



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:23 AM UTC

PDB ID : 3RFR / pdb_00003rfr
Title : Crystal Structure of particulate methane monooxygenase (pMMO) from
Methylocystis sp. strain M
Authors : Smith, S.M.; Rosenzweig, A.C.
Deposited on : 2011-04-06
Resolution : 2.68 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

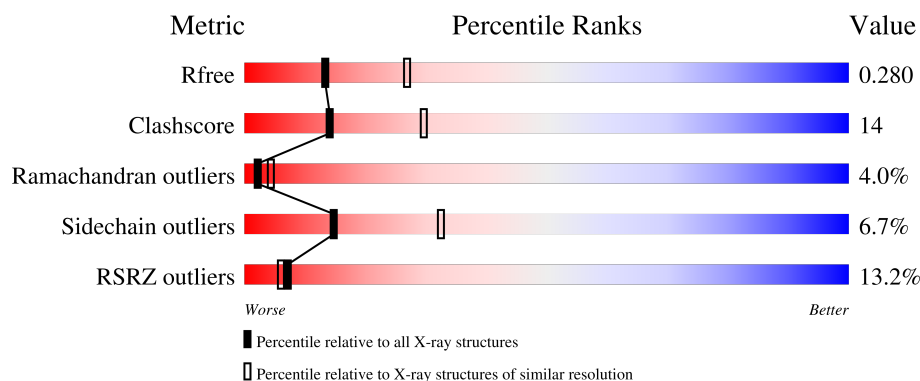
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	419	12% 66% 21% • • 8%
1	E	419	13% 65% 22% 5% • 8%
1	I	419	4% 53% 32% 6% • 8%
2	D	19	53% 68% 32%
2	H	19	47% 68% 16% 16%

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Mol	Chain	Length	Quality of chain
3	B	252	8% 68% 23%
3	F	252	10% 66% 26%
3	J	252	8% 63% 26% 6%
4	C	256	19% 57% 22% 18%
4	G	256	18% 57% 22% 18%
4	K	256	15% 60% 19% 18%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20224 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 PmoB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			3012	1937	521	551	3			
1	E	386	Total	C	N	O	S	0	0	0
			3012	1937	521	551	3			
1	I	386	Total	C	N	O	S	0	0	0
			3012	1937	521	551	3			

- Molecule 2 is a protein called peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	19	Total	C	N	O	0	0	0
			94	57	19	18			
2	H	16	Total	C	N	O	0	0	0
			79	48	16	15			

- Molecule 3 is a protein called PmoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	242	Total	C	N	O	S	0	0	0
			1964	1326	312	313	13			
3	B	242	Total	C	N	O	S	0	0	0
			1964	1326	312	313	13			
3	F	242	Total	C	N	O	S	0	0	0
			1964	1326	312	313	13			

- Molecule 4 is a protein called PmoC.

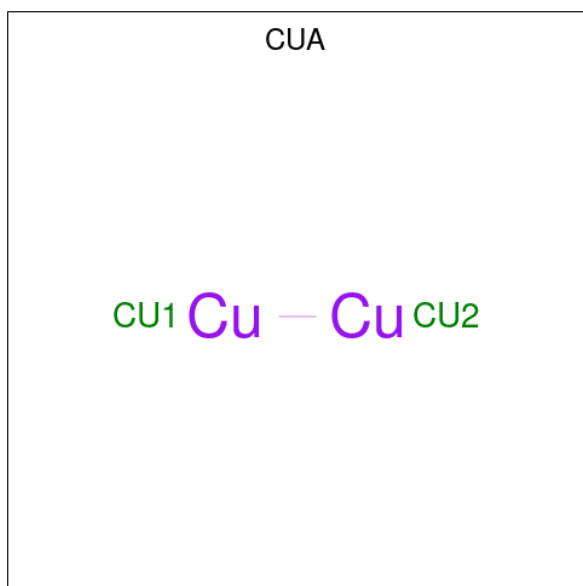
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	210	Total	C	N	O	S	0	0	0
			1695	1137	271	280	7			
4	G	211	Total	C	N	O	S	0	0	0
			1706	1146	272	281	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	211	Total	C	N	O	S	0	0	0
			1706	1146	272	281	7			

- Molecule 5 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cu	0	0
			2	2		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	C	2	Total	Zn	0	0
			2	2		
6	G	2	Total	Zn	0	0
			2	2		
6	K	2	Total	Zn	0	0
			2	2		
6	E	1	Total	Zn	0	0
			1	1		
6	I	1	Total	Zn	0	0
			1	1		

- Molecule 7 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total 1	Cu 1	0	0
7	I	1	Total 1	Cu 1	0	0

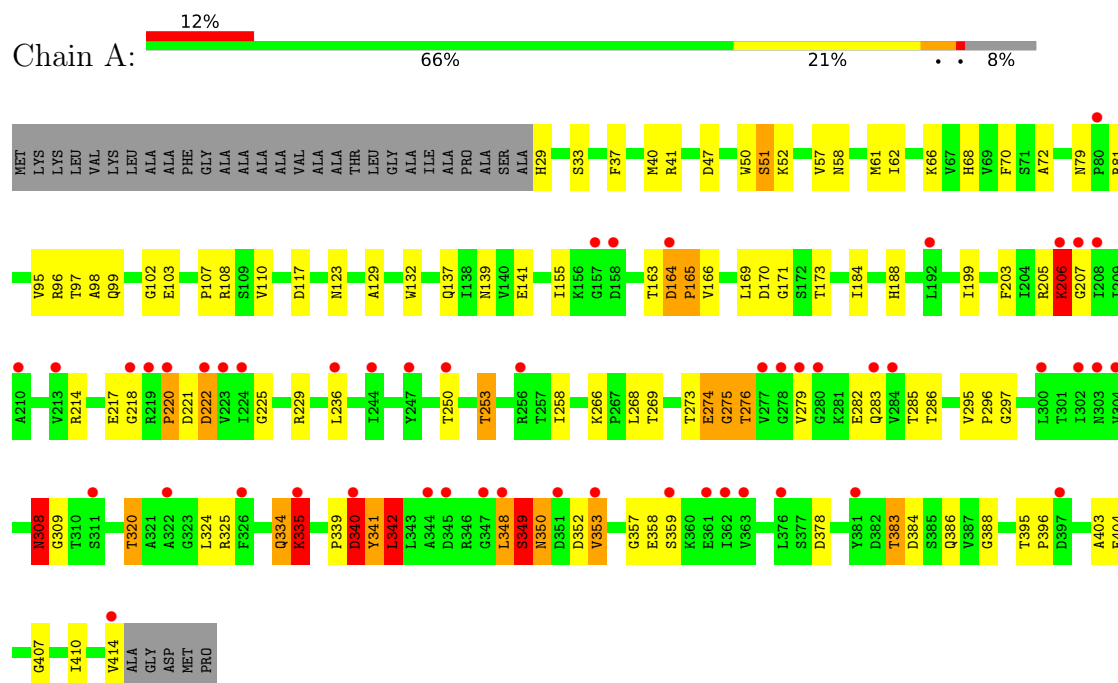
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total 1	O 1	0	0
8	G	1	Total 1	O 1	0	0
8	K	1	Total 1	O 1	0	0

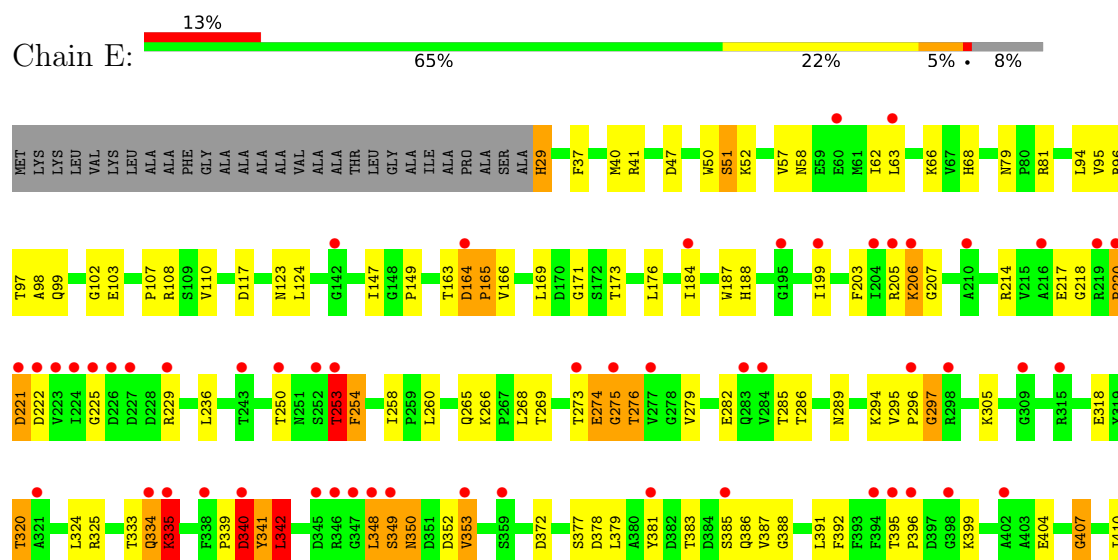
3 Residue-property plots [i](#)

