



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:20 AM UTC

PDB ID : 1OS2 / pdb_00001os2
Title : Ternary enzyme-product-inhibitor complexes of human MMP12
Authors : Bertini, I.; Calderone, V.; Fragai, M.; Luchinat, C.; Mangani, S.; Terni, B.
Deposited on : 2003-03-18
Resolution : 2.15 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:

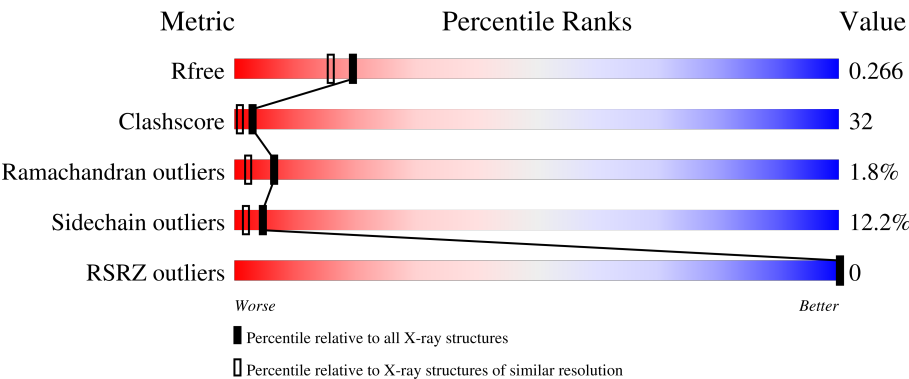
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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

Mol	Chain	Length	Quality of chain
1	A	165	49%42%7%•
1	B	165	44%39%15%•
1	C	165	48%33%15%•
1	D	165	53%37%7%•
1	E	165	45%38%15%•

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Mol	Chain	Length	Quality of chain
1	F	165	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	B	374	-	X	-	-
6	AZI	C	474	-	X	-	-
6	AZI	F	774	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8132 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 Macrophage metalloelastase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	7	0
			1295	823	225	242	5			
1	B	165	Total	C	N	O	S	0	7	0
			1295	823	225	242	5			
1	C	165	Total	C	N	O	S	0	6	0
			1295	823	225	242	5			
1	D	165	Total	C	N	O	S	0	7	0
			1295	823	225	242	5			
1	E	165	Total	C	N	O	S	0	7	0
			1295	823	225	242	5			
1	F	165	Total	C	N	O	S	0	7	0
			1295	823	225	242	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	MET	-	cloning artifact	UNP P39900
A	105	MET	-	cloning artifact	UNP P39900
A	171	ASP	PHE	engineered mutation	UNP P39900
B	104	MET	-	cloning artifact	UNP P39900
B	105	MET	-	cloning artifact	UNP P39900
B	171	ASP	PHE	engineered mutation	UNP P39900
C	104	MET	-	cloning artifact	UNP P39900
C	105	MET	-	cloning artifact	UNP P39900
C	171	ASP	PHE	engineered mutation	UNP P39900
D	104	MET	-	cloning artifact	UNP P39900
D	105	MET	-	cloning artifact	UNP P39900
D	171	ASP	PHE	engineered mutation	UNP P39900
E	104	MET	-	cloning artifact	UNP P39900
E	105	MET	-	cloning artifact	UNP P39900
E	171	ASP	PHE	engineered mutation	UNP P39900
F	104	MET	-	cloning artifact	UNP P39900
F	105	MET	-	cloning artifact	UNP P39900

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Chain	Residue	Modelled	Actual	Comment	Reference
F	171	ASP	PHE	engineered mutation	UNP P39900

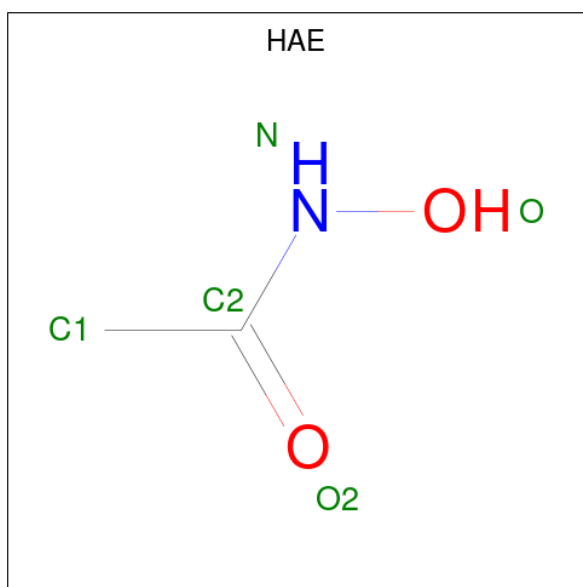
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		
3	B	3	Total	Ca	0	0
			3	3		
3	C	3	Total	Ca	0	0
			3	3		
3	D	3	Total	Ca	0	0
			3	3		
3	E	3	Total	Ca	0	0
			3	3		
3	F	3	Total	Ca	0	0
			3	3		

- Molecule 4 is ACETOHYDROXAMIC ACID (CCD ID: HAE) (formula: C₂H₅NO₂).



