THR:HG21	1:C:228:GLN:O	2.21	0.41
1:B:355:MET:HE3	1:B:355:MET:HA	2.02	0.41
1:B:446:ALA:HB2	1:B:482:VAL:HG21	2.01	0.41
1:B:939:ALA:O	1:B:943:ILE:HG13	2.21	0.41
2:D:89:ARG:NH1	3:D:172:HOH:O	2.48	0.41
1:A:14:VAL:HG13	1:B:886:LEU:HB3	2.01	0.41
1:C:369:THR:O	1:C:373:PRO:HD3	2.20	0.41
1:A:66:GLU:HG2	1:A:78:MET:CE	2.49	0.41
1:A:987:MET:N	1:A:988:PRO:CD	2.83	0.41
1:B:200:PRO:O	1:B:204:ILE:HG13	2.21	0.41
1:B:676:THR:O	1:B:676:THR:CG2	2.66	0.41
1:C:632:LYS:HG2	1:C:632:LYS:H	1.72	0.41
1:C:780:ARG:HD2	3:C:1089:HOH:O	2.20	0.41
2:E:60:LEU:O	2:E:62:ILE:N	2.54	0.41
1:A:1007:VAL:O	1:A:1011:MET:HB2	2.20	0.41
1:B:967:ALA:HA	1:B:970:MET:HE3	2.02	0.41
1:C:85:THR:OG1	1:C:87:THR:HG22	2.21	0.41
1:A:567:GLU:OE1	1:A:996:GLY:HA2	2.21	0.41
1:A:616:GLY:C	1:A:618:ALA:N	2.77	0.41
1:B:396:PHE:HA	1:B:399:VAL:HG22	2.03	0.41
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:ILE:O	1:C:448:VAL:HG12	2.21	0.41
2:D:59:HIS:CD2	2:D:59:HIS:H	2.39	0.41
2:D:134:LYS:HG3	2:D:135:ASN:ND2	2.35	0.41
1:B:223:PRO:HG3	1:C:275:TYR:CD2	2.55	0.41
1:C:64:VAL:HG12	1:C:114:ALA:HB1	2.03	0.41
1:C:420:MET:HG3	1:C:425:LEU:O	2.20	0.41
1:C:775:SER:OG	1:C:789:TRP:HZ2	2.03	0.41
1:A:165:ALA:O	1:A:169:THR:HG23	2.20	0.41
1:A:774:MET:HE2	1:A:780:ARG:NE	2.35	0.41
1:A:781:MET:CE	1:C:224:PRO:HA	2.50	0.41
1:B:415:ASN:HB3	3:B:1119:HOH:O	2.20	0.41
1:B:493:CYS:O	1:B:497:LEU:HB2	2.21	0.41
1:B:643:LYS:O	1:B:647:ILE:HG13	2.21	0.41
1:B:764:ASP:OD1	1:B:765:ARG:HD3	2.21	0.41
1:B:799:VAL:HA	1:B:800:PRO:HD3	1.87	0.41
1:C:903:LEU:O	1:C:906:PRO:HD2	2.21	0.41
1:C:960:LEU:HD22	1:C:1027:VAL:HG22	2.03	0.41
2:E:139:VAL:O	2:E:139:VAL:CG1	2.67	0.41
1:A:75:LEU:C	1:A:75:LEU:HD23	2.46	0.41
1:A:448:VAL:HG12	1:A:887:CYS:HB3	2.03	0.41
1:A:897:ILE:N	1:A:898:PRO:CD	2.84	0.41