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: PmoB

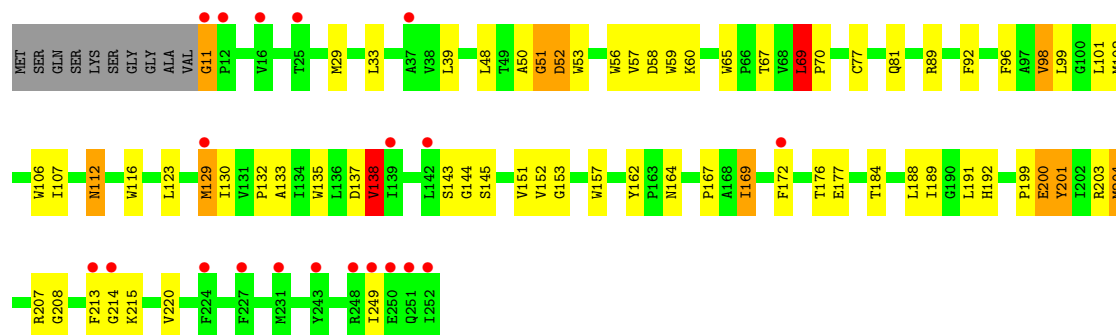


• Molecule 1: PmoB

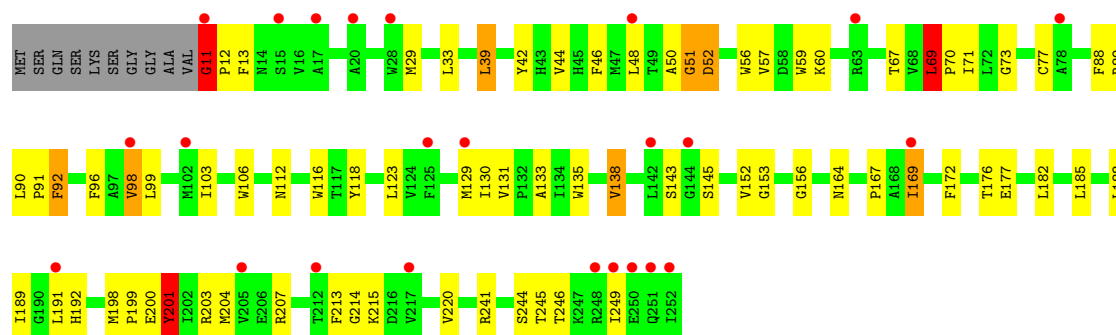




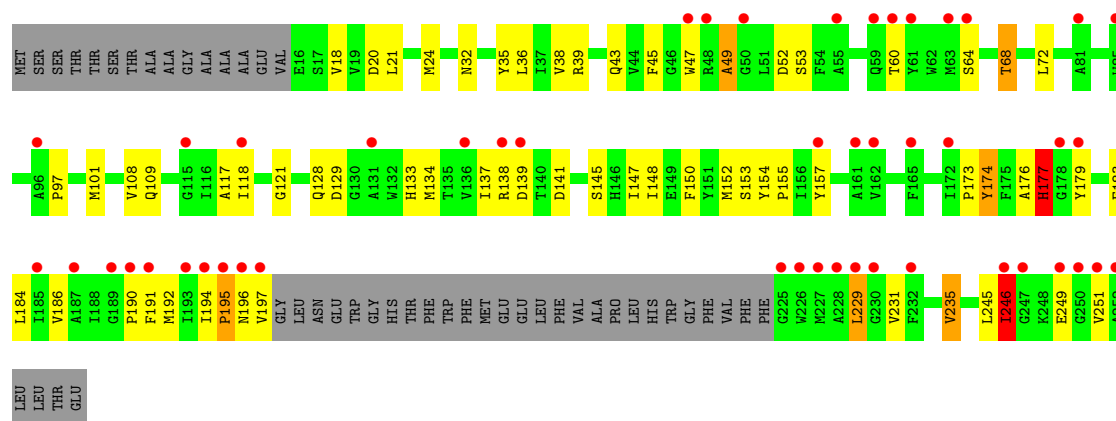
• Molecule 3: PmoA



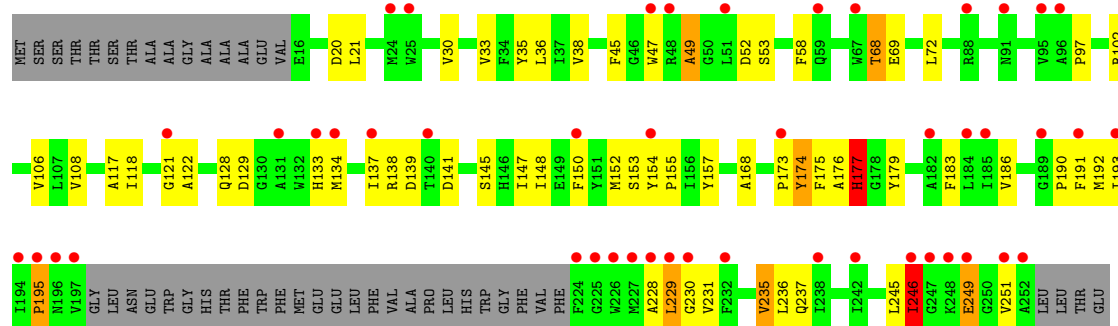
• Molecule 3: PmoA



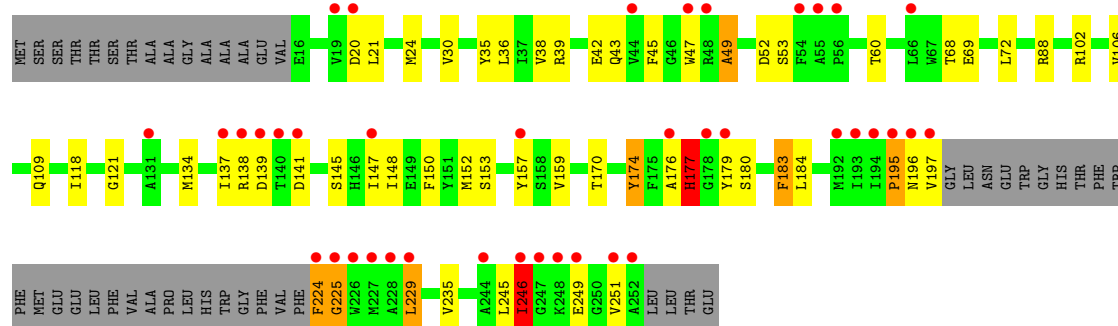
• Molecule 4: PmoC



• Molecule 4: PmoC



• Molecule 4: PmoC



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.72Å 178.31Å 183.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.79 – 2.68 45.79 – 2.68	Depositor EDS
% Data completeness (in resolution range)	88.9 (45.79-2.68) 88.9 (45.79-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.249 , 0.281 0.250 , 0.280	Depositor DCC
R_{free} test set	4440 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20224	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, CUA, ZN

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	0.86	0/3087	1.10	13/4205 (0.3%)
1	E	0.90	2/3087 (0.1%)	1.12	14/4205 (0.3%)
1	I	1.25	8/3087 (0.3%)	1.27	16/4205 (0.4%)
2	D	1.40	1/93 (1.1%)	1.27	0/129
2	H	1.23	0/78	1.49	0/108
3	B	0.94	1/2041 (0.0%)	1.13	10/2795 (0.4%)
3	F	1.01	1/2041 (0.0%)	1.19	7/2795 (0.3%)
3	J	1.08	3/2041 (0.1%)	1.21	11/2795 (0.4%)
4	C	0.87	0/1749	1.05	2/2386 (0.1%)
4	G	0.81	0/1761	1.04	3/2402 (0.1%)
4	K	0.85	1/1761 (0.1%)	1.02	1/2402 (0.0%)
All	All	0.98	17/20826 (0.1%)	1.14	77/28427 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	E	0	3
1	I	0	4
3	B	0	3
3	F	0	3
3	J	0	2
4	G	0	1
4	K	0	1
All	All	0	21

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	387	VAL	CA-CB	7.01	1.64	1.54
1	E	254	PHE	N-CA	6.67	1.51	1.46
1	I	314	VAL	CA-CB	6.52	1.63	1.54
1	I	148	GLY	N-CA	6.27	1.53	1.44
3	J	152	VAL	CA-CB	6.11	1.62	1.54
2	D	5	ALA	CA-CB	6.05	1.60	1.52
1	I	310	THR	CA-CB	5.99	1.62	1.53
3	F	69	LEU	N-CA	-5.76	1.41	1.46
3	B	138	VAL	CA-CB	5.73	1.62	1.54
1	I	84	PHE	CA-C	5.41	1.58	1.52
1	I	139	ASN	CA-C	-5.38	1.46	1.52
4	K	159	VAL	CA-CB	5.30	1.59	1.54
1	E	254	PHE	CA-CB	5.28	1.56	1.52
3	J	120	PRO	CA-C	5.24	1.58	1.52
1	I	120	PHE	C-O	5.23	1.30	1.23
1	I	86	ASN	C-O	5.06	1.29	1.23
3	J	124	VAL	CA-CB	5.03	1.61	1.54

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	11	GLY	CA-C-N	12.54	135.51	119.84
3	F	11	GLY	C-N-CA	12.54	135.51	119.84
1	A	253	THR	N-CA-C	-8.61	99.16	110.53
3	J	162	TYR	CA-C-N	-7.79	110.71	119.28
3	J	162	TYR	C-N-CA	-7.79	110.71	119.28
1	E	341	TYR	CA-C-N	7.70	135.56	121.70
1	E	341	TYR	C-N-CA	7.70	135.56	121.70
1	A	341	TYR	CA-C-N	7.64	135.45	121.70
1	A	341	TYR	C-N-CA	7.64	135.45	121.70
3	J	249	ILE	N-CA-C	7.49	120.87	113.53
3	B	249	ILE	N-CA-C	7.47	120.85	113.53
1	I	341	TYR	CA-C-N	7.00	134.31	121.70
1	I	341	TYR	C-N-CA	7.00	134.31	121.70
3	B	162	TYR	CA-C-N	-6.90	112.52	119.56
3	B	162	TYR	C-N-CA	-6.90	112.52	119.56
1	E	407	GLY	CA-C-N	6.82	126.78	119.76
1	E	407	GLY	C-N-CA	6.82	126.78	119.76
1	E	399	LYS	N-CA-C	6.74	120.62	110.64
3	F	249	ILE	N-CA-C	6.74	120.28	113.47
3	J	237	TRP	N-CA-C	-6.65	103.95	111.07
1	A	141	GLU	N-CA-C	6.58	118.14	110.97
1	A	269	THR	CA-C-N	-6.55	114.04	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	THR	C-N-CA	-6.55	114.04	120.52
4	G	186	VAL	N-CA-C	6.51	116.67	110.42
4	K	225	GLY	N-CA-C	6.26	128.03	113.18
1	E	253	THR	N-CA-C	-6.20	102.34	110.53
1	I	86	ASN	N-CA-C	6.20	117.96	108.42
1	I	141	GLU	N-CA-C	6.16	118.53	111.02
1	I	341	TYR	N-CA-CB	6.14	119.09	110.98
1	I	226	ASP	N-CA-C	-6.09	101.53	110.42
1	I	181	ILE	N-CA-C	6.01	116.75	110.62
3	J	118	TYR	N-CA-C	6.00	120.19	112.86
1	A	308	ASN	CA-C-N	5.99	133.14	121.41
1	A	308	ASN	C-N-CA	5.99	133.14	121.41
1	E	269	THR	CA-C-N	-5.95	114.48	120.31
1	E	269	THR	C-N-CA	-5.95	114.48	120.31
4	C	186	VAL	N-CA-C	5.90	116.08	110.42
3	J	51	GLY	CA-C-N	5.87	132.26	121.70
3	J	51	GLY	C-N-CA	5.87	132.26	121.70
1	E	342	LEU	N-CA-C	5.80	127.23	111.00
1	E	253	THR	CA-C-N	-5.71	116.66	122.83
1	E	253	THR	C-N-CA	-5.71	116.66	122.83
1	A	342	LEU	N-CA-C	5.71	126.98	111.00
3	B	107	ILE	N-CA-C	-5.69	104.82	110.62
4	G	230	GLY	N-CA-C	-5.66	106.73	115.73
1	E	275	GLY	CA-C-N	5.61	131.81	121.70
1	E	275	GLY	C-N-CA	5.61	131.81	121.70
3	B	129	MET	N-CA-C	5.49	122.36	114.39
1	I	324	LEU	N-CA-C	5.49	117.98	110.24
4	G	249	GLU	N-CA-C	5.48	118.77	112.57
3	B	69	LEU	CA-CB-CG	-5.45	97.23	116.30
3	F	245	THR	N-CA-C	5.44	117.91	110.24
1	E	341	TYR	N-CA-CB	5.44	119.09	111.15
1	I	413	PHE	N-CA-C	5.36	118.21	110.28
1	A	341	TYR	N-CA-CB	5.34	118.94	111.15
1	I	338	PHE	CA-C-N	5.31	126.48	119.84
1	I	338	PHE	C-N-CA	5.31	126.48	119.84
3	J	202	ILE	N-CA-C	-5.29	105.88	113.07
3	B	112	ASN	N-CA-C	5.28	119.05	111.02
3	F	69	LEU	CA-CB-CG	-5.26	97.87	116.30
1	I	399	LYS	N-CA-C	5.24	118.07	110.42
3	B	11	GLY	CA-C-N	5.24	126.39	119.84
3	B	11	GLY	C-N-CA	5.24	126.39	119.84
3	J	214	GLY	N-CA-C	-5.24	103.93	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	275	GLY	CA-C-N	5.22	131.09	121.70
1	I	275	GLY	C-N-CA	5.22	131.09	121.70
3	F	71	ILE	CB-CA-C	-5.21	105.10	112.14
1	I	73	TRP	CA-C-N	5.21	125.50	119.92
1	I	73	TRP	C-N-CA	5.21	125.50	119.92
3	F	118	TYR	N-CA-C	5.21	118.91	112.24
3	J	69	LEU	CA-CB-CG	-5.13	98.34	116.30
1	A	275	GLY	CA-C-N	5.09	130.86	121.70
1	A	275	GLY	C-N-CA	5.09	130.86	121.70
4	C	32	ASN	N-CA-C	5.07	116.88	111.36
3	B	189	ILE	N-CA-C	-5.06	105.61	110.72
1	A	222	ASP	N-CA-C	-5.04	107.09	113.18
3	J	165	ASN	N-CA-C	-5.03	107.81	114.04

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	LYS	Peptide
1	A	308	ASN	Peptide
1	A	335	LYS	Peptide
1	A	340	ASP	Peptide
3	B	11	GLY	Peptide
3	B	50	ALA	Peptide
3	B	51	GLY	Peptide
1	E	206	LYS	Peptide
1	E	335	LYS	Peptide
1	E	340	ASP	Peptide
3	F	11	GLY	Peptide
3	F	50	ALA	Peptide
3	F	51	GLY	Peptide
4	G	228	ALA	Peptide
1	I	206	LYS	Peptide
1	I	335	LYS	Peptide
1	I	340	ASP	Peptide
1	I	341	TYR	Peptide
3	J	50	ALA	Peptide
3	J	51	GLY	Peptide
4	K	224	PHE	Peptide

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	3012	0	3009	98	0
1	E	3012	0	3009	100	0
1	I	3012	0	3009	139	0
2	D	94	0	97	2	0
2	H	79	0	79	2	0
3	B	1964	0	1924	60	0
3	F	1964	0	1924	67	0
3	J	1964	0	1924	64	0
4	C	1695	0	1692	41	0
4	G	1706	0	1701	42	0
4	K	1706	0	1701	42	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
6	C	2	0	0	0	0
6	E	1	0	0	0	0
6	G	2	0	0	0	0
6	I	1	0	0	0	0
6	K	2	0	0	0	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0
8	C	1	0	0	0	0
8	G	1	0	0	0	0
8	K	1	0	0	0	0
All	All	20224	0	20069	576	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 14.