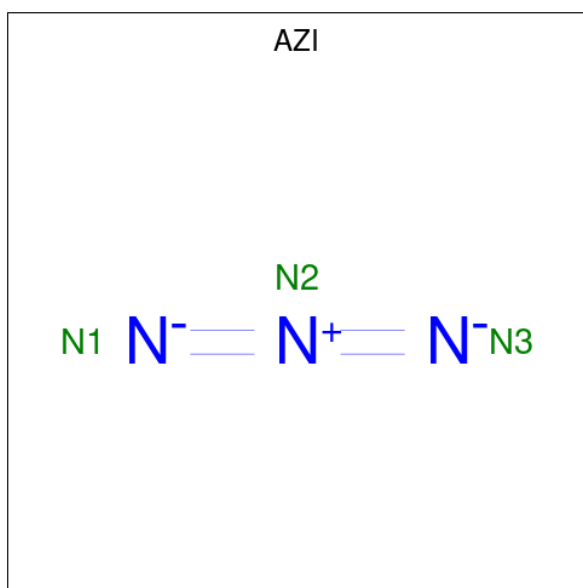
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			5	2	1	2		
4	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is AZIDE ION (CCD ID: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total N 3 3	0	0
6	F	1	Total N 3 3	0	0

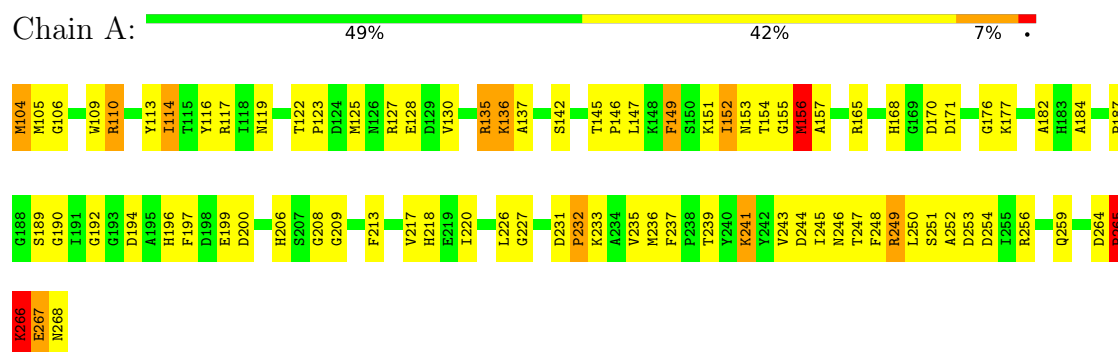
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	46	Total O 46 46	0	0
7	B	67	Total O 67 67	0	0
7	C	51	Total O 51 51	0	0
7	D	44	Total O 44 44	0	0
7	E	59	Total O 59 59	0	0
7	F	41	Total O 41 41	0	0

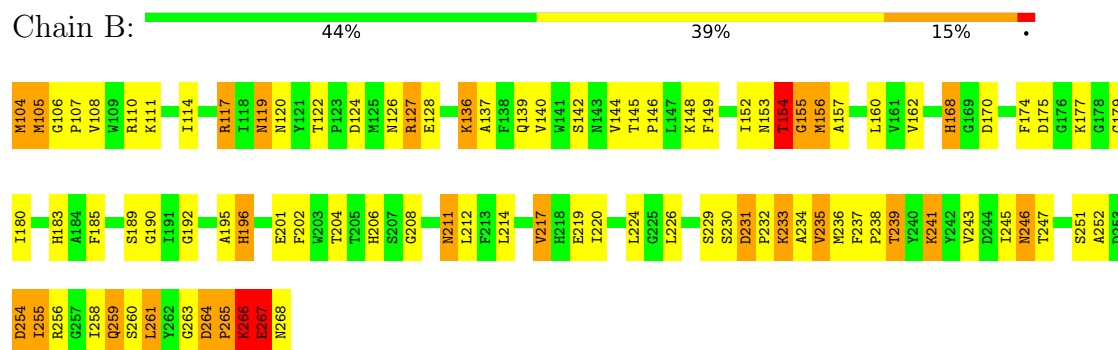
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

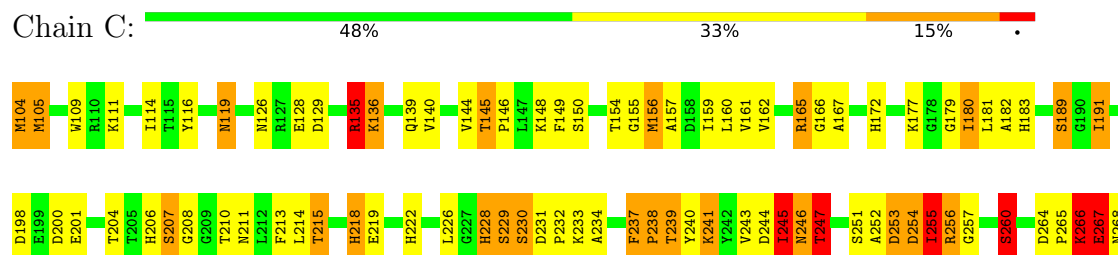
• Molecule 1: Macrophage metalloelastase



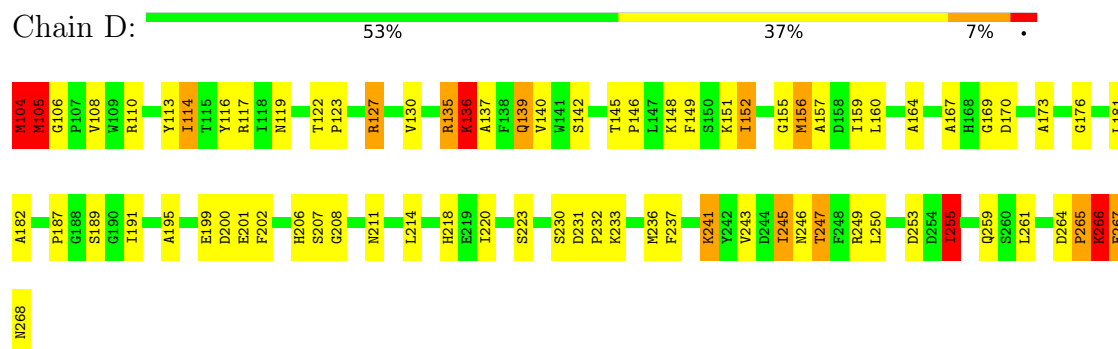
• Molecule 1: Macrophage metalloelastase