1:B:187:TRP:HA	1:B:774:MET:O	2.21	0.41
1:B:1020:PHE:C	1:B:1023:PRO:HD2	2.46	0.41
1:C:443:VAL:O	1:C:447:MET:HB2	2.20	0.41
1:C:941:ASN:ND2	1:C:1011:MET:HE1	2.36	0.41
1:A:478:MET:HE2	1:A:478:MET:HB3	1.92	0.40
1:A:535:LEU:HD22	1:A:1027:VAL:HG21	2.03	0.40
1:A:953:MET:SD	1:A:960:LEU:HA	2.61	0.40
1:B:207:ILE:O	1:B:211:ASN:HB3	2.21	0.40
1:C:135:SER:CB	1:C:672:VAL:HG12	2.52	0.40
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.56	0.40
1:C:564:LEU:HA	1:C:565:PRO:HD3	1.94	0.40
1:C:681:ASP:CB	3:C:1143:HOH:O	2.65	0.40
1:C:876:LEU:O	1:C:876:LEU:HD22	2.20	0.40
2:D:49:THR:HB	2:D:50:PRO:HD2	2.03	0.40
2:E:60:LEU:C	2:E:62:ILE:H	2.28	0.40
1:A:101:ASP:O	1:A:105:VAL:HG23	2.20	0.40
1:A:185:ARG:HA	1:A:185:ARG:HD2	1.99	0.40
1:B:218:GLN:NE2	1:B:231:ASN:HD21	2.20	0.40
1:B:919:ARG:CD	1:B:1005:THR:HG21	2.52	0.40
1:C:23:GLY:HA3	1:C:377:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LEU:HD23	1:C:75:LEU:HA	1.91	0.40
1:C:897:ILE:N	1:C:898:PRO:CD	2.82	0.40
1:A:454:VAL:HB	1:A:455:PRO:HD3	2.03	0.40
1:A:498:LYS:HA	1:A:499:PRO:HD3	1.94	0.40
1:A:712:MET:HB2	1:A:712:MET:HE2	1.78	0.40
1:B:293:LEU:HD22	1:B:297:ALA:HB3	2.02	0.40
1:B:896:SER:C	1:B:898:PRO:HD2	2.46	0.40
1:B:927:PHE:CE2	1:B:931:LEU:HD11	2.56	0.40
1:C:189:ASN:HA	1:C:190:PRO:HD2	1.83	0.40
1:C:243:THR:HG23	3:C:1194:HOH:O	2.20	0.40
1:C:330:THR:N	1:C:331:PRO:CD	2.85	0.40
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.52	0.40
1:A:983:ILE:HD13	1:A:1012:VAL:HG22	2.02	0.40
1:B:217:GLY:HA3	1:C:754:TRP:O	2.22	0.40
1:B:446:ALA:HA	1:B:478:MET:SD	2.62	0.40
1:B:459:PHE:O	1:B:464:GLY:HA3	2.22	0.40
1:B:681:ASP:HB3	1:B:860:THR:HG23	2.03	0.40
1:C:404:LEU:HG	1:C:449:LEU:HD13	2.03	0.40
1:B:194:ASN:HD22	1:B:798:MET:HG3	1.86	0.40
1:C:892:TYR:CG	1:C:897:ILE:HD11	2.56	0.40