All (576) 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)
3:J:116:TRP:O	4:K:47:TRP:HH2	1.31	1.13
1:I:275:GLY:HA3	1:I:276:THR:HG22	1.29	1.11
3:F:11:GLY:HA3	3:F:13:PHE:H	1.02	1.10
1:A:340:ASP:HB3	1:A:341:TYR:HB3	1.33	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:51:GLY:HA3	3:B:52:ASP:HB2	1.28	1.08
1:A:274:GLU:H	1:A:275:GLY:CA	1.66	1.08
1:A:275:GLY:HA3	1:A:276:THR:HG22	1.28	1.08
1:E:340:ASP:HB3	1:E:341:TYR:HB3	1.28	1.07
3:J:116:TRP:O	4:K:47:TRP:CH2	2.08	1.07
3:J:51:GLY:HA3	3:J:52:ASP:HB2	1.36	1.06
1:E:274:GLU:H	1:E:275:GLY:CA	1.67	1.06
3:B:116:TRP:O	4:C:47:TRP:HH2	1.38	1.06
4:K:245:LEU:O	4:K:246:ILE:HG13	1.54	1.05
3:F:51:GLY:HA3	3:F:52:ASP:HB2	1.36	1.05
3:B:116:TRP:O	4:C:47:TRP:CH2	2.12	1.02
1:A:348:LEU:HB2	1:A:349:SER:HB3	1.44	1.00
1:I:274:GLU:H	1:I:275:GLY:CA	1.74	0.99
1:A:274:GLU:H	1:A:275:GLY:HA3	1.30	0.97
4:C:245:LEU:O	4:C:246:ILE:HG13	1.64	0.97
4:K:121:GLY:HA2	4:K:153:SER:OG	1.63	0.97
1:I:340:ASP:HB3	1:I:341:TYR:HB3	1.46	0.96
4:K:245:LEU:C	4:K:246:ILE:HG13	1.89	0.96
4:G:245:LEU:O	4:G:246:ILE:HG13	1.65	0.95
4:G:245:LEU:C	4:G:246:ILE:HG13	1.90	0.94
1:A:275:GLY:HA3	1:A:276:THR:CG2	1.95	0.94
1:I:96:ARG:HH21	1:I:99:GLN:HE22	1.02	0.93
1:I:58:ASN:HD21	1:I:163:THR:H	1.16	0.92
1:I:275:GLY:HA3	1:I:276:THR:CG2	2.00	0.91
1:I:274:GLU:H	1:I:275:GLY:HA3	1.34	0.91
3:F:116:TRP:O	4:G:47:TRP:HH2	1.54	0.89
2:D:3:ALA:HA	2:D:6:ALA:HB3	1.55	0.89
3:F:11:GLY:HA3	3:F:13:PHE:N	1.87	0.88
3:F:116:TRP:O	4:G:47:TRP:CH2	2.27	0.88
4:C:121:GLY:HA2	4:C:153:SER:OG	1.73	0.88
1:E:340:ASP:HB3	1:E:341:TYR:CB	2.02	0.88
4:C:245:LEU:C	4:C:246:ILE:HG13	1.95	0.87
1:I:164:ASP:CB	1:I:165:PRO:HA	2.02	0.87
3:F:11:GLY:CA	3:F:13:PHE:H	1.88	0.87
1:I:137:GLN:HE21	1:I:139:ASN:HD21	1.23	0.86
1:A:340:ASP:HB3	1:A:341:TYR:CB	2.07	0.85
1:I:205:ARG:O	1:I:206:LYS:HB2	1.77	0.84
1:E:274:GLU:H	1:E:275:GLY:HA3	1.42	0.83
1:I:348:LEU:HB2	1:I:349:SER:HB3	1.61	0.81
4:K:245:LEU:O	4:K:246:ILE:CG1	2.30	0.80
1:A:164:ASP:CB	1:A:165:PRO:HA	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:143:SER:O	3:J:145:SER:N	2.14	0.80
3:B:51:GLY:CA	3:B:52:ASP:HB2	2.12	0.80
3:J:214:GLY:HA2	3:J:215:LYS:HB2	1.62	0.79
1:E:68:HIS:HE1	1:E:404:GLU:OE1	1.66	0.79
1:A:58:ASN:HD21	1:A:163:THR:H	1.30	0.79
1:I:96:ARG:HH21	1:I:99:GLN:NE2	1.80	0.79
3:F:214:GLY:HA2	3:F:215:LYS:HB2	1.65	0.78
1:E:58:ASN:HD21	1:E:163:THR:H	1.30	0.78
3:B:200:GLU:O	3:B:201:TYR:HB3	1.83	0.77
4:G:245:LEU:O	4:G:246:ILE:CG1	2.32	0.77
4:G:53:SER:OG	4:G:139:ASP:HB2	1.84	0.77
1:I:68:HIS:HE1	1:I:404:GLU:OE1	1.67	0.76
1:I:164:ASP:HB2	1:I:165:PRO:HA	1.67	0.76
1:A:164:ASP:HB2	1:A:165:PRO:HA	1.68	0.76
1:E:274:GLU:N	1:E:275:GLY:CA	2.47	0.76
1:I:225:GLY:HA2	1:I:229:ARG:NH2	2.00	0.76
1:E:164:ASP:CB	1:E:165:PRO:HA	2.16	0.75
3:B:98:VAL:HG21	3:B:133:ALA:HB2	1.66	0.75
1:E:274:GLU:H	1:E:275:GLY:HA2	1.48	0.75
1:A:98:ALA:HB3	1:A:123:ASN:HD22	1.52	0.75
1:I:220:PRO:O	1:I:222:ASP:N	2.16	0.75
3:J:106:TRP:HE1	1:I:188:HIS:CD2	2.04	0.75
1:E:340:ASP:CB	1:E:341:TYR:HB3	2.15	0.75
2:H:8:ALA:HB1	4:G:68:THR:HG21	1.68	0.74
3:J:98:VAL:HG21	3:J:133:ALA:HB2	1.67	0.74
4:C:53:SER:OG	4:C:139:ASP:HB2	1.85	0.74
1:E:275:GLY:HA3	1:E:276:THR:HG22	1.68	0.74
1:A:348:LEU:CB	1:A:349:SER:HB3	2.18	0.73
1:E:334:GLN:HA	1:E:335:LYS:HB2	1.71	0.73
3:J:177:GLU:HG3	1:E:410:ILE:HG12	1.69	0.73
3:B:214:GLY:HA2	3:B:215:LYS:HB2	1.70	0.73
1:A:220:PRO:O	1:A:222:ASP:N	2.15	0.73
1:I:70:PHE:HE1	1:I:72:ALA:HB3	1.53	0.72
3:B:143:SER:O	3:B:145:SER:N	2.21	0.72
1:E:348:LEU:HB2	1:E:349:SER:HB3	1.72	0.72
3:B:60:LYS:HD2	3:B:169:ILE:HD11	1.70	0.72
4:K:52:ASP:HB2	1:I:29:HIS:HD2	1.55	0.72
4:C:245:LEU:O	4:C:246:ILE:CG1	2.39	0.71
1:I:334:GLN:HA	1:I:335:LYS:HB2	1.71	0.71
1:E:220:PRO:O	1:E:222:ASP:N	2.20	0.71
3:J:203:ARG:O	3:J:204:MET:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:HIS:CD2	3:B:106:TRP:HE1	2.08	0.70
3:J:184:THR:HG22	1:I:258:ILE:HG13	1.74	0.70
1:I:68:HIS:HD2	1:I:117:ASP:OD1	1.75	0.69
3:F:200:GLU:O	3:F:201:TYR:HB3	1.92	0.69
1:E:164:ASP:HB2	1:E:165:PRO:HA	1.73	0.69
3:J:51:GLY:CA	3:J:52:ASP:HB2	2.19	0.69
3:B:98:VAL:HG22	3:B:129:MET:HE2	1.75	0.69
1:I:164:ASP:CB	1:I:165:PRO:CA	2.71	0.68
1:E:50:TRP:O	1:E:52:LYS:N	2.26	0.68
1:E:98:ALA:HB3	1:E:123:ASN:HD22	1.59	0.68
3:B:143:SER:C	3:B:145:SER:H	2.01	0.68
1:E:275:GLY:HA3	1:E:276:THR:CG2	2.23	0.68
1:E:40:MET:HE2	1:E:388:GLY:H	1.59	0.68
1:A:334:GLN:HA	1:A:335:LYS:HB2	1.76	0.67
3:F:60:LYS:HD2	3:F:169:ILE:HD11	1.76	0.67
1:I:68:HIS:CD2	1:I:117:ASP:OD1	2.48	0.67
4:G:121:GLY:HA2	4:G:153:SER:OG	1.95	0.67
4:K:45:PHE:O	4:K:49:ALA:HB3	1.94	0.67
3:B:203:ARG:O	3:B:204:MET:HB2	1.94	0.67
1:I:220:PRO:C	1:I:222:ASP:H	2.03	0.67
1:I:96:ARG:NH2	1:I:99:GLN:HE22	1.86	0.66
1:I:276:THR:HG23	1:I:279:VAL:HB	1.77	0.66
1:I:70:PHE:CE1	1:I:72:ALA:HB3	2.30	0.66
1:I:225:GLY:HA2	1:I:229:ARG:HH21	1.58	0.66
1:A:220:PRO:C	1:A:222:ASP:H	2.02	0.66
1:A:68:HIS:HD2	1:A:117:ASP:OD1	1.79	0.66
1:I:386:GLN:HG3	1:I:407:GLY:C	2.21	0.66
1:A:340:ASP:CB	1:A:341:TYR:HB3	2.18	0.65
4:K:53:SER:OG	4:K:139:ASP:HB2	1.96	0.65
1:A:274:GLU:N	1:A:275:GLY:CA	2.48	0.65
1:A:274:GLU:H	1:A:275:GLY:HA2	1.60	0.65
3:J:214:GLY:CA	3:J:215:LYS:HB2	2.27	0.65
3:J:143:SER:C	3:J:145:SER:H	2.05	0.64
1:A:29:HIS:HD2	4:C:52:ASP:HB2	1.62	0.64
1:A:96:ARG:HH21	1:A:99:GLN:HE22	1.45	0.64
4:K:52:ASP:HB2	1:I:29:HIS:CD2	2.31	0.64
1:A:68:HIS:HE1	1:A:404:GLU:OE1	1.81	0.64
3:B:213:PHE:HA	1:I:33:SER:O	1.98	0.64
3:J:98:VAL:HG22	3:J:129:MET:HE2	1.79	0.64
4:C:246:ILE:HB	4:C:249:GLU:HG2	1.78	0.64
3:J:59:TRP:CZ3	3:J:203:ARG:O	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:45:PHE:O	4:G:49:ALA:HB3	1.98	0.63
1:A:275:GLY:HA3	1:A:276:THR:CB	2.28	0.63
1:A:352:ASP:O	1:A:353:VAL:C	2.41	0.63
3:F:214:GLY:CA	3:F:215:LYS:HB2	2.29	0.63
1:I:164:ASP:OD2	1:I:176:LEU:HB2	1.99	0.63
1:I:250:THR:O	1:I:253:THR:O	2.17	0.63
1:A:410:ILE:HG12	3:F:177:GLU:HG3	1.79	0.62
4:G:246:ILE:HB	4:G:249:GLU:HG2	1.79	0.62
4:G:35:TYR:HE1	4:G:152:MET:HE3	1.65	0.62
1:A:274:GLU:N	1:A:275:GLY:HA3	2.11	0.62
1:A:276:THR:HG23	1:A:279:VAL:HB	1.80	0.62
3:F:98:VAL:HG21	3:F:133:ALA:HB2	1.81	0.62
1:I:110:VAL:HB	1:I:268:LEU:HD11	1.81	0.62
3:J:138:VAL:HG21	1:I:236:LEU:HB2	1.80	0.62
4:K:246:ILE:HB	4:K:249:GLU:HG2	1.81	0.62
1:E:274:GLU:N	1:E:275:GLY:HA3	2.13	0.62
1:E:275:GLY:HA3	1:E:276:THR:CB	2.30	0.62
1:E:225:GLY:HA2	1:E:229:ARG:NH2	2.15	0.61
3:F:106:TRP:HE1	1:E:188:HIS:CD2	2.18	0.61
1:A:236:LEU:HB2	3:B:138:VAL:HG21	1.83	0.61
3:B:214:GLY:CA	3:B:215:LYS:HB2	2.31	0.61
3:F:46:PHE:HZ	3:F:69:LEU:HD11	1.65	0.61
3:F:51:GLY:CA	3:F:52:ASP:HB2	2.22	0.61
3:F:138:VAL:HG21	1:E:236:LEU:HB2	1.82	0.61
1:A:225:GLY:HA2	1:A:229:ARG:NH2	2.15	0.61
1:A:283:GLN:O	1:A:309:GLY:HA3	2.00	0.61
1:E:352:ASP:O	1:E:353:VAL:C	2.43	0.61
4:C:150:PHE:CZ	4:C:195:PRO:HG3	2.36	0.61
3:F:69:LEU:HB3	3:F:70:PRO:HD3	1.81	0.61
4:G:150:PHE:CZ	4:G:195:PRO:HG3	2.36	0.61
1:I:348:LEU:CA	1:I:349:SER:HB3	2.31	0.60
1:A:348:LEU:CA	1:A:349:SER:HB3	2.30	0.60
3:B:69:LEU:HB3	3:B:70:PRO:HD3	1.82	0.60
1:E:205:ARG:O	1:E:206:LYS:HB2	2.01	0.60
1:I:164:ASP:HB3	1:I:165:PRO:HA	1.81	0.60
1:I:48:VAL:HG21	1:I:149:PRO:HG2	1.83	0.60
1:I:50:TRP:O	1:I:52:LYS:N	2.35	0.60
4:K:20:ASP:O	4:K:21:LEU:HB2	2.02	0.60
1:E:214:ARG:NH1	1:E:222:ASP:O	2.34	0.60
1:I:164:ASP:HB3	1:I:165:PRO:CA	2.31	0.60
3:B:207:ARG:HD3	1:I:75:GLN:NE2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:348:LEU:HB2	1:E:349:SER:CB	2.30	0.60
1:I:170:ASP:OD1	1:I:170:ASP:C	2.44	0.60
4:G:138:ARG:NH1	4:G:141:ASP:HA	2.17	0.60
1:I:320:THR:HG22	1:I:324:LEU:O	2.01	0.60
3:J:203:ARG:O	3:J:204:MET:CB	2.50	0.60
1:I:348:LEU:CB	1:I:349:SER:HB3	2.31	0.60
3:F:98:VAL:HG22	3:F:129:MET:HE2	1.84	0.59
1:A:205:ARG:O	1:A:206:LYS:HB2	2.01	0.59
1:A:275:GLY:CA	1:A:276:THR:HG22	2.20	0.59
4:K:69:GLU:OE1	4:K:152:MET:HB2	2.02	0.59
3:F:143:SER:C	3:F:145:SER:H	2.09	0.59
4:C:45:PHE:O	4:C:49:ALA:HB3	2.02	0.59
1:I:340:ASP:HB3	1:I:341:TYR:CB	2.27	0.59
4:K:121:GLY:HA2	4:K:153:SER:HG	1.65	0.59
1:I:207:GLY:O	1:I:211:SER:HB2	2.03	0.59
1:A:164:ASP:CB	1:A:165:PRO:CA	2.80	0.59
3:J:172:PHE:CE2	1:I:184:ILE:HD11	2.37	0.59
3:B:59:TRP:CZ3	3:B:203:ARG:O	2.55	0.59
4:K:150:PHE:CZ	4:K:195:PRO:HG3	2.38	0.59
3:J:176:THR:HG21	3:J:188:LEU:HD22	1.84	0.59
3:F:191:LEU:HD13	1:E:107:PRO:HA	1.85	0.59
1:I:214:ARG:NH1	1:I:222:ASP:O	2.36	0.59
1:E:275:GLY:CA	1:E:276:THR:HB	2.31	0.59
1:E:275:GLY:HA3	1:E:276:THR:HB	1.84	0.59
1:I:349:SER:OG	1:I:350:ASN:N	2.36	0.59
4:G:52:ASP:HB2	1:E:29:HIS:HD2	1.67	0.58
3:B:215:LYS:HA	1:I:381:TYR:CZ	2.39	0.58
3:J:200:GLU:O	3:J:201:TYR:HB3	2.03	0.58