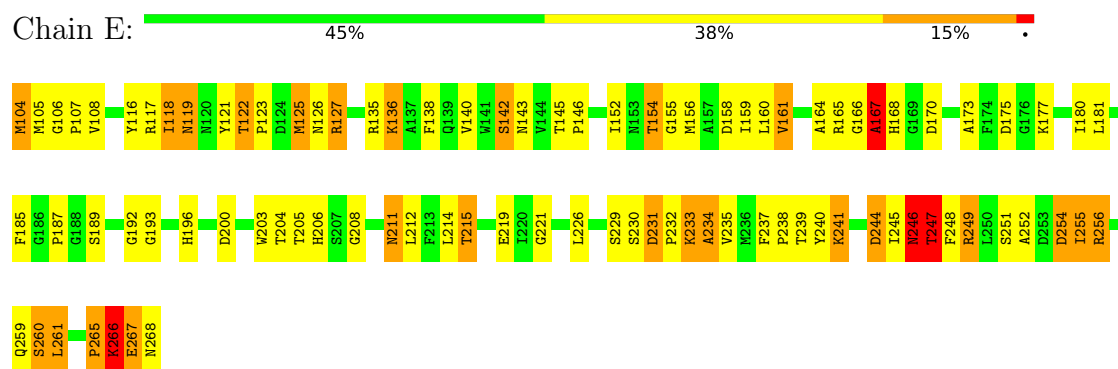
• Molecule 1: Macrophage metalloelastase



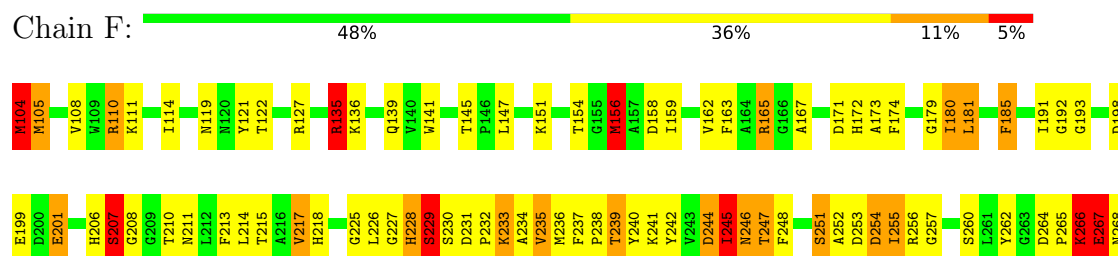
• Molecule 1: Macrophage metalloelastase



• Molecule 1: Macrophage metalloelastase



• Molecule 1: Macrophage metalloelastase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	123.84Å 123.84Å 69.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	69.01 – 2.15 69.01 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (69.01-2.15) 100.0 (69.01-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.1.80	Depositor
R, R_{free}	0.212 , 0.271 0.216 , 0.266	Depositor DCC
R_{free} test set	3296 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l 0.488 for h,-h-k,-l 0.029 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8132	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: ACT, AZI, HAE, CA, 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	1.90	26/1333 (2.0%)	1.74	25/1805 (1.4%)
1	B	2.01	28/1333 (2.1%)	1.81	31/1805 (1.7%)
1	C	1.91	25/1333 (1.9%)	1.83	33/1805 (1.8%)
1	D	1.85	31/1333 (2.3%)	1.70	22/1805 (1.2%)
1	E	2.05	36/1333 (2.7%)	1.97	40/1805 (2.2%)
1	F	1.84	21/1333 (1.6%)	1.77	25/1805 (1.4%)
All	All	1.93	167/7998 (2.1%)	1.81	176/10830 (1.6%)

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	1	2
1	B	0	2
1	C	0	2
1	E	0	4
1	F	1	2
All	All	2	12