There are no symmetry-related clashes.

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	1020/1049 (97%)	981 (96%)	39 (4%)	0	100	100
1	B	1020/1049 (97%)	985 (97%)	34 (3%)	1 (0%)	48	73
1	C	1032/1049 (98%)	993 (96%)	39 (4%)	0	100	100
2	D	152/169 (90%)	150 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	150/169 (89%)	141 (94%)	9 (6%)	0	100	100
All	All	3374/3485 (97%)	3250 (96%)	123 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	677	ALA

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	766/854 (90%)	721 (94%)	45 (6%)	18	42
1	B	780/854 (91%)	746 (96%)	34 (4%)	25	53
1	C	792/854 (93%)	753 (95%)	39 (5%)	22	49
2	D	108/133 (81%)	95 (88%)	13 (12%)	5	12
2	E	104/133 (78%)	85 (82%)	19 (18%)	2	5
All	All	2550/2828 (90%)	2400 (94%)	150 (6%)	18	42

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	62	THR
1	A	70	ASN
1	A	92	LEU
1	A	98	THR
1	A	130	GLU
1	A	143	ILE
1	A	146	ASP
1	A	148	THR
1	A	185	ARG
1	A	240	LEU

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Mol	Chain	Res	Type
1	A	244	GLU
1	A	258	SER
1	A	259	ARG
1	A	262	LEU
1	A	263	ARG
1	A	274	ASN
1	A	293	LEU
1	A	310	LEU
1	A	321	LEU
1	A	330	THR
1	A	348	ILE
1	A	376	LEU
1	A	410	ILE
1	A	537	SER
1	A	538	THR
1	A	577	GLN
1	A	587	THR
1	A	612	VAL
1	A	659	LYS
1	A	695	LEU
1	A	712	MET
1	A	713	LEU
1	A	714	THR
1	A	729	ILE
1	A	749	THR
1	A	828	LEU
1	A	902	MET
1	A	953	MET
1	A	960	LEU
1	A	961	ILE
1	A	968	VAL
1	A	984	LEU
1	A	990	VAL
1	A	997	SER
1	B	70	ASN
1	B	88	VAL
1	B	121	GLU
1	B	163	LYS
1	B	172	VAL
1	B	197	GLN
1	B	225	VAL
1	B	243	THR

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Mol	Chain	Res	Type
1	B	259	ARG
1	B	267	LYS
1	B	268	ILE
1	B	274	ASN
1	B	293	LEU
1	B	306	ILE
1	B	355	MET
1	B	366	LEU
1	B	429	GLU
1	B	471	SER
1	B	472	ILE
1	B	497	LEU
1	B	577	GLN
1	B	578	LEU
1	B	672	VAL
1	B	687	GLN
1	B	695	LEU
1	B	716	VAL
1	B	825	MET
1	B	837	THR
1	B	844	MET
1	B	860	THR
1	B	914	LEU
1	B	956	GLU
1	B	972	LEU
1	B	980	LEU
1	C	10	ILE
1	C	55	LYS
1	C	81	ASN
1	C	88	VAL
1	C	125	GLN
1	C	127	VAL
1	C	129	VAL
1	C	177	LEU
1	C	239	ARG
1	C	244	GLU
1	C	249	ILE
1	C	274	ASN
1	C	289	LEU
1	C	310	LEU
1	C	372	VAL
1	C	394	THR

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Mol	Chain	Res	Type
1	C	404	LEU
1	C	415	ASN
1	C	448	VAL
1	C	482	VAL
1	C	510	LYS
1	C	544	LEU
1	C	571	VAL
1	C	587	THR
1	C	626	ILE
1	C	632	LYS
1	C	684	LEU
1	C	695	LEU
1	C	743	ILE
1	C	799	VAL
1	C	860	THR
1	C	876	LEU
1	C	891	LEU
1	C	897	ILE
1	C	901	VAL
1	C	960	LEU
1	C	968	VAL
1	C	976	LEU
1	C	1011	MET
2	D	17	LYS
2	D	26	GLN
2	D	34	MET
2	D	51	LEU
2	D	59	HIS
2	D	62	ILE
2	D	81	VAL
2	D	84	LEU
2	D	93	LEU
2	D	117	LEU
2	D	122	LYS
2	D	139	VAL
2	D	140	ASN
2	E	14	LEU
2	E	18	LEU
2	E	40	VAL
2	E	59	HIS
2	E	64	GLU
2	E	76	LYS

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Mol	Chain	Res	Type
2	E	77	ASP
2	E	81	VAL
2	E	89	ARG
2	E	90	ARG
2	E	93	LEU
2	E	95	ILE
2	E	100	LEU
2	E	122	LYS
2	E	138	ASP
2	E	140	ASN
2	E	152	ILE
2	E	154	ILE
2	E	164	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	63	GLN
1	A	70	ASN
1	A	109	ASN
1	A	125	GLN
1	A	151	GLN
1	A	181	GLN
1	A	191	ASN
1	A	194	ASN
1	A	229	GLN
1	A	237	GLN
1	A	338	HIS
1	A	361	ASN
1	A	687	GLN
1	A	923	ASN
1	A	1000	GLN
1	A	1001	ASN
1	B	3	ASN
1	B	63	GLN
1	B	70	ASN
1	B	123	GLN
1	B	124	GLN
1	B	194	ASN
1	B	197	GLN
1	B	213	GLN