1:I:102:GLY:HA3	1:I:268:LEU:HD22	1.85	0.58
4:K:137:ILE:HD13	1:I:147:ILE:CD1	2.34	0.58
1:E:320:THR:HG22	1:E:324:LEU:O	2.04	0.57
1:I:219:ARG:HB3	1:I:221:ASP:OD1	2.05	0.57
4:C:138:ARG:NH1	4:C:141:ASP:HA	2.19	0.57
1:I:96:ARG:CD	1:I:99:GLN:NE2	2.68	0.57
1:I:352:ASP:O	1:I:353:VAL:C	2.46	0.57
3:F:203:ARG:O	3:F:204:MET:HB2	2.04	0.57
4:G:148:ILE:HG23	4:G:152:MET:HE2	1.86	0.57
4:G:176:ALA:O	4:G:177:HIS:CD2	2.58	0.57
1:A:47:ASP:OD2	1:A:66:LYS:NZ	2.36	0.57
1:E:386:GLN:HG3	1:E:407:GLY:C	2.29	0.56
3:F:167:PRO:HA	1:E:250:THR:HG21	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:HIS:HD2	1:E:117:ASP:OD1	1.88	0.56
1:I:68:HIS:CE1	1:I:404:GLU:OE1	2.54	0.56
1:A:214:ARG:NH1	1:A:222:ASP:O	2.39	0.56
3:J:29:MET:HE1	4:K:109:GLN:HG3	1.87	0.56
1:E:395:THR:OG1	1:E:396:PRO:HD2	2.05	0.56
1:A:68:HIS:CD2	1:A:117:ASP:OD1	2.57	0.56
4:K:176:ALA:O	4:K:177:HIS:CD2	2.59	0.56
3:B:208:GLY:O	1:I:76:ALA:HB1	2.06	0.56
1:I:51:SER:HB3	1:I:62:ILE:O	2.05	0.55
3:J:98:VAL:HG12	3:J:99:LEU:N	2.20	0.55
3:B:203:ARG:O	3:B:204:MET:CB	2.53	0.55
1:I:203:PHE:O	1:I:207:GLY:HA2	2.07	0.55
1:A:349:SER:OG	1:A:350:ASN:N	2.39	0.54
3:J:201:TYR:CD1	3:J:201:TYR:C	2.85	0.54
1:A:220:PRO:HB3	3:B:89:ARG:HG3	1.89	0.54
3:F:46:PHE:CZ	3:F:69:LEU:HD11	2.41	0.54
3:F:96:PHE:HA	1:E:199:ILE:HD11	1.88	0.54
1:A:386:GLN:HG3	1:A:407:GLY:C	2.32	0.54
1:E:164:ASP:CB	1:E:165:PRO:CA	2.84	0.54
1:I:274:GLU:N	1:I:275:GLY:CA	2.55	0.54
3:F:89:ARG:HG3	1:E:220:PRO:HB3	1.89	0.54
1:I:275:GLY:HA3	1:I:276:THR:CB	2.38	0.54
4:K:24:MET:HB2	4:K:109:GLN:HG2	1.90	0.54
1:I:58:ASN:HD22	1:I:125:ARG:HH21	1.56	0.54
1:I:367:GLN:O	1:I:368:ASP:HB2	2.07	0.54
3:J:57:VAL:HG12	3:J:123:LEU:HD12	1.90	0.54
1:I:358:GLU:HG2	1:I:359:SER:N	2.23	0.54
1:A:70:PHE:HE1	1:A:72:ALA:HB3	1.73	0.53
3:F:57:VAL:HG12	3:F:123:LEU:HD12	1.90	0.53
3:B:200:GLU:O	3:B:201:TYR:CB	2.55	0.53
1:I:79:ASN:C	1:I:81:ARG:H	2.14	0.53
1:I:334:GLN:HA	1:I:335:LYS:CB	2.37	0.53
1:A:102:GLY:HA3	1:A:268:LEU:HD22	1.89	0.53
3:F:200:GLU:HG2	3:F:203:ARG:HH11	1.73	0.53
1:A:395:THR:OG1	1:A:396:PRO:HD2	2.09	0.53
1:E:220:PRO:C	1:E:222:ASP:H	2.13	0.53
1:E:110:VAL:HB	1:E:268:LEU:HD11	1.90	0.53
3:B:57:VAL:HG12	3:B:123:LEU:HD12	1.91	0.53
3:B:201:TYR:CD1	3:B:201:TYR:C	2.86	0.53
1:E:320:THR:CG2	1:E:325:ARG:HG2	2.39	0.53
3:F:135:TRP:NE1	3:F:156:GLY:HA3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:92:PHE:O	3:J:96:PHE:HB2	2.09	0.52
4:K:180:SER:HB3	4:K:183:PHE:HB2	1.92	0.52
1:I:82:VAL:HG11	1:I:141:GLU:OE1	2.08	0.52
1:I:286:THR:HG21	1:I:391:LEU:HD12	1.91	0.52
3:F:42:TYR:OH	3:F:73:GLY:O	2.25	0.52
1:I:358:GLU:HG2	1:I:359:SER:H	1.73	0.52
1:A:275:GLY:CA	1:A:276:THR:CB	2.87	0.52
3:J:101:LEU:HD23	3:J:129:MET:HE1	1.90	0.52
3:B:132:PRO:HB2	3:B:157:TRP:CE3	2.45	0.52
1:I:273:THR:HB	1:I:274:GLU:HB2	1.91	0.52
1:E:340:ASP:HB3	1:E:341:TYR:CA	2.38	0.52
1:I:348:LEU:HA	1:I:349:SER:HB3	1.92	0.52
1:I:395:THR:HG22	1:I:399:LYS:O	2.10	0.52
1:E:318:GLU:HB3	1:E:392:PHE:HB2	1.91	0.52
1:A:50:TRP:O	1:A:52:LYS:N	2.43	0.51
2:D:2:ALA:O	2:D:6:ALA:HB2	2.11	0.51
4:K:148:ILE:HG23	4:K:152:MET:HE2	1.92	0.51
1:A:250:THR:HG21	3:B:167:PRO:HA	1.93	0.51
3:J:69:LEU:HB3	3:J:70:PRO:HD3	1.92	0.51
3:F:204:MET:H	3:F:207:ARG:HH12	1.59	0.51
1:E:276:THR:HG23	1:E:279:VAL:HB	1.92	0.51
3:F:77:CYS:SG	3:F:98:VAL:HG23	2.50	0.51
4:G:246:ILE:HG21	4:G:249:GLU:OE2	2.11	0.51
3:J:89:ARG:HG3	1:I:220:PRO:HB3	1.91	0.51
1:A:40:MET:HE2	1:A:388:GLY:H	1.74	0.51
1:A:203:PHE:O	1:A:207:GLY:HA2	2.10	0.51
4:C:246:ILE:HG21	4:C:249:GLU:OE2	2.11	0.51
3:F:59:TRP:CZ3	3:F:203:ARG:O	2.64	0.51
3:F:176:THR:HG21	3:F:188:LEU:HD22	1.93	0.51
4:C:173:PRO:O	4:C:174:TYR:CB	2.59	0.51
4:G:102:ARG:O	4:G:106:VAL:HG23	2.10	0.51
1:E:102:GLY:HA3	1:E:268:LEU:HD22	1.92	0.51
1:E:339:PRO:O	1:E:340:ASP:C	2.54	0.50
1:E:37:PHE:O	1:E:41:ARG:HG3	2.12	0.50
1:A:341:TYR:H	1:A:342:LEU:CA	2.24	0.50
3:J:56:TRP:CH2	4:K:134:MET:HG3	2.46	0.50
4:G:53:SER:OG	4:G:139:ASP:CB	2.59	0.50
1:I:96:ARG:HD3	1:I:99:GLN:NE2	2.26	0.50
2:H:13:ALA:O	2:H:17:ALA:HB3	2.11	0.50
3:B:176:THR:HG21	3:B:188:LEU:HD22	1.93	0.50
3:B:204:MET:H	3:B:207:ARG:HH12	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:MET:HE1	1:E:387:VAL:HB	1.93	0.50
1:I:273:THR:CA	1:I:274:GLU:HB2	2.40	0.50
1:A:184:ILE:HD11	3:B:172:PHE:CE2	2.47	0.50
1:E:149:PRO:HB3	1:E:342:LEU:HD21	1.93	0.50
4:C:231:VAL:O	4:C:235:VAL:HG13	2.11	0.50
1:I:274:GLU:H	1:I:275:GLY:HA2	1.70	0.50
1:A:275:GLY:CA	1:A:276:THR:HB	2.41	0.50
1:E:341:TYR:H	1:E:342:LEU:CA	2.25	0.50
4:G:168:ALA:O	4:G:175:PHE:HB2	2.12	0.49
4:K:137:ILE:HD13	1:I:147:ILE:HD11	1.93	0.49
1:E:349:SER:OG	1:E:350:ASN:N	2.45	0.49
1:E:57:VAL:O	1:E:58:ASN:HB2	2.12	0.49
1:A:33:SER:O	3:F:213:PHE:HA	2.12	0.49
1:A:96:ARG:HH21	1:A:99:GLN:NE2	2.09	0.49
1:I:58:ASN:ND2	1:I:163:THR:H	1.97	0.49
1:I:205:ARG:O	1:I:206:LYS:CB	2.52	0.49
3:B:29:MET:HE2	4:C:108:VAL:HG12	1.95	0.49
1:I:96:ARG:HD2	1:I:99:GLN:NE2	2.27	0.49
3:J:184:THR:CG2	1:I:258:ILE:HG13	2.42	0.49
3:F:246:THR:HG22	4:G:237:GLN:HG3	1.93	0.49
1:E:348:LEU:HA	1:E:349:SER:HB2	1.94	0.49
1:I:56:ASN:HA	1:I:156:LYS:O	2.12	0.49
1:I:101:ILE:HG13	1:I:120:PHE:HB3	1.95	0.49
1:A:70:PHE:CE1	1:A:72:ALA:HB3	2.48	0.49
3:J:191:LEU:HD13	1:I:107:PRO:HA	1.95	0.49
3:F:135:TRP:CD1	3:F:153:GLY:O	2.66	0.49
3:F:138:VAL:CG2	1:E:236:LEU:HD22	2.43	0.49
4:G:20:ASP:O	4:G:21:LEU:HB2	2.13	0.49
1:E:334:GLN:HG2	1:E:335:LYS:HB2	1.95	0.49
1:I:338:PHE:HB3	1:I:343:LEU:HD22	1.95	0.49
1:A:79:ASN:C	1:A:81:ARG:H	2.20	0.48
1:A:334:GLN:HA	1:A:335:LYS:CB	2.42	0.48
1:A:340:ASP:HB3	1:A:341:TYR:CA	2.42	0.48
1:E:203:PHE:O	1:E:207:GLY:HA2	2.13	0.48
3:J:102:MET:HG3	3:J:130:ILE:CD1	2.43	0.48
1:E:107:PRO:HD2	1:E:265:GLN:HE22	1.79	0.48
1:I:320:THR:CG2	1:I:325:ARG:HG2	2.43	0.48
4:C:35:TYR:HE1	4:C:152:MET:HE3	1.77	0.48
4:K:35:TYR:HE1	4:K:152:MET:HE3	1.78	0.48
4:K:39:ARG:NH2	4:K:43:GLN:HB2	2.27	0.48
4:C:148:ILE:HG23	4:C:152:MET:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:176:ALA:O	4:C:177:HIS:CD2	2.67	0.48
1:I:334:GLN:HG2	1:I:335:LYS:HB2	1.96	0.48
1:A:108:ARG:NH2	1:I:384:ASP:OD1	2.46	0.48
1:A:320:THR:CG2	1:A:325:ARG:HG2	2.44	0.48
3:F:172:PHE:CZ	1:E:184:ILE:HD11	2.48	0.48
1:I:410:ILE:HG23	1:I:411:PRO:HD2	1.95	0.48
3:F:99:LEU:HG	3:F:103:ILE:HD12	1.95	0.48
4:C:129:ASP:O	4:C:133:HIS:HD2	1.96	0.48
1:A:188:HIS:HD2	3:B:106:TRP:HE1	1.60	0.48
3:J:53:TRP:CE3	3:J:68:VAL:HG21	2.49	0.48
3:F:56:TRP:NE1	3:F:198:MET:HE3	2.29	0.48
4:G:35:TYR:CE1	4:G:152:MET:HE3	2.48	0.48
1:I:58:ASN:HD21	1:I:163:THR:N	1.98	0.48
3:F:203:ARG:O	3:F:204:MET:CB	2.62	0.48
1:I:80:PRO:HA	1:I:140:VAL:HG13	1.96	0.48
3:F:185:LEU:O	3:F:189:ILE:HG13	2.13	0.47
1:A:384:ASP:OD1	1:E:108:ARG:NH2	2.46	0.47
3:J:215:LYS:HA	1:E:381:TYR:CZ	2.49	0.47
3:J:39:LEU:HD11	3:J:104:GLY:HA3	1.97	0.47
4:G:190:PRO:C	4:G:192:MET:H	2.20	0.47
1:I:105:PHE:CE2	1:I:107:PRO:HG3	2.50	0.47
1:A:110:VAL:HB	1:A:268:LEU:HD11	1.97	0.47
3:B:112:ASN:CG	4:C:128:GLN:HE21	2.22	0.47
1:E:275:GLY:CA	1:E:276:THR:CB	2.92	0.47
1:I:40:MET:HE2	1:I:388:GLY:H	1.80	0.47
1:A:258:ILE:HG13	3:B:184:THR:HG22	1.97	0.47
3:B:199:PRO:HB2	3:B:201:TYR:CE2	2.49	0.47
3:F:192:HIS:HD2	1:E:164:ASP:OD2	1.98	0.47
4:K:20:ASP:O	4:K:21:LEU:CB	2.62	0.47
3:F:112:ASN:CG	4:G:128:GLN:HE21	2.23	0.47
3:F:200:GLU:HG2	3:F:203:ARG:NH1	2.30	0.47
3:F:192:HIS:CD2	1:E:164:ASP:OD2	2.68	0.46
3:F:199:PRO:HB2	3:F:201:TYR:CE2	2.50	0.46
3:F:59:TRP:CZ2	3:F:203:ARG:HA	2.51	0.46
3:F:167:PRO:HG2	1:E:187:TRP:CZ2	2.50	0.46
4:C:190:PRO:C	4:C:192:MET:H	2.23	0.46
1:I:55:VAL:O	1:I:155:ILE:HA	2.15	0.46
1:I:56:ASN:O	1:I:57:VAL:C	2.56	0.46
1:A:132:TRP:CD1	1:A:155:ILE:HD12	2.50	0.46
3:J:151:VAL:HG12	3:J:152:VAL:N	2.29	0.46
4:G:173:PRO:O	4:G:174:TYR:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:177:GLU:HG3	1:I:410:ILE:HG12	1.97	0.46
1:I:58:ASN:ND2	1:I:125:ARG:HH21	2.13	0.46
1:A:273:THR:HB	1:A:274:GLU:HB2	1.97	0.46
3:B:98:VAL:HG12	3:B:99:LEU:N	2.29	0.46
1:E:79:ASN:OD1	1:E:81:ARG:HB2	2.16	0.46
1:A:348:LEU:HA	1:A:349:SER:CB	2.45	0.46
4:C:173:PRO:O	4:C:174:TYR:HB2	2.15	0.46
4:K:138:ARG:NH1	4:K:141:ASP:HA	2.31	0.46
3:F:98:VAL:HG12	3:F:99:LEU:N	2.30	0.46
3:F:201:TYR:CD1	3:F:201:TYR:C	2.93	0.46
1:A:137:GLN:HE21	1:A:139:ASN:HD21	1.64	0.46
3:B:135:TRP:CD1	3:B:153:GLY:O	2.69	0.46
4:G:69:GLU:OE1	4:G:152:MET:HB2	2.15	0.46
1:E:334:GLN:HA	1:E:335:LYS:CB	2.38	0.46
4:C:24:MET:HB2	4:C:109:GLN:HG2	1.98	0.45
1:I:275:GLY:CA	1:I:276:THR:CB	2.94	0.45
4:C:20:ASP:O	4:C:21:LEU:HB2	2.15	0.45
4:C:53:SER:OG	4:C:139:ASP:CB	2.60	0.45
1:E:385:SER:H	1:I:261:GLN:HE22	1.63	0.45
3:J:39:LEU:HD22	3:J:100:GLY:HA2	1.97	0.45