All (167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	MET	C-O	12.73	1.39	1.23
1	E	167	ALA	C-O	-9.28	1.11	1.23
1	F	252	ALA	CA-CB	9.24	1.67	1.53
1	A	137	ALA	CA-CB	9.11	1.67	1.53
1	E	166	GLY	C-N	8.96	1.45	1.33
1	E	212	LEU	C-O	8.92	1.34	1.24
1	C	140	VAL	CA-CB	8.52	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	136	LYS	CA-C	8.51	1.63	1.52
1	A	170	ASP	CA-C	-7.79	1.42	1.53
1	B	177	LYS	N-CA	-7.77	1.36	1.46
1	D	137	ALA	CA-CB	7.76	1.65	1.53
1	A	239	THR	C-O	-7.74	1.14	1.24
1	B	236	MET	SD-CE	7.59	1.98	1.79
1	B	192	GLY	CA-C	7.50	1.59	1.52
1	B	140	VAL	CA-C	7.36	1.61	1.52
1	C	140	VAL	C-O	-7.33	1.15	1.24
1	E	158	ASP	C-O	-7.24	1.15	1.24
1	E	161	VAL	CA-CB	7.20	1.62	1.54
1	F	180	ILE	C-O	-7.11	1.17	1.23
1	B	185	PHE	CA-C	-6.98	1.44	1.52
1	C	119	ASN	CA-C	6.96	1.61	1.52
1	E	234	ALA	CA-CB	6.96	1.64	1.53
1	D	140	VAL	CA-CB	6.87	1.63	1.54
1	D	220	ILE	CA-CB	6.85	1.63	1.54
1	A	116	TYR	CA-C	-6.83	1.44	1.52
1	D	130	VAL	CA-CB	-6.82	1.46	1.54
1	D	139	GLN	CG-CD	6.81	1.69	1.52
1	E	204	THR	C-O	6.81	1.32	1.23
1	A	237	PHE	CA-C	-6.80	1.46	1.53
1	E	117	ARG	CA-C	-6.72	1.44	1.52
1	F	135	ARG	NE-CZ	6.71	1.40	1.33
1	E	240	TYR	N-CA	6.70	1.54	1.46
1	E	219	GLU	C-O	6.70	1.31	1.24
1	A	187	PRO	CA-C	6.65	1.60	1.52
1	F	165	ARG	N-CA	6.61	1.53	1.45
1	E	140	VAL	CA-C	6.61	1.60	1.52
1	D	116	TYR	CA-C	-6.59	1.44	1.52
1	B	155	GLY	C-N	-6.59	1.24	1.33
1	E	177	LYS	N-CA	-6.58	1.37	1.46
1	A	114	ILE	CA-C	-6.51	1.44	1.52
1	E	118	ILE	CA-CB	-6.49	1.46	1.53
1	A	252	ALA	CA-CB	6.48	1.63	1.53
1	E	104	MET	SD-CE	-6.47	1.63	1.79
1	F	228	HIS	CA-C	-6.47	1.44	1.52
1	D	246	ASN	CB-CG	6.45	1.68	1.52
1	B	127	ARG	C-O	6.44	1.31	1.24
1	C	145	THR	N-CA	6.44	1.51	1.46
1	C	267	GLU	CA-C	6.41	1.61	1.52
1	C	228	HIS	C-O	-6.41	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	207	SER	CA-C	-6.39	1.43	1.52
1	F	145	THR	CA-C	6.36	1.58	1.52
1	E	135	ARG	NE-CZ	6.34	1.40	1.33
1	C	165	ARG	N-CA	6.31	1.53	1.45
1	E	192	GLY	CA-C	6.29	1.60	1.51
1	C	252	ALA	CA-CB	6.25	1.63	1.53
1	A	227	GLY	C-O	6.24	1.29	1.23
1	E	185	PHE	CA-C	-6.23	1.45	1.52
1	D	230	SER	CA-C	6.20	1.61	1.52
1	E	247	THR	CA-C	6.19	1.61	1.52
1	B	196	HIS	CA-C	-6.18	1.45	1.52
1	F	114	ILE	CA-CB	6.18	1.63	1.54
1	F	185	PHE	C-O	6.18	1.31	1.23
1	E	119	ASN	C-O	-6.17	1.16	1.24
1	A	125	MET	SD-CE	-6.13	1.64	1.79
1	F	199	GLU	C-O	6.09	1.31	1.24
1	D	187	PRO	CA-C	6.09	1.60	1.52
1	A	220	ILE	CA-CB	6.08	1.62	1.54
1	D	195	ALA	CA-CB	-6.07	1.43	1.53
1	E	231	ASP	CA-C	6.02	1.59	1.52
1	B	211[A]	ASN	CA-CB	6.00	1.61	1.53
1	E	165	ARG	CA-C	5.99	1.59	1.52
1	B	117	ARG	NE-CZ	5.99	1.39	1.33
1	D	104	MET	CB-CG	5.98	1.70	1.52
1	D	114	ILE	CA-C	-5.96	1.45	1.52
1	C	182	ALA	CA-C	5.95	1.60	1.52
1	B	212	LEU	C-O	5.94	1.30	1.24
1	B	239	THR	CA-CB	5.91	1.61	1.53
1	D	170	ASP	CA-C	-5.90	1.45	1.53
1	B	120	ASN	CA-C	-5.86	1.45	1.52
1	C	218	HIS	CA-CB	5.84	1.62	1.53
1	A	189	SER	CA-C	-5.84	1.45	1.53
1	C	180	ILE	C-O	-5.84	1.18	1.24
1	B	236	MET	CG-SD	5.83	1.95	1.80