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Mol	Chain	Res	Type
1	B	218	GLN
1	B	231	ASN
1	B	274	ASN
1	B	284	GLN
1	B	360	GLN
1	B	517	ASN
1	B	577	GLN
1	B	592	ASN
1	B	687	GLN
1	B	701	GLN
1	B	733	GLN
1	B	744	ASN
1	B	747	ASN
1	B	871	ASN
1	B	941	ASN
1	B	1000	GLN
1	B	1001	ASN
1	C	3	ASN
1	C	34	GLN
1	C	67	GLN
1	C	68	ASN
1	C	81	ASN
1	C	125	GLN
1	C	194	ASN
1	C	197	GLN
1	C	213	GLN
1	C	229	GLN
1	C	231	ASN
1	C	237	GLN
1	C	274	ASN
1	C	284	GLN
1	C	298	ASN
1	C	360	GLN
1	C	437	GLN
1	C	517	ASN
1	C	525	HIS
1	C	569	GLN
1	C	604	ASN
1	C	692	HIS
1	C	701	GLN
1	C	744	ASN
1	C	830	GLN

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Mol	Chain	Res	Type
1	C	871	ASN
1	C	1001	ASN
2	D	36	ASN
2	D	52	HIS
2	D	59	HIS
2	D	125	HIS
2	D	135	ASN
2	D	140	ASN
2	D	142	GLN
2	D	156	ASN
2	E	26	GLN
2	E	41	ASN
2	E	59	HIS
2	E	85	HIS
2	E	92	HIS
2	E	102	ASN
2	E	112	HIS
2	E	118	HIS
2	E	135	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	A	1	1	8,9,10	0.36	0	8,9,11	11.89	2 (25%)
1	FME	C	1	1	8,9,10	0.35	0	8,9,11	1.09	1 (12%)
1	FME	B	1	1	8,9,10	0.35	0	8,9,11	8.31	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	1/7/9/11	-
1	FME	C	1	1	-	1/7/9/11	-
1	FME	B	1	1	-	1/7/9/11	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	CA-N-CN	27.93	165.77	122.82
1	A	1	FME	O1-CN-N	18.64	173.45	125.32
1	B	1	FME	CA-N-CN	17.80	150.20	122.82
1	B	1	FME	O1-CN-N	15.23	164.66	125.32
1	C	1	FME	C-CA-N	2.02	113.41	109.50

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	B	1	FME	O1-CN-N-CA
1	C	1	FME	O1-CN-N-CA

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	1	FME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	1026/1049 (97%)	0.79	122 (11%) 9 7	26, 61, 114, 188	0
1	B	1025/1049 (97%)	0.61	90 (8%) 15 13	22, 56, 89, 154	1 (0%)
1	C	1033/1049 (98%)	0.51	86 (8%) 17 14	27, 53, 88, 168	0
2	D	154/169 (91%)	0.63	15 (9%) 13 11	33, 64, 104, 162	0
2	E	152/169 (89%)	1.56	44 (28%) 1 1	14, 97, 140, 200	2 (1%)
All	All	3390/3485 (97%)	0.68	357 (10%) 11 9	14, 57, 107, 200	3 (0%)