3:B:59:TRP:CZ2	3:B:203:ARG:HA	2.51	0.45
1:E:96:ARG:HH21	1:E:99:GLN:HE22	1.63	0.45
3:J:162:TYR:O	3:J:163:PRO:C	2.56	0.45
4:G:53:SER:HA	4:G:58:PHE:CG	2.52	0.45
1:E:94:LEU:HB3	1:E:124:LEU:HB3	1.98	0.45
1:I:302:ILE:HG13	1:I:364:VAL:HB	1.98	0.45
4:C:38:VAL:HG11	4:C:152:MET:HE1	1.99	0.45
4:K:38:VAL:HG11	4:K:152:MET:HE1	1.99	0.45
1:E:68:HIS:CE1	1:E:404:GLU:OE1	2.57	0.45
3:J:39:LEU:HD22	3:J:100:GLY:CA	2.47	0.45
1:E:220:PRO:HB2	1:E:221:ASP:H	1.51	0.45
3:J:123:LEU:HD13	3:J:189:ILE:HG22	1.99	0.45
1:A:308:ASN:O	1:A:357:GLY:N	2.50	0.45
1:A:341:TYR:CG	1:A:342:LEU:HB2	2.51	0.45
3:J:67:THR:HG22	3:J:68:VAL:N	2.31	0.45
3:F:172:PHE:CE2	1:E:184:ILE:HD11	2.51	0.45
4:C:18:VAL:HG11	4:C:101:MET:HG3	1.98	0.45
4:K:184:LEU:HD23	4:K:184:LEU:HA	1.88	0.45
1:E:341:TYR:CG	1:E:342:LEU:HB2	2.52	0.45
1:I:274:GLU:N	1:I:275:GLY:HA3	2.17	0.45
1:A:348:LEU:CA	1:A:349:SER:CB	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:348:LEU:CA	1:E:349:SER:CB	2.95	0.45
1:A:358:GLU:HG2	1:A:359:SER:N	2.33	0.44
1:A:61:MET:O	1:A:61:MET:HG3	2.17	0.44
1:A:79:ASN:OD1	1:A:81:ARG:HB2	2.17	0.44
1:A:199:ILE:HD11	3:B:96:PHE:HA	2.00	0.44
3:J:105:GLU:O	3:J:109:ARG:HG2	2.17	0.44
3:J:233:TYR:C	3:J:233:TYR:CD2	2.96	0.44
4:G:154:TYR:HB2	4:G:155:PRO:HD3	2.00	0.44
4:K:137:ILE:HG22	4:K:137:ILE:O	2.17	0.44
1:I:94:LEU:HG	1:I:155:ILE:HD11	1.99	0.44
1:E:297:GLY:O	1:E:372:ASP:HB2	2.18	0.44
1:E:289:ASN:ND2	1:E:305:LYS:HE2	2.33	0.44
1:I:293:TYR:CZ	1:I:411:PRO:HB3	2.53	0.44
1:A:225:GLY:HA2	1:A:229:ARG:HH21	1.80	0.44
3:F:29:MET:HE2	4:G:108:VAL:HG12	1.98	0.44
1:A:184:ILE:HD11	3:B:172:PHE:CZ	2.52	0.44
3:J:132:PRO:HD3	3:J:164:ASN:ND2	2.33	0.44
4:K:38:VAL:O	4:K:42:GLU:HG2	2.17	0.44
1:I:93:VAL:HG11	1:I:132:TRP:CE2	2.52	0.44
1:A:164:ASP:HB3	1:A:165:PRO:CA	2.48	0.44
4:G:231:VAL:O	4:G:235:VAL:HG13	2.18	0.44
1:I:318:GLU:HB3	1:I:392:PHE:HB2	1.99	0.44
1:A:37:PHE:O	1:A:41:ARG:HG3	2.17	0.44
3:J:135:TRP:NE1	3:J:156:GLY:HA3	2.33	0.44
3:J:172:PHE:HE2	1:I:184:ILE:HD11	1.79	0.44
3:B:77:CYS:SG	3:B:98:VAL:HG23	2.58	0.43
3:B:81:GLN:HE21	3:B:137:ASP:HA	1.84	0.43
1:A:96:ARG:HD2	1:A:99:GLN:NE2	2.33	0.43
1:A:320:THR:HG22	1:A:324:LEU:O	2.18	0.43
3:J:178:GLN:HG3	3:J:188:LEU:HD11	2.00	0.43
3:B:188:LEU:HD12	3:B:188:LEU:HA	1.86	0.43
4:G:137:ILE:HD13	1:E:147:ILE:CD1	2.49	0.43
1:I:61:MET:O	1:I:61:MET:HG3	2.17	0.43
3:F:192:HIS:HA	1:E:96:ARG:O	2.18	0.43
4:G:148:ILE:HG23	4:G:152:MET:CE	2.48	0.43
1:E:273:THR:O	1:E:273:THR:OG1	2.36	0.43
3:F:185:LEU:HD22	1:E:176:LEU:HD21	2.01	0.43
1:I:167:THR:HG22	1:I:168:LEU:O	2.18	0.43
1:A:295:VAL:HA	1:A:296:PRO:HA	1.92	0.43
3:J:112:ASN:O	3:J:113:PHE:C	2.61	0.43
3:J:204:MET:H	3:J:207:ARG:HH12	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:295:VAL:HA	1:E:296:PRO:HA	1.90	0.43
3:B:143:SER:C	3:B:145:SER:N	2.67	0.43
4:C:184:LEU:HD23	4:C:184:LEU:HA	1.76	0.43
1:I:306:VAL:HG12	1:I:360:LYS:O	2.19	0.43
3:J:59:TRP:CH2	3:J:203:ARG:O	2.71	0.43
3:B:101:LEU:HD23	3:B:129:MET:HE1	2.01	0.43
1:I:98:ALA:HB3	1:I:123:ASN:HD22	1.82	0.43
1:I:341:TYR:CG	1:I:342:LEU:HB2	2.53	0.43
3:F:90:LEU:HA	3:F:91:PRO:HD3	1.87	0.43
4:K:139:ASP:OD1	1:I:30:GLY:HA2	2.19	0.43
1:I:40:MET:HE1	1:I:387:VAL:HB	2.01	0.43
3:J:92:PHE:CD1	3:J:92:PHE:C	2.96	0.42
1:I:129:ALA:HA	1:I:155:ILE:O	2.19	0.42
1:I:276:THR:CG2	1:I:279:VAL:HB	2.48	0.42
1:A:107:PRO:HA	3:B:191:LEU:HD13	2.01	0.42
1:A:334:GLN:HG2	1:A:335:LYS:HB2	2.00	0.42
3:J:116:TRP:CD1	4:K:47:TRP:CZ3	3.07	0.42
3:B:98:VAL:O	3:B:102:MET:HG2	2.19	0.42
4:C:196:ASN:HA	4:C:197:VAL:HA	1.81	0.42
1:A:57:VAL:O	1:A:58:ASN:HB2	2.19	0.42
3:F:92:PHE:O	3:F:96:PHE:HB2	2.19	0.42
4:K:157:TYR:CD2	4:K:157:TYR:C	2.97	0.42
4:K:174:TYR:CD2	4:K:174:TYR:C	2.96	0.42
1:I:58:ASN:HD22	1:I:125:ARG:NH2	2.17	0.42
3:J:11:GLY:C	3:J:13:PHE:H	2.27	0.42
3:J:178:GLN:HG3	3:J:188:LEU:CD1	2.49	0.42
3:F:39:LEU:C	3:F:39:LEU:HD12	2.44	0.42
4:C:39:ARG:NH2	4:C:43:GLN:HB2	2.34	0.42
4:C:64:SER:O	4:C:68:THR:HB	2.20	0.42
4:K:196:ASN:HA	4:K:197:VAL:HA	1.87	0.42
1:E:225:GLY:HA2	1:E:229:ARG:HH21	1.81	0.42
1:I:149:PRO:HB3	1:I:342:LEU:HD21	2.02	0.42
3:F:44:VAL:HG23	4:G:122:ALA:HB1	2.00	0.42
4:K:88:ARG:HB2	4:K:170:THR:HB	2.01	0.42
1:E:333:THR:O	1:E:334:GLN:CB	2.68	0.42
3:J:241:ARG:O	3:J:244:SER:HB2	2.19	0.42
3:B:29:MET:HE1	4:C:109:GLN:HG3	2.00	0.42
3:F:182:LEU:HD21	1:E:258:ILE:HD13	2.02	0.42
4:G:38:VAL:HG11	4:G:152:MET:HE1	2.02	0.42
1:I:201:PHE:HZ	1:I:231:ILE:HD13	1.84	0.42
3:F:56:TRP:CZ2	4:G:134:MET:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:143:SER:C	3:F:145:SER:N	2.77	0.42
1:I:273:THR:CB	1:I:274:GLU:HB2	2.49	0.42
1:A:220:PRO:C	1:A:222:ASP:N	2.67	0.42
1:A:286:THR:OG1	1:A:403:ALA:HB1	2.19	0.42
3:B:116:TRP:CD1	4:C:47:TRP:CZ3	3.07	0.42
4:C:137:ILE:HG22	4:C:137:ILE:O	2.20	0.42
1:I:37:PHE:O	1:I:41:ARG:HG3	2.20	0.42
1:I:220:PRO:C	1:I:222:ASP:N	2.68	0.42
1:I:342:LEU:H	1:I:370:ARG:HD3	1.84	0.42
4:C:174:TYR:CD2	4:C:174:TYR:C	2.97	0.42
1:I:108:ARG:HD2	1:I:262:ALA:HA	2.02	0.42
3:B:143:SER:O	3:B:143:SER:OG	2.38	0.42
1:E:62:ILE:HG22	1:E:123:ASN:OD1	2.20	0.42
1:I:225:GLY:O	1:I:226:ASP:C	2.61	0.42
1:I:297:GLY:O	1:I:372:ASP:HB2	2.20	0.42
3:B:53:TRP:O	3:B:60:LYS:NZ	2.53	0.41
1:I:201:PHE:CZ	1:I:231:ILE:HD13	2.55	0.41
1:A:341:TYR:CZ	1:A:342:LEU:HD22	2.56	0.41
4:K:246:ILE:HG21	4:K:249:GLU:OE2	2.19	0.41
1:E:276:THR:CG2	1:E:279:VAL:HB	2.50	0.41
1:I:102:GLY:HA3	1:I:268:LEU:HB3	2.02	0.41
1:A:51:SER:HB3	1:A:62:ILE:O	2.21	0.41
4:G:129:ASP:O	4:G:133:HIS:HD2	2.02	0.41
1:E:47:ASP:OD2	1:E:66:LYS:NZ	2.43	0.41
1:I:275:GLY:CA	1:I:276:THR:HB	2.50	0.41
1:I:286:THR:OG1	1:I:403:ALA:HB1	2.20	0.41
3:J:98:VAL:HG22	3:J:129:MET:CE	2.47	0.41
1:A:164:ASP:OD2	3:B:192:HIS:CD2	2.73	0.41
1:E:377:SER:C	1:E:379:LEU:H	2.28	0.41
3:J:45:HIS:HE1	4:K:224:PHE:HA	1.85	0.41
4:K:137:ILE:HD13	1:I:147:ILE:HD12	2.02	0.41
1:I:73:TRP:HA	1:I:74:PRO:HD3	1.91	0.41
3:B:92:PHE:O	3:B:96:PHE:HB2	2.20	0.41
1:E:348:LEU:HA	1:E:349:SER:CB	2.50	0.41
1:I:77:VAL:O	1:I:78:ALA:C	2.63	0.41
1:A:129:ALA:HA	1:A:155:ILE:O	2.21	0.41
4:C:154:TYR:HB2	4:C:155:PRO:HD3	2.03	0.41
1:E:286:THR:HG21	1:E:391:LEU:HD12	2.02	0.41
1:I:295:VAL:HA	1:I:296:PRO:HA	1.92	0.41
1:A:170:ASP:OD1	1:A:170:ASP:C	2.63	0.41
3:B:56:TRP:CH2	4:C:134:MET:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:59:TRP:CH2	3:B:203:ARG:O	2.74	0.41
4:G:117:ALA:HB1	4:G:157:TYR:HB3	2.03	0.41
4:G:190:PRO:C	4:G:192:MET:N	2.78	0.41
1:E:294:LYS:O	1:E:297:GLY:HA2	2.21	0.41
1:I:83:SER:O	1:I:109:SER:HB2	2.21	0.41
1:A:96:ARG:NH2	1:A:99:GLN:HE22	2.16	0.41
3:J:30:LEU:HD23	3:J:33:LEU:HD21	2.03	0.41
3:B:98:VAL:HG11	3:B:130:ILE:HA	2.03	0.41
3:F:51:GLY:HA3	3:F:52:ASP:CB	2.26	0.41
3:F:244:SER:O	4:G:236:LEU:HD12	2.20	0.41
1:E:169:LEU:C	1:E:171:GLY:H	2.29	0.41
3:B:58:ASP:HB2	3:B:203:ARG:HH21	1.86	0.40
3:B:60:LYS:HD3	3:B:65:TRP:CZ2	2.56	0.40
3:F:188:LEU:HD12	3:F:188:LEU:HA	1.97	0.40
4:C:117:ALA:HB1	4:C:157:TYR:HB3	2.02	0.40
4:G:190:PRO:O	4:G:193:ILE:HG13	2.21	0.40
1:E:253:THR:O	1:E:254:PHE:C	2.63	0.40
1:A:102:GLY:HA3	1:A:268:LEU:HB3	2.03	0.40
1:A:169:LEU:C	1:A:171:GLY:H	2.30	0.40
3:J:239:MET:HE1	4:K:225:GLY:O	2.21	0.40
3:F:44:VAL:CG2	4:G:122:ALA:HB1	2.51	0.40
1:E:163:THR:HG22	1:E:164:ASP:N	2.36	0.40
3:J:143:SER:C	3:J:145:SER:N	2.69	0.40
3:J:150:ALA:O	3:J:230:MET:HG2	2.22	0.40
3:J:199:PRO:HB2	3:J:201:TYR:CE2	2.57	0.40
1:A:334:GLN:HG2	1:A:335:LYS:CB	2.52	0.40
3:J:129:MET:O	3:J:132:PRO:HD2	2.21	0.40
3:J:172:PHE:CZ	1:I:184:ILE:HD11	2.57	0.40
3:F:241:ARG:O	3:F:244:SER:HB2	2.21	0.40
1:E:51:SER:HB3	1:E:62:ILE:O	2.21	0.40
1:E:220:PRO:C	1:E:222:ASP:N	2.73	0.40
1:I:48:VAL:HG21	1:I:149:PRO:CG	2.51	0.40
1:A:339:PRO:O	1:A:340:ASP:C	2.63	0.40
1:A:383:THR:HG22	1:E:260:LEU:O	2.22	0.40
4:C:39:ARG:HH22	4:C:43:GLN:HB2	1.86	0.40
4:C:194:ILE:HA	4:C:195:PRO:HD3	2.00	0.40
4:K:102:ARG:O	4:K:106:VAL:HG23	2.22	0.40
1:I:275:GLY:CA	1:I:276:THR:HG22	2.22	0.40
1:I:287:GLU:HB2	1:I:305:LYS:HB2	2.03	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	384/419 (92%)	338 (88%)	27 (7%)	19 (5%)	1	3
1	E	384/419 (92%)	340 (88%)	26 (7%)	18 (5%)	2	3
1	I	384/419 (92%)	330 (86%)	31 (8%)	23 (6%)	1	2
2	D	17/19 (90%)	13 (76%)	2 (12%)	2 (12%)	0	0
2	H	14/19 (74%)	12 (86%)	2 (14%)	0	100	100
3	B	240/252 (95%)	218 (91%)	16 (7%)	6 (2%)	4	10
3	F	240/252 (95%)	215 (90%)	22 (9%)	3 (1%)	9	22
3	J	240/252 (95%)	214 (89%)	19 (8%)	7 (3%)	3	8
4	C	206/256 (80%)	188 (91%)	10 (5%)	8 (4%)	2	4
4	G	207/256 (81%)	181 (87%)	18 (9%)	8 (4%)	2	4
4	K	207/256 (81%)	184 (89%)	16 (8%)	7 (3%)	3	6
All	All	2523/2819 (90%)	2233 (88%)	189 (8%)	101 (4%)	2	4