1	A	235	VAL	CA-CB	5.82	1.62	1.54
1	E	211[A]	ASN	C-O	5.81	1.30	1.24
1	E	215	THR	C-O	5.79	1.30	1.24
1	C	215	THR	CA-C	5.79	1.60	1.52
1	B	226	LEU	C-O	5.79	1.31	1.23
1	E	127	ARG	C-O	5.79	1.30	1.24
1	A	151	LYS	CA-C	5.77	1.60	1.52
1	B	217	VAL	CA-C	5.77	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	237	PHE	N-CA	5.77	1.52	1.45
1	A	168	HIS	CA-C	-5.76	1.45	1.53
1	C	119	ASN	C-O	5.75	1.30	1.24
1	E	226	LEU	C-O	5.73	1.31	1.23
1	D	127	ARG	C-O	5.73	1.30	1.24
1	C	260	SER	CA-C	-5.72	1.45	1.52
1	B	126	ASN	C-N	5.70	1.41	1.33
1	F	119	ASN	N-CA	-5.69	1.39	1.46
1	E	164	ALA	N-CA	5.69	1.52	1.46
1	B	119	ASN	CA-CB	5.69	1.63	1.53
1	C	154	THR	CA-C	-5.68	1.45	1.52
1	A	130	VAL	CA-C	-5.67	1.46	1.52
1	E	196	HIS	CA-C	-5.67	1.45	1.52
1	C	226	LEU	CA-C	-5.65	1.45	1.52
1	A	250	LEU	C-O	-5.63	1.16	1.23
1	E	136	LYS	CA-C	5.62	1.60	1.52
1	B	235	VAL	CA-CB	5.60	1.63	1.54
1	A	142[A]	SER	N-CA	5.59	1.53	1.46
1	C	253	ASP	CA-C	5.58	1.60	1.52
1	A	110[A]	ARG	CA-CB	5.57	1.60	1.53
1	D	237	PHE	CA-C	-5.56	1.47	1.53
1	D	195	ALA	CA-C	-5.56	1.45	1.52
1	F	158	ASP	C-O	-5.56	1.17	1.24
1	F	110[A]	ARG	N-CA	5.55	1.53	1.46
1	D	164	ALA	CA-C	-5.53	1.45	1.52
1	D	236	MET	SD-CE	5.51	1.93	1.79
1	C	135	ARG	NE-CZ	5.51	1.39	1.33
1	D	253	ASP	C-O	-5.51	1.17	1.24
1	E	143	ASN	C-O	-5.50	1.17	1.24
1	C	256	ARG	CA-C	-5.48	1.46	1.52
1	D	142[A]	SER	N-CA	5.47	1.53	1.46
1	B	211[A]	ASN	C-O	5.46	1.30	1.24
1	F	154	THR	CA-C	-5.45	1.46	1.52
1	B	204	THR	C-O	5.45	1.30	1.23
1	F	158	ASP	CA-C	5.44	1.59	1.52
1	F	141	TRP	CA-C	5.44	1.60	1.52
1	A	152	ILE	CA-C	-5.43	1.46	1.52
1	D	151	LYS	CA-C	5.43	1.59	1.52
1	C	149	PHE	CA-C	-5.42	1.46	1.52
1	D	156	MET	C-N	-5.42	1.25	1.33
1	E	261	LEU	CA-C	-5.40	1.45	1.52
1	E	123	PRO	CA-C	-5.38	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	217	VAL	CA-C	5.38	1.59	1.52
1	C	162	VAL	CA-CB	-5.37	1.47	1.54
1	E	160	LEU	CB-CG	-5.36	1.42	1.53
1	A	236	MET	SD-CE	5.34	1.92	1.79
1	E	241[A]	LYS	C-O	-5.33	1.17	1.23
1	A	155	GLY	C-N	-5.33	1.25	1.33
1	B	153	ASN	CA-C	-5.32	1.45	1.52
1	E	230	SER	N-CA	5.31	1.53	1.46
1	B	128	GLU	CA-CB	5.31	1.62	1.53
1	D	218	HIS	C-O	-5.30	1.18	1.24
1	C	116	TYR	C-O	5.30	1.30	1.23
1	D	104	MET	SD-CE	-5.28	1.66	1.79
1	D	202	PHE	CA-C	5.27	1.59	1.53
1	C	114	ILE	CA-CB	5.26	1.60	1.54
1	C	105	MET	SD-CE	5.21	1.92	1.79
1	B	195	ALA	CA-CB	5.21	1.63	1.53
1	F	229[A]	SER	CA-C	5.19	1.58	1.52
1	E	117	ARG	NE-CZ	5.19	1.38	1.33
1	B	117	ARG	CA-C	-5.17	1.46	1.52
1	D	155	GLY	C-O	5.17	1.28	1.23
1	A	197	PHE	N-CA	-5.15	1.39	1.46
1	D	255	ILE	CG1-CD1	-5.15	1.31	1.51
1	D	130	VAL	CA-C	-5.14	1.46	1.52
1	F	207	SER	CA-C	-5.14	1.45	1.52
1	D	207	SER	N-CA	5.12	1.52	1.46
1	F	251	SER	C-O	5.09	1.30	1.23
1	B	219	GLU	C-O	5.08	1.29	1.24
1	D	159	ILE	CA-CB	5.07	1.60	1.53
1	B	201	GLU	CA-C	5.07	1.60	1.53
1	D	189	SER	CA-C	-5.06	1.46	1.53
1	A	104	MET	CG-SD	5.06	1.93	1.80
1	E	166	GLY	C-O	5.03	1.30	1.24
1	F	135	ARG	CG-CD	5.02	1.67	1.52
1	A	232	PRO	C-O	-5.01	1.17	1.24