All (357) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	672	VAL	12.5
1	B	676	THR	8.1
2	E	14	LEU	7.8
2	E	38	ALA	7.1
1	B	562	SER	7.0
1	A	865	GLN	6.9
1	B	134	SER	6.8
1	C	1034	SER	6.8
1	B	660	ASP	6.7
1	C	670	ALA	6.7
1	A	1035	ARG	6.5
1	A	408	ASP	5.8
1	C	7	ASP	5.6
1	C	918	PHE	5.6
1	B	424	GLY	5.3
1	B	617	PHE	5.1
1	A	407	ASP	5.1
1	A	538	THR	5.1
1	C	513	PHE	5.0
2	E	45	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	256	ASP	4.9
1	A	1044	HIS	4.9
1	A	229	GLN	4.9
1	A	681	ASP	4.9
1	A	670	ALA	4.8
1	C	70	ASN	4.8
1	C	28	LEU	4.8
1	B	871	ASN	4.7
1	C	495	THR	4.7
2	E	47	GLY	4.7
1	A	668	LEU	4.6
1	C	1033	PHE	4.6
1	A	1042	HIS	4.6
1	B	135	SER	4.6
1	A	617	PHE	4.5
2	E	44	ASP	4.4
1	C	674	LEU	4.4
1	B	659	LYS	4.4
1	A	810	GLU	4.4
1	A	671	ILE	4.4
1	A	833	PRO	4.3
1	B	216	ALA	4.3
2	E	158	ASN	4.2
1	B	877	TYR	4.2
1	C	508	GLY	4.2
2	D	124	GLY	4.2
1	B	678	THR	4.1
2	D	140	ASN	4.1
1	A	534	ILE	4.1
1	A	515	TRP	4.1
1	B	600	THR	4.1
1	C	248	LYS	4.0
1	B	865	GLN	4.0
1	C	618	ALA	4.0
1	C	566	ASP	4.0
1	A	406	VAL	4.0
1	C	509	LYS	4.0
2	E	161	LEU	3.9
1	C	862	MET	3.9
2	E	143	ASP	3.9
1	A	542	LEU	3.9
1	B	671	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	71	GLY	3.9
1	C	809	TRP	3.9
2	E	156	ASN	3.8
1	C	124	GLN	3.8
1	B	863	SER	3.8
1	C	511	GLY	3.8
1	A	386	PHE	3.8
1	A	1039	ASP	3.8
1	A	719	ASN	3.8
2	D	150	PHE	3.8
1	B	407	ASP	3.7
1	A	284	GLN	3.7
2	D	31	ARG	3.7
1	A	961	ILE	3.6
1	C	152	GLU	3.6
2	E	165	LEU	3.6
1	B	232	ALA	3.6
1	C	994	GLY	3.6
1	B	563	PHE	3.6
1	B	133	SER	3.6
2	E	51	LEU	3.6
1	C	993	THR	3.6
2	E	150	PHE	3.6
2	E	122	LYS	3.6
1	A	874	PRO	3.5
1	A	1016	VAL	3.5
1	A	1033	PHE	3.4
2	D	139	VAL	3.4
2	E	144	LYS	3.4
2	E	77	ASP	3.4
1	A	938	SER	3.4
1	C	505	HIS	3.4
1	B	386	PHE	3.4
1	A	1019	ILE	3.4
1	C	811	TYR	3.4
1	A	403	GLY	3.4
1	C	256	ASP	3.4
1	A	669	PRO	3.3
1	C	514	GLY	3.3
1	B	708	LYS	3.3
1	B	837	THR	3.3
1	A	994	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	37	GLY	3.3
1	C	510	LYS	3.3
1	B	148	THR	3.3
1	C	255	GLN	3.3
1	B	332	PHE	3.3
1	C	3	ASN	3.3
1	A	969	ARG	3.3
1	A	518	ARG	3.2
1	B	147	GLY	3.2
1	B	561	SER	3.2
2	E	58	GLY	3.2
1	A	541	TYR	3.2
1	C	363	ARG	3.1
1	A	526	HIS	3.1
1	A	501	ALA	3.1
1	A	1031	ARG	3.1
2	D	13	ASP	3.1