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	GLU
1	A	164	ASP
1	A	220	PRO
1	A	221	ASP
1	A	274	GLU
1	A	276	THR
1	A	340	ASP
1	A	342	LEU
1	A	349	SER
2	D	4	ALA
3	J	52	ASP
3	J	201	TYR
3	B	201	TYR

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Mol	Chain	Res	Type
3	F	12	PRO
3	F	52	ASP
4	C	229	LEU
4	G	49	ALA
4	G	229	LEU
4	K	229	LEU
1	E	51	SER
1	E	103	GLU
1	E	164	ASP
1	E	217	GLU
1	E	220	PRO
1	E	221	ASP
1	E	276	THR
1	E	334	GLN
1	E	340	ASP
1	E	342	LEU
1	E	349	SER
1	I	51	SER
1	I	103	GLU
1	I	164	ASP
1	I	220	PRO
1	I	221	ASP
1	I	274	GLU
1	I	276	THR
1	I	335	LYS
1	I	340	ASP
1	I	342	LEU
1	I	349	SER
1	I	353	VAL
1	A	51	SER
1	A	217	GLU
1	A	353	VAL
3	J	204	MET
3	B	52	ASP
3	F	201	TYR
4	C	49	ALA
4	C	174	TYR
4	C	177	HIS
4	C	246	ILE
4	G	174	TYR
4	G	177	HIS
4	G	246	ILE