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	166	GLY	CA-C-N	-19.57	89.94	122.82
1	E	166	GLY	C-N-CA	-19.57	89.94	122.82
1	C	155	GLY	CA-C-N	-11.12	107.32	122.99
1	C	155	GLY	C-N-CA	-11.12	107.32	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	246	ASN	N-CA-C	10.84	127.82	113.30
1	A	155	GLY	CA-C-N	-10.45	106.31	122.62
1	A	155	GLY	C-N-CA	-10.45	106.31	122.62
1	F	245	ILE	CA-C-N	-10.10	106.84	122.49
1	F	245	ILE	C-N-CA	-10.10	106.84	122.49
1	A	267	GLU	N-CA-C	-9.60	94.82	109.41
1	D	267	GLU	N-CA-C	-9.21	95.25	109.52
1	B	119	ASN	CB-CA-C	8.97	128.73	109.99
1	B	170	ASP	CA-C-N	-8.92	108.37	122.73
1	B	170	ASP	C-N-CA	-8.92	108.37	122.73
1	C	201	GLU	N-CA-C	-8.91	97.33	110.52
1	E	170	ASP	CA-C-N	-8.84	109.22	122.83
1	E	170	ASP	C-N-CA	-8.84	109.22	122.83
1	A	265	PRO	N-CA-C	-8.54	98.40	111.13
1	F	105	MET	N-CA-C	8.44	122.72	109.81
1	B	254	ASP	N-CA-C	-8.17	101.64	111.69
1	E	167	ALA	CA-C-O	8.17	131.05	121.58
1	D	136	LYS	N-CA-C	-8.12	102.40	111.82
1	F	201	GLU	N-CA-C	-7.88	98.85	110.52
1	B	231	ASP	N-CA-C	7.87	119.68	109.93
1	E	155	GLY	CA-C-N	-7.82	111.00	122.65
1	E	155	GLY	C-N-CA	-7.82	111.00	122.65
1	C	119	ASN	N-CA-C	7.81	119.80	111.28
1	A	266	LYS	CB-CA-C	7.62	124.58	110.10
1	D	245	ILE	N-CA-C	7.49	118.26	110.62
1	B	246	ASN	N-CA-C	7.43	122.17	113.18
1	E	254	ASP	N-CA-C	-7.32	102.68	111.69
1	E	231	ASP	N-CA-C	7.27	118.81	109.65
1	E	205	THR	N-CA-C	-7.26	103.74	112.59
1	B	168	HIS	N-CA-C	-7.24	102.55	112.03
1	E	212	LEU	N-CA-C	7.21	118.78	111.07
1	C	144	VAL	N-CA-C	7.12	119.17	111.77
1	E	142[A]	SER	CA-CB-OG	-7.08	96.93	111.10
1	E	119	ASN	CB-CA-C	7.08	125.10	110.31
1	D	265	PRO	CA-C-N	6.88	134.09	121.70
1	D	265	PRO	C-N-CA	6.88	134.09	121.70
1	E	168	HIS	N-CA-C	-6.80	102.59	111.71
1	B	245	ILE	CA-C-N	-6.79	108.33	121.58
1	B	245	ILE	C-N-CA	-6.79	108.33	121.58
1	E	265	PRO	CA-C-N	6.79	133.92	121.70
1	E	265	PRO	C-N-CA	6.79	133.92	121.70
1	C	156	MET	CA-C-O	6.78	127.68	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	265	PRO	N-CA-C	-6.76	101.26	111.41
1	F	255	ILE	N-CA-C	-6.75	103.74	110.62
1	D	156	MET	CA-C-O	-6.74	113.72	121.47
1	F	156	MET	CB-CA-C	6.70	121.05	110.19
1	B	154	THR	N-CA-CB	-6.69	101.19	111.56
1	C	204	THR	N-CA-C	6.67	119.08	109.14
1	E	246	ASN	N-CA-CB	6.67	121.75	110.49
1	E	245	ILE	CA-C-N	-6.65	108.85	121.54
1	E	245	ILE	C-N-CA	-6.65	108.85	121.54
1	C	159	ILE	N-CA-CB	-6.64	103.31	111.67
1	A	226	LEU	CA-C-N	-6.55	115.34	122.55
1	A	226	LEU	C-N-CA	-6.55	115.34	122.55
1	B	212	LEU	N-CA-C	6.54	118.07	111.07
1	A	156	MET	O-C-N	-6.53	115.21	123.24
1	B	243	VAL	CA-C-N	-6.52	110.57	121.39
1	B	243	VAL	C-N-CA	-6.52	110.57	121.39
1	F	248	PHE	N-CA-C	6.44	119.56	110.23
1	E	230	SER	N-CA-C	-6.41	105.45	113.28
1	F	210	THR	N-CA-C	-6.39	97.99	108.41
1	D	247	THR	N-CA-CB	-6.27	101.31	110.53
1	C	162	VAL	CB-CA-C	-6.25	101.30	110.62
1	A	168	HIS	CA-C-N	-6.21	113.61	122.00
1	A	168	HIS	C-N-CA	-6.21	113.61	122.00
1	A	156	MET	CA-C-O	-6.19	113.87	121.11
1	B	127	ARG	CB-CA-C	6.19	121.06	110.79
1	C	156	MET	CB-CA-C	6.18	121.02	109.71
1	F	119	ASN	N-CA-C	6.16	118.00	111.28
1	D	246	ASN	N-CA-CB	6.15	120.11	110.46
1	F	199	GLU	N-CA-C	6.12	118.75	111.71
1	F	111	LYS	CB-CA-C	-6.11	98.86	109.86
1	C	245	ILE	CA-C-N	-6.09	111.50	122.46
1	C	245	ILE	C-N-CA	-6.09	111.50	122.46
1	E	119	ASN	CA-CB-CG	6.05	118.65	112.60
1	B	111	LYS	N-CA-C	-6.01	99.17	108.42
1	C	207	SER	N-CA-C	-6.01	105.44	112.89
1	C	222	HIS	CB-CA-C	-6.00	99.15	110.67
1	C	246	ASN	N-CA-C	5.99	120.39	112.72
1	F	227	GLY	N-CA-C	-5.99	104.54	112.81
1	B	175	ASP	CA-C-N	-5.94	112.30	121.45
1	B	175	ASP	C-N-CA	-5.94	112.30	121.45
1	B	155	GLY	O-C-N	5.94	128.41	122.77