1	A	502	LYS	3.1
1	B	744	ASN	3.1
1	B	566	ASP	3.1
1	B	404	LEU	3.1
1	A	531	VAL	3.1
1	A	872	GLN	3.0
1	A	438	ILE	3.0
1	A	359	LEU	3.0
1	B	633	ASP	3.0
1	C	500	ILE	3.0
1	A	376	LEU	3.0
1	B	180	SER	3.0
1	B	864	TYR	3.0
1	A	143	ILE	3.0
1	B	253	VAL	3.0
1	A	907	LEU	2.9
1	A	148	THR	2.9
1	C	423	GLU	2.9
2	E	134	LYS	2.9
2	E	155	ASP	2.9
1	A	513	PHE	2.9
1	A	1014	ALA	2.9
1	B	688	ALA	2.9
1	A	380	PHE	2.9
1	B	542	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	620	ARG	2.9
1	C	786	ILE	2.9
1	A	954	ASP	2.9
1	C	676	THR	2.9
1	A	972	LEU	2.9
1	B	555	LEU	2.9
1	A	618	ALA	2.8
1	C	564	LEU	2.8
1	C	244	GLU	2.8
1	C	737	GLN	2.8
1	A	863	SER	2.8
1	B	269	GLU	2.8
1	A	659	LYS	2.8
1	B	132	SER	2.8
1	A	387	GLY	2.8
1	B	270	LEU	2.8
1	B	854	GLY	2.8
1	A	276	ASP	2.8
1	C	501	ALA	2.8
2	E	163	GLU	2.8
1	A	511	GLY	2.7
1	C	724	THR	2.7
2	E	130	GLU	2.7
1	A	31	PRO	2.7
1	A	619	GLY	2.7
2	D	156	ASN	2.7
2	E	111	SER	2.7
1	A	616	GLY	2.7
1	C	84	SER	2.7
2	D	111	SER	2.7
2	E	124	GLY	2.7
1	B	670	ALA	2.7
1	A	146	ASP	2.7
1	B	669	PRO	2.7
1	C	496	MET	2.7
1	A	893	GLU	2.7
1	C	269	GLU	2.7
2	E	159	GLU	2.7
1	C	515	TRP	2.7
1	C	723	ASP	2.7
1	B	862	MET	2.6
1	C	258	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	617	PHE	2.6
2	E	25	GLY	2.6
2	E	76	LYS	2.6
1	A	836	SER	2.6
1	A	255	GLN	2.6
1	C	151	GLN	2.6
2	E	91	GLY	2.6
1	B	112	GLN	2.6
1	C	48	SER	2.6
1	C	134	SER	2.6
1	C	726	GLN	2.6
2	D	77	ASP	2.6
1	B	337	ILE	2.6
1	A	539	GLY	2.6
1	A	566	ASP	2.5
1	A	952	LEU	2.5
2	E	123	ARG	2.5
2	E	20	GLU	2.5
1	C	51	GLY	2.5
1	C	424	GLY	2.5
1	B	993	THR	2.5
2	E	39	ASP	2.5
1	A	717	ARG	2.5
1	C	835	LYS	2.5
1	A	877	TYR	2.5
1	B	567	GLU	2.5
2	D	97	GLU	2.5
1	A	993	THR	2.5
1	A	729	ILE	2.5
1	A	960	LEU	2.5
1	C	620	ARG	2.5
1	B	499	PRO	2.5
2	E	40	VAL	2.5
1	A	832	ALA	2.5
1	B	677	ALA	2.5
1	B	131	LYS	2.5
1	C	518	ARG	2.5
1	A	257	GLY	2.5
1	A	424	GLY	2.5
1	A	32	VAL	2.5
1	A	405	LEU	2.4
1	C	83	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	520	PHE	2.4
1	B	635	ALA	2.4
1	B	982	PHE	2.4
1	B	408	ASP	2.4
1	A	962	GLU	2.4
2	D	159	GLU	2.4
1	A	71	GLY	2.4
1	C	116	PRO	2.4
2	E	103	GLY	2.4
1	A	553	ALA	2.4
1	C	832	ALA	2.4
2	D	141	ALA	2.4
1	A	922	THR	2.4
1	B	405	LEU	2.4
1	B	130	GLU	2.4
1	B	255	GLN	2.4