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Mol	Chain	Res	Type
4	K	49	ALA
4	K	174	TYR
4	K	177	HIS
1	E	274	GLU
1	E	353	VAL
1	A	218	GLY
1	A	297	GLY
1	A	335	LYS
3	B	204	MET
4	G	195	PRO
4	K	179	TYR
1	E	297	GLY
1	E	335	LYS
1	I	217	GLU
1	I	218	GLY
1	I	264	LEU
1	I	334	GLN
1	I	350	ASN
1	A	334	GLN
1	A	350	ASN
4	C	179	TYR
4	C	191	PHE
4	C	195	PRO
4	G	191	PHE
4	K	246	ILE
1	E	218	GLY
1	E	350	ASN
1	I	165	PRO
1	I	206	LYS
1	I	297	GLY
3	J	144	GLY
3	J	250	GLU
4	G	179	TYR
4	K	195	PRO
1	A	206	LYS
2	D	18	ALA
3	J	203	ARG
3	B	144	GLY
3	B	200	GLU
1	I	368	ASP
3	J	151	VAL
1	I	357	GLY

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Mol	Chain	Res	Type
3	B	151	VAL
1	I	208	ILE
1	A	165	PRO
1	E	165	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	318/335 (95%)	303 (95%)	15 (5%)	23	47
1	E	318/335 (95%)	301 (95%)	17 (5%)	20	43
1	I	318/335 (95%)	296 (93%)	22 (7%)	14	31
3	B	201/208 (97%)	190 (94%)	11 (6%)	19	41
3	F	201/208 (97%)	185 (92%)	16 (8%)	11	25
3	J	201/208 (97%)	185 (92%)	16 (8%)	11	25
4	C	173/209 (83%)	159 (92%)	14 (8%)	11	25
4	G	174/209 (83%)	159 (91%)	15 (9%)	10	22
4	K	174/209 (83%)	160 (92%)	14 (8%)	11	25
All	All	2078/2256 (92%)	1938 (93%)	140 (7%)	15	32

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	VAL
1	A	97	THR
1	A	166	VAL
1	A	173	THR
1	A	253	THR
1	A	266	LYS
1	A	282	GLU
1	A	285	THR
1	A	320	THR
1	A	335	LYS

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Mol	Chain	Res	Type
1	A	348	LEU
1	A	349	SER
1	A	378	ASP
1	A	383	THR
1	A	414	VAL
3	J	16	VAL
3	J	33	LEU
3	J	39	LEU
3	J	48	LEU
3	J	52	ASP
3	J	67	THR
3	J	69	LEU
3	J	98	VAL
3	J	130	ILE
3	J	138	VAL
3	J	152	VAL
3	J	164	ASN
3	J	169	ILE
3	J	177	GLU
3	J	220	VAL
3	J	234	PHE
3	B	33	LEU
3	B	39	LEU
3	B	48	LEU
3	B	67	THR
3	B	69	LEU
3	B	98	VAL
3	B	138	VAL
3	B	152	VAL
3	B	164	ASN
3	B	169	ILE
3	B	220	VAL
3	F	33	LEU
3	F	39	LEU
3	F	48	LEU
3	F	67	THR
3	F	69	LEU
3	F	88	PHE
3	F	92	PHE
3	F	98	VAL
3	F	130	ILE
3	F	131	VAL

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Mol	Chain	Res	Type
3	F	138	VAL
3	F	152	VAL
3	F	164	ASN
3	F	169	ILE
3	F	201	TYR
3	F	220	VAL
4	C	36	LEU
4	C	60	THR
4	C	68	THR
4	C	72	LEU
4	C	97	PRO
4	C	118	ILE
4	C	145	SER
4	C	147	ILE
4	C	177	HIS
4	C	183	PHE
4	C	229	LEU
4	C	235	VAL
4	C	246	ILE
4	C	251	VAL
4	G	30	VAL
4	G	33	VAL
4	G	36	LEU
4	G	68	THR
4	G	72	LEU
4	G	97	PRO
4	G	118	ILE
4	G	145	SER
4	G	147	ILE
4	G	177	HIS
4	G	183	PHE
4	G	229	LEU
4	G	235	VAL
4	G	246	ILE
4	G	251	VAL
4	K	30	VAL
4	K	36	LEU
4	K	60	THR
4	K	68	THR
4	K	72	LEU
4	K	118	ILE
4	K	145	SER

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Mol	Chain	Res	Type
4	K	147	ILE
4	K	177	HIS
4	K	183	PHE
4	K	229	LEU
4	K	235	VAL
4	K	246	ILE
4	K	251	VAL
1	E	29	HIS
1	E	63	LEU
1	E	95	VAL
1	E	97	THR
1	E	166	VAL
1	E	173	THR
1	E	253	THR
1	E	266	LYS
1	E	282	GLU
1	E	285	THR
1	E	320	THR
1	E	335	LYS
1	E	342	LEU
1	E	348	LEU
1	E	378	ASP
1	E	383	THR
1	E	414	VAL
1	I	51	SER
1	I	60	GLU
1	I	63	LEU
1	I	95	VAL
1	I	97	THR
1	I	133	HIS
1	I	166	VAL
1	I	173	THR
1	I	184	ILE
1	I	204	ILE
1	I	253	THR
1	I	266	LYS
1	I	282	GLU
1	I	285	THR
1	I	310	THR
1	I	320	THR
1	I	335	LYS
1	I	342	LEU

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Mol	Chain	Res	Type
1	I	348	LEU
1	I	353	VAL
1	I	378	ASP
1	I	414	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	44	ASN
1	A	58	ASN
1	A	68	HIS
1	A	99	GLN
1	A	139	ASN
1	A	188	HIS
1	A	261	GLN
1	A	265	GLN
3	J	45	HIS
3	J	174	GLN
3	B	178	GLN
3	B	179	HIS
3	B	192	HIS
3	F	174	GLN
3	F	178	GLN
3	F	192	HIS
4	C	59	GLN
4	C	109	GLN
4	C	128	GLN
4	C	177	HIS
4	G	59	GLN
4	G	109	GLN
4	G	128	GLN
4	G	177	HIS
4	K	59	GLN
4	K	109	GLN
4	K	128	GLN
4	K	177	HIS
1	E	34	GLN
1	E	44	ASN
1	E	58	ASN
1	E	68	HIS
1	E	99	GLN

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Mol	Chain	Res	Type
1	E	104	GLN
1	E	188	HIS
1	E	261	GLN
1	E	265	GLN
1	E	289	ASN
1	E	350	ASN
1	I	58	ASN
1	I	68	HIS
1	I	99	GLN
1	I	137	GLN
1	I	188	HIS
1	I	261	GLN
1	I	265	GLN
1	I	350	ASN
1	I	386	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 11 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
5	CUA	A	420	1	0,1,1	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	386/419 (92%)	0.96	50 (12%) 7 6	50, 69, 98, 114	0
1	E	386/419 (92%)	0.96	56 (14%) 6 4	48, 68, 101, 123	0
1	I	386/419 (92%)	0.38	15 (3%) 43 38	34, 50, 74, 90	0
2	D	19/19 (100%)	2.30	10 (52%) 0 0	78, 80, 83, 83	0
2	H	16/19 (84%)	2.65	9 (56%) 0 0	97, 99, 104, 104	0
3	B	242/252 (96%)	0.76	20 (8%) 17 14	43, 58, 90, 109	0
3	F	242/252 (96%)	0.71	24 (9%) 13 10	42, 57, 93, 117	0
3	J	242/252 (96%)	0.55	20 (8%) 17 14	40, 55, 89, 109	0
4	C	210/256 (82%)	1.22	48 (22%) 2 1	53, 69, 101, 114	0
4	G	211/256 (82%)	1.24	46 (21%) 2 2	53, 78, 112, 125	0
4	K	211/256 (82%)	1.13	39 (18%) 3 2	54, 72, 106, 119	0
All	All	2551/2819 (90%)	0.87	337 (13%) 7 6	34, 63, 100, 125	0