1	E	221	GLY	N-CA-C	-5.93	105.61	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	122	THR	OG1-CB-CG2	-5.92	97.46	109.30
1	C	257	GLY	N-CA-C	-5.90	105.51	113.24
1	C	161	VAL	N-CA-C	-5.89	99.26	107.80
1	E	126	ASN	CA-C-O	-5.86	115.34	121.55
1	E	156	MET	CA-C-O	5.83	127.27	120.80
1	A	119	ASN	CB-CA-C	-5.79	101.13	110.74
1	A	265	PRO	CA-C-N	5.78	132.10	121.70
1	A	265	PRO	C-N-CA	5.78	132.10	121.70
1	E	233	LYS	CA-C-N	-5.75	113.19	121.42
1	E	233	LYS	C-N-CA	-5.75	113.19	121.42
1	A	153	ASN	CA-C-N	-5.75	110.59	121.63
1	A	153	ASN	C-N-CA	-5.75	110.59	121.63
1	F	235	VAL	N-CA-C	-5.74	103.62	111.89
1	C	239	THR	OG1-CB-CG2	-5.71	97.88	109.30
1	A	149	PHE	CA-C-N	-5.70	112.88	122.29
1	A	149	PHE	C-N-CA	-5.70	112.88	122.29
1	C	255	ILE	N-CA-C	-5.69	104.81	110.62
1	F	256	ARG	CA-C-N	-5.69	112.99	120.22
1	F	256	ARG	C-N-CA	-5.69	112.99	120.22
1	C	238	PRO	CA-C-N	-5.66	114.44	122.94
1	C	238	PRO	C-N-CA	-5.66	114.44	122.94
1	D	167	ALA	CA-C-N	-5.65	113.09	122.08
1	D	167	ALA	C-N-CA	-5.65	113.09	122.08
1	A	136	LYS	N-CA-C	-5.63	105.14	111.28
1	C	254	ASP	N-CA-C	-5.63	104.53	111.40
1	F	158	ASP	N-CA-C	-5.60	105.09	111.14
1	C	148	LYS	CB-CA-C	-5.59	102.08	110.24
1	A	156	MET	CB-CA-C	5.58	121.05	109.38
1	B	247	THR	OG1-CB-CG2	-5.57	98.15	109.30
1	F	162	VAL	CB-CA-C	-5.57	101.92	110.50
1	E	155	GLY	N-CA-C	-5.55	103.73	112.61
1	D	267	GLU	CA-C-N	5.54	131.68	121.70
1	D	267	GLU	C-N-CA	5.54	131.68	121.70
1	B	190	GLY	N-CA-C	5.50	120.99	110.86
1	C	166	GLY	N-CA-C	5.50	121.35	111.34
1	E	138	PHE	N-CA-C	5.50	117.27	111.28
1	B	252	ALA	CA-C-N	5.47	128.16	120.28
1	B	252	ALA	C-N-CA	5.47	128.16	120.28
1	F	159	ILE	N-CA-CB	-5.46	105.12	111.83
1	A	253	ASP	CB-CA-C	-5.45	102.32	110.88
1	E	175	ASP	CA-C-N	-5.45	115.09	121.85
1	E	175	ASP	C-N-CA	-5.45	115.09	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	225	GLY	N-CA-C	5.44	123.09	115.43
1	F	254	ASP	N-CA-C	-5.43	104.78	111.40
1	E	229[A]	SER	N-CA-C	-5.43	100.55	109.40
1	D	255	ILE	N-CA-C	-5.42	105.43	110.53
1	F	257	GLY	N-CA-C	-5.41	106.13	113.37
1	F	181	LEU	N-CA-C	5.38	118.07	111.82
1	D	130	VAL	CB-CA-C	-5.38	105.08	111.97
1	B	119	ASN	CA-CB-CG	5.37	117.97	112.60
1	D	169	GLY	CA-C-N	-5.37	113.58	122.39
1	D	169	GLY	C-N-CA	-5.37	113.58	122.39
1	B	153	ASN	CA-C-N	-5.36	111.80	121.62
1	B	153	ASN	C-N-CA	-5.36	111.80	121.62
1	B	185	PHE	N-CA-CB	-5.34	102.31	110.85
1	A	254	ASP	CB-CA-C	-5.32	102.52	110.88
1	E	181	LEU	N-CA-C	-5.32	106.92	113.41
1	C	189	SER	N-CA-C	-5.31	103.68	110.53
1	F	228	HIS	CA-CB-CG	-5.30	108.50	113.80
1	F	174	PHE	N-CA-CB	-5.28	102.42	110.39
1	E	226	LEU	N-CA-C	5.27	117.34	110.43
1	E	233	LYS	CB-CA-C	-5.26	100.07	110.27
1	B	230	SER	N-CA-C	-5.21	106.43	112.89
1	B	154	THR	CB-CA-C	5.21	120.30	110.62
1	E	200	ASP	CA-C-N	-5.20	112.19	122.02
1	E	200	ASP	C-N-CA	-5.20	112.19	122.02
1	D	173	ALA	N-CA-C	5.19	117.56	110.24
1	E	142[A]	SER	N-CA-C	5.19	117.34	111.11
1	D	119	ASN	N-CA-C	5.19	117.34	111.11
1	C	237	PHE	CA-C-N	5.19	124.85	119.56
1	C	237	PHE	C-N-CA	5.19	124.85	119.56
1	D	253	ASP	N-CA-C	5.13	116.56	111.07
1	A	249	ARG	CA-CB-CG	-5.12	103.85	114.10
1	C	210	THR	N-CA-C	-5.12	100.07	108.41
1	C	157	ALA	N-CA-C	-5.09	102.52	110.42
1	B	142[A]	SER	CA-CB-OG	-5.08	100.94	111.10
1	A	218	HIS	N-CA-C	-5.06	105.68	111.14
1	D	223	SER	N-CA-C	5.05	118.21	111.75
1	B	261	LEU	CB-CG-CD1	-5.03	95.61	110.70
1	C	167	ALA	CA-C-N	-5.03	111.85	121.15
1	C	167	ALA	C-N-CA	-5.03	111.85	121.15
1	C	226	LEU	CA-C-N	-5.01	117.97	122.43
1	C	226	LEU	C-N-CA	-5.01	117.97	122.43
1	B	189	SER	CB-CA-C	-5.01	100.77	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	105	MET	CG-SD-CE	-5.01	89.87	100.90
1	E	167	ALA	CA-C-N	-5.01	112.09	121.81
1	E	167	ALA	C-N-CA	-5.01	112.09	121.81
1	A	109	TRP	N-CA-CB	5.01	117.35	109.69

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	266	LYS	CA
1	F	246	ASN	CA

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	MET	Mainchain
1	A	265	PRO	Peptide
1	B	265	PRO	Peptide
1	B	266	LYS	Peptide
1	C	245	ILE	Peptide
1	C	266	LYS	Peptide
1	E	125	MET	Mainchain
1	E	167	ALA	Peptide,Mainchain
1	E	266	LYS	Peptide
1	F	104	MET	Peptide
1	F	245	ILE	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	1295	0	1210	59	0
1	B	1295	0	1210	122	1
1	C	1295	0	1212	108	0
1	D	1295	0	1210	48	0
1	E	1295	0	1210	78	1
1	F	1295	0	1210	113	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
4	A	5	0	4	0	0
4	D	5	0	4	0	0
5	B	4	0	3	1	0
5	E	4	0	3	1	0
6	C	3	0	0	1	0
6	F	3	0	0	1	0
7	A	46	0	0	11	0
7	B	67	0	0	10	0
7	C	51	0	0	2	0
7	D	44	0	0	4	0
7	E	59	0	0	9	0
7	F	41	0	0	5	0
All	All	8132	0	7276	483	1

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 32.

All (483) 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:F:136:LYS:CE	1:F:245:ILE:HD11	1.33	1.58
1:C:136:LYS:CE	1:C:245:ILE:HD11	1.32	1.55
1:F:136:LYS:HE2	1:F:245:ILE:CD1	1.42	1.49
1:C:136:LYS:HE2	1:C:245:ILE:CD1	1.58	1.32
1:C:136:LYS:CE	1:C:245:ILE:CD1	2.08	1.31
1:C:267:GLU:CB	1:C:268:ASN:HB2	1.61	1.29
1:F:267:GLU:HB2	1:F:268:ASN:CA	1.66	1.25
1:C:264:ASP:O	1:C:266:LYS:HG2	1.36	1.25
1:B:266:LYS:HA	1:B:266:LYS:NZ	1.54	1.23
1:F:206:HIS:CD2	1:F:208:GLY:H	1.57	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:MET:HA	1:B:105:MET:CE	1.67	1.21
1:E:167:ALA:HB1	7:E:688:HOH:O	1.37	1.20
1:C:265:PRO:HA	1:C:266:LYS:HB2	1.21	1.19
1:C:267:GLU:HB2	1:C:268:ASN:CB	1.73	1.19
1:E:231:ASP:OD2	1:E:232:PRO:CD	1.91	1.19
1:B:105:MET:CA	1:B:105:MET:HE3	1.75	1.16
1:B:231:ASP:OD2	1:B:232:PRO:CD	1.94	1.16
1:A:267:GLU:HB2	1:A:268:ASN:HB2	1.23	1.15
1:E:246:ASN:O	1:E:248:PHE:N	1.78	1.15
1:F:136:LYS:HE3	1:F:245:ILE:HD11	1.24	1.14
1:B:231:ASP:OD2	1:B:232:PRO:HD2	1.46	1.12
1:E:105:MET:HA	1:E:105:MET:HE3	1.30	1.12
1:E:231:ASP:OD2	1:E:232:PRO:HD2	1.45	1.12
1:B:263:GLY:O	1:B:264:ASP:CB	1.97	1.12
1:C:265:PRO:HA	1:C:266:LYS:CB	1.79	1.10
1:B:266:LYS:HA	1:B:266:LYS:HZ2	1.02	1.09
1:F:230:SER:O	1:F:232:PRO:HD3	1.52	1.09
1:F:136:LYS:CE	1:F:245:ILE:CD1	2.14	1.08
1:B:104:MET:HE3	1:C:240:TYR:HD2	1.19	1.07
1:F:267:GLU:CB	1:F:268:ASN:HA	1.80	1.07
1:A:267:GLU:HB2	1:A:268:ASN:CB	1.84	1.07
1:C:267:GLU:HG3	1:C:268:ASN:HB3	1.33	1.05
1:C:244:ASP:H	1:C:247:THR:HG21	1.21	1.05
1:B:156:MET:HE3	1:B:156:MET:HA	1.39	1.05
1:B:107:PRO:HD2	7:B:431:HOH:O	1.57	1.04
1:D:241[A]:LYS:HE3	7:D:615:HOH:O	1.54	1.04
1:B:263:GLY:O	1:B:264:ASP:HB2	1.52	1.03
1:F:244:ASP:CG	1:F:247:THR:HG22	1.83	1.03
1:F:136:LYS:HG2	1:F:213:PHE:CE2	1.94	1.02
1:B:105:MET:HA	1:B:105:MET:HE3	1.06	1.02
1:C:206:HIS:CD2	1:C:208:GLY:H	1.77	1.01
1:B:267:GLU:HG2	1:B:268:ASN:HB2	1.42	1.00
1:A:117:ARG:NH1	1:A:154:THR:HA	1.77	1.00
1:B:206:HIS:HD2	1:B:208:GLY:H	1.08	1.00
1:C:136:LYS:HE2	1:C:245:ILE:HD13	1.40	1.00
1:E:167:ALA:HB2	1:E:173:ALA:CB	1.93	0.99
1:C:266:LYS:HE2	1:C:266:LYS:HA	1.45	0.98
1:C:136:LYS:HE3	1:C:245:ILE:CD1	1.83	0.98
1:E:127:ARG:NH2	7:E:731:HOH:O	1.97	0.98
1:F:136:LYS:HE2	1:F:245:ILE:HD13	1.40	0.98
1:F:265:PRO:HA	1:F:266:LYS:HE2	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:267:GLU:HB2	1:F:268:ASN:HA	0.97	0.96
1:F:206:HIS:HD2	1:F:208:GLY:N	1.63	0.95
1:E:206:HIS:HD2	1:E:208:GLY:H	0.97	0.95
1:A:231:ASP:OD2	1:A:233:LYS:HE3	1.65	0.95
1:E:107:PRO:HD2	7:E:705:HOH:O	1.65	0.95
1:B:105:MET:HG3	1:B:261:LEU:CD2	1.98	0.93
1:B:267:GLU:HG2	1:B:268:ASN:CB	1.98	0.93
1:C:206:HIS:HD2	1:C:208:GLY:H	0.93	0.92
1:C:244:ASP:H	1:C:247:THR:CG2	1.81	0.92
1:C:136:LYS:HE3	1:C:245:ILE:HD11	0.94	0.92
1:E:106:GLY:HA2	1:F:181:LEU:HD11	1.51	0.92
1:C:267:GLU:CB	1:C:268:ASN:CB	2.42	0.91
1:C:267:GLU:HG3	1:C:268:ASN:CB	2.00	0.91
1:F:