1	A	363	ARG	2.4
2	E	93	LEU	2.4
1	C	319	SER	2.4
1	A	125	GLN	2.4
1	A	212	ALA	2.4
1	A	402	ILE	2.3
1	A	987	MET	2.3
1	B	569	GLN	2.3
1	C	117	LEU	2.3
2	E	104	ALA	2.3
1	A	860	THR	2.3
1	C	833	PRO	2.3
1	A	506	GLY	2.3
1	B	919	ARG	2.3
1	A	535	LEU	2.3
2	E	52	HIS	2.3
1	A	95	GLU	2.3
1	B	640	GLU	2.3
1	B	874	PRO	2.3
2	E	157	GLY	2.3
2	E	101	LYS	2.3
1	A	807	SER	2.3
1	B	258	SER	2.3
1	B	730	ASP	2.3
2	D	138	ASP	2.3
1	C	846	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	139	VAL	2.3
1	B	987	MET	2.2
1	B	748	THR	2.2
1	A	432	ARG	2.2
1	A	370	ILE	2.2
2	E	145	PHE	2.2
1	B	866	GLU	2.2
1	C	87	THR	2.2
1	A	275	TYR	2.2
1	C	35	TYR	2.2
1	A	530	SER	2.2
1	A	1034	SER	2.2
1	B	631	LEU	2.2
1	A	712	MET	2.2
1	A	873	ALA	2.2
1	A	919	ARG	2.2
1	B	653	ARG	2.2
1	A	608	SER	2.2
1	B	544	LEU	2.2
2	E	78	SER	2.2
2	E	92	HIS	2.2
1	C	47	ALA	2.2
1	A	322	LYS	2.2
1	A	366	LEU	2.2
1	B	998	GLY	2.2
1	C	834	GLY	2.2
1	B	515	TRP	2.1
1	B	832	ALA	2.1
1	B	1013	THR	2.1
1	C	307	ARG	2.1
1	C	1030	ARG	2.1
1	A	426	PRO	2.1
1	B	554	TYR	2.1
1	C	425	LEU	2.1
1	A	461	GLY	2.1
1	C	691	GLY	2.1
1	A	537	SER	2.1
1	A	802	SER	2.1
1	B	402	ILE	2.1
1	A	11	PHE	2.1
1	B	553	ALA	2.1
1	B	618	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	422	GLU	2.1
1	C	312	LYS	2.1
1	A	34	GLN	2.1
1	B	657	GLN	2.1
1	C	497	LEU	2.1
1	C	675	GLY	2.1
1	C	959	GLY	2.1
1	A	459	PHE	2.1
1	C	896	SER	2.1
1	B	995	ALA	2.1
1	A	259	ARG	2.1
1	B	363	ARG	2.1
1	A	835	LYS	2.1
2	E	68	LYS	2.1
1	C	86	GLY	2.1
1	B	731	ILE	2.1
1	B	1003	VAL	2.1
1	C	671	ILE	2.1
1	A	470	PHE	2.1
1	C	784	ASP	2.1
1	A	805	SER	2.1
1	A	285	PRO	2.1
1	B	577	GLN	2.1
1	B	872	GLN	2.1
1	B	191	ASN	2.1
2	E	125	HIS	2.1
1	B	1028	VAL	2.1
1	C	362	PHE	2.1
1	B	457	ALA	2.0
1	C	96	SER	2.0
1	B	573	MET	2.0
1	C	901	VAL	2.0
1	C	926	TYR	2.0
2	E	81	VAL	2.0
2	D	123	ARG	2.0
1	A	244	GLU	2.0
1	B	478	MET	2.0
1	C	662	MET	2.0
1	C	898	PRO	2.0
1	A	921	LEU	2.0
2	D	166	GLN	2.0
1	C	283	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	904	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	FME	A	1	10/11	0.62	0.25	47,80,97,110	0
1	FME	B	1	10/11	0.82	0.16	42,74,88,109	0
1	FME	C	1	10/11	0.85	0.18	65,71,86,87	0

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.