All (337) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	K	252	ALA	9.0
2	H	19	ALA	8.5
4	C	252	ALA	7.8
4	G	252	ALA	7.6
4	C	60	THR	7.2
1	E	394	PHE	6.8
1	A	222	ASP	6.4
4	C	61	TYR	6.3
1	E	396	PRO	6.3
4	K	139	ASP	6.1
4	K	48	ARG	6.0
4	C	251	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
4	C	187	ALA	5.8
4	G	224	PHE	5.5
3	B	251	GLN	5.4
1	E	226	ASP	5.4
3	J	252	ILE	5.2
2	D	19	ALA	5.2
1	E	414	VAL	5.2
1	A	353	VAL	5.1
1	A	361	GLU	5.0
4	K	196	ASN	5.0
1	E	275	GLY	4.9
4	C	48	ARG	4.9
4	K	178	GLY	4.7
4	K	54	PHE	4.7
1	A	414	VAL	4.7
1	E	402	ALA	4.7
3	J	249	ILE	4.7
4	G	197	VAL	4.6
1	E	225	GLY	4.6
3	B	252	ILE	4.5
1	I	311	SER	4.5
4	C	194	ILE	4.4
3	J	11	GLY	4.4
4	K	224	PHE	4.4
1	E	219	ARG	4.3
4	C	249	GLU	4.3
4	C	139	ASP	4.3
4	K	197	VAL	4.3
3	F	11	GLY	4.3
4	G	194	ILE	4.2
2	H	7	ALA	4.2
2	D	1	ALA	4.1
4	K	228	ALA	4.1
4	G	226	TRP	4.1
1	A	303	ASN	4.1
1	E	220	PRO	4.0
4	C	190	PRO	4.0
1	A	362	ILE	4.0
4	G	196	ASN	4.0
3	J	13	PHE	4.0
1	A	359	SER	4.0
4	K	244	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
3	J	248	ARG	4.0
1	E	184	ILE	4.0
4	K	246	ILE	4.0
4	K	140	THR	3.9
4	K	226	TRP	3.9
1	E	221	ASP	3.9
3	B	250	GLU	3.9
3	F	251	GLN	3.9
2	D	5	ALA	3.9
1	A	363	VAL	3.9
1	I	414	VAL	3.9
2	H	18	ALA	3.8
1	A	220	PRO	3.8
4	K	56	PRO	3.7
1	A	340	ASP	3.7
1	A	344	ALA	3.7
4	K	247	GLY	3.7
1	A	164	ASP	3.7
4	G	48	ARG	3.6
2	D	3	ALA	3.6
1	E	252	SER	3.6
2	H	5	ALA	3.6
4	K	47	TRP	3.6
4	G	96	ALA	3.5
3	B	227	PHE	3.5
1	E	353	VAL	3.5
1	E	345	ASP	3.5
4	C	85	TRP	3.5
1	A	348	LEU	3.5
4	K	179	TYR	3.5
4	K	194	ILE	3.5
1	E	349	SER	3.4
2	H	8	ALA	3.4
4	C	193	ILE	3.4
4	G	227	MET	3.4
1	E	398	GLY	3.4
4	G	228	ALA	3.4
1	E	348	LEU	3.4
1	A	304	VAL	3.4
3	B	249	ILE	3.4
3	F	252	ILE	3.4
3	B	231	MET	3.4

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Mol	Chain	Res	Type	RSRZ
4	C	131	ALA	3.3
3	F	212	THR	3.3
1	E	210	ALA	3.3
4	G	230	GLY	3.3
2	H	6	ALA	3.3
4	K	55	ALA	3.3
4	K	248	LYS	3.3
4	C	225	GLY	3.3
3	F	249	ILE	3.3
3	F	102	MET	3.2
1	E	253	THR	3.2
2	D	17	ALA	3.2
4	K	229	LEU	3.2
1	A	218	GLY	3.2
3	B	172	PHE	3.2
4	C	179	TYR	3.2
1	A	236	LEU	3.1
4	G	246	ILE	3.1
1	E	340	ASP	3.1
4	G	249	GLU	3.1
1	A	283	GLN	3.1
1	E	224	ILE	3.1
2	D	2	ALA	3.1
4	K	227	MET	3.1
1	E	283	GLN	3.1
4	G	140	THR	3.1
1	E	229	ARG	3.1
1	E	142	GLY	3.1
1	E	277	VAL	3.1
4	K	249	GLU	3.0
1	A	224	ILE	3.0
3	B	213	PHE	3.0
3	F	217	VAL	3.0
1	E	346	ARG	3.0
1	E	347	GLY	3.0
3	F	248	ARG	3.0
4	C	189	GLY	3.0
4	G	242	ILE	3.0
1	A	322	ALA	3.0
4	G	193	ILE	3.0
4	K	195	PRO	3.0
3	J	251	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
3	J	19	ALA	3.0
3	F	125	PHE	3.0
1	A	397	ASP	2.9
1	I	345	ASP	2.9
1	E	321	ALA	2.9
4	C	191	PHE	2.9
4	C	229	LEU	2.9
4	G	67	TRP	2.9
2	D	18	ALA	2.9
4	G	131	ALA	2.9
3	B	248	ARG	2.9
4	K	138	ARG	2.9
4	C	228	ALA	2.9
4	C	47	TRP	2.9
4	G	154	TYR	2.9
4	G	191	PHE	2.9
1	E	250	THR	2.8
1	E	223	VAL	2.8
3	F	250	GLU	2.8
1	A	351	ASP	2.8
3	F	129	MET	2.8
1	E	298	ARG	2.8
4	C	59	GLN	2.8
4	C	246	ILE	2.8
4	C	226	TRP	2.8
4	G	25	TRP	2.8
4	G	91	ASN	2.8
4	K	176	ALA	2.8
4	C	232	PHE	2.8
3	F	63	ARG	2.8
1	E	199	ILE	2.7
1	A	300	LEU	2.7
3	F	144	GLY	2.7
1	I	353	VAL	2.7
2	H	14	ALA	2.7
3	J	224	PHE	2.7
1	A	381	TYR	2.7
3	J	28	TRP	2.7
1	E	222	ASP	2.7
3	B	16	VAL	2.7
4	C	161	ALA	2.7
4	C	115	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
4	C	165	PHE	2.7
4	C	197	VAL	2.7
1	A	345	ASP	2.7
4	G	238	ILE	2.7
4	K	193	ILE	2.7
3	B	142	LEU	2.7
1	I	347	GLY	2.7
1	A	311	SER	2.7
4	K	192	MET	2.6
4	K	131	ALA	2.6
1	A	302	ILE	2.6
4	C	136	VAL	2.6
1	E	315	ARG	2.6
1	E	206	LYS	2.6
1	A	347	GLY	2.6
1	E	309	GLY	2.6
4	G	225	GLY	2.6
1	A	210	ALA	2.6
4	G	251	VAL	2.6
1	E	164	ASP	2.6
1	E	227	ASP	2.6
3	J	213	PHE	2.6
3	F	20	ALA	2.6
3	F	15	SER	2.5
3	F	169	ILE	2.5
1	A	206	LYS	2.5
3	B	243	TYR	2.5
3	B	11	GLY	2.5
3	J	98	VAL	2.5
4	C	195	PRO	2.5
1	E	395	THR	2.5
3	J	211	ARG	2.5
4	C	230	GLY	2.5
3	B	25	THR	2.5
3	F	28	TRP	2.5
4	G	137	ILE	2.5
4	K	147	ILE	2.5
4	K	157	TYR	2.5
4	K	19	VAL	2.5
3	J	22	CYS	2.5
1	E	205	ARG	2.5
1	I	182	SER	2.5

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Mol	Chain	Res	Type	RSRZ
4	G	189	GLY	2.5
4	G	247	GLY	2.5
1	I	210	ALA	2.5
4	G	150	PHE	2.5
1	A	219	ARG	2.4
4	C	138	ARG	2.4
1	A	208	ILE	2.4
1	E	359	SER	2.4
4	C	227	MET	2.4
3	J	17	ALA	2.4
3	J	250	GLU	2.4
1	A	280	GLY	2.4
2	D	14	ALA	2.4
4	C	96	ALA	2.4
4	C	196	ASN	2.4
4	G	133	HIS	2.4
1	E	385	SER	2.4
3	F	98	VAL	2.4
1	E	216	ALA	2.4
2	H	16	ALA	2.4
4	G	185	ILE	2.3
3	B	129	MET	2.3
1	A	158	ASP	2.3
1	E	335	LYS	2.3
4	G	195	PRO	2.3
3	B	214	GLY	2.3
4	C	250	GLY	2.3
1	A	279	VAL	2.3
3	B	224	PHE	2.3
3	F	191	LEU	2.3
4	C	55	ALA	2.3
4	K	66	LEU	2.3
1	E	273	THR	2.3
1	I	365	LYS	2.3
1	A	80	PRO	2.3
4	G	88	ARG	2.3
1	E	284	VAL	2.3
3	J	16	VAL	2.3
4	C	81	ALA	2.3
1	E	243	THR	2.3
4	G	173	PRO	2.3
4	K	20	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
4	G	59	GLN	2.3
4	K	225	GLY	2.3
4	K	44	VAL	2.3
4	K	251	VAL	2.3
2	H	11	ALA	2.3
3	B	139	ILE	2.3
1	A	223	VAL	2.3
3	J	23	VAL	2.3
1	A	335	LYS	2.2
4	C	157	TYR	2.2
1	I	252	SER	2.2
3	J	15	SER	2.2
4	C	247	GLY	2.2
1	I	348	LEU	2.2
3	F	48	LEU	2.2
1	E	338	PHE	2.2
4	G	232	PHE	2.2
2	D	9	ALA	2.2
4	K	137	ILE	2.2
1	A	250	THR	2.2
4	G	47	TRP	2.2
4	C	63	MET	2.2
4	G	134	MET	2.2
3	F	17	ALA	2.2
3	J	243	TYR	2.2
1	E	411	PRO	2.2
3	F	142	LEU	2.2
1	A	213	VAL	2.2
1	A	326	PHE	2.2
1	A	157	GLY	2.2
1	A	278	GLY	2.2
1	A	376	LEU	2.2
1	E	195	GLY	2.2
4	G	121	GLY	2.2
1	A	277	VAL	2.2
4	C	64	SER	2.2
4	C	172	ILE	2.2
3	B	12	PRO	2.1
1	E	334	GLN	2.1
1	A	192	LEU	2.1
1	A	284	VAL	2.1
1	E	204	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
4	C	118	ILE	2.1
1	I	160	LYS	2.1
1	E	296	PRO	2.1
3	J	204	MET	2.1
4	G	184	LEU	2.1
1	I	303	ASN	2.1
1	A	207	GLY	2.1
1	E	381	TYR	2.1
4	C	50	GLY	2.1
4	C	178	GLY	2.1
4	C	162	VAL	2.1
1	E	60	GLU	2.1
4	G	182	ALA	2.1
4	G	24	MET	2.1
1	E	63	LEU	2.1
4	G	229	LEU	2.1
1	A	247	TYR	2.1
3	F	205	VAL	2.1
4	K	141	ASP	2.0
1	I	283	GLN	2.0
4	G	51	LEU	2.0
1	I	387	VAL	2.0
4	G	95	VAL	2.0
2	D	11	ALA	2.0
3	B	37	ALA	2.0
3	F	78	ALA	2.0
4	G	248	LYS	2.0
1	I	273	THR	2.0
1	A	244	ILE	2.0
4	C	185	ILE	2.0
1	A	256	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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
6	ZN	G	258	1/1	0.79	0.19	129,129,129,129	0
6	ZN	K	258	1/1	0.93	0.08	141,141,141,141	0
6	ZN	I	421	1/1	0.95	0.22	70,70,70,70	0
7	CU	I	420	1/1	0.95	0.08	76,76,76,76	0
5	CUA	A	420	2/2	0.96	0.09	72,72,72,93	0
6	ZN	E	421	1/1	0.96	0.19	90,90,90,90	0
6	ZN	A	421	1/1	0.97	0.13	88,88,88,88	0
6	ZN	C	258	1/1	0.98	0.05	87,87,87,87	0
7	CU	E	420	1/1	0.99	0.04	63,63,63,63	0
6	ZN	K	257	1/1	0.99	0.03	70,70,70,70	0
6	ZN	G	257	1/1	1.00	0.04	64,64,64,64	0
6	ZN	C	257	1/1	1.00	0.06	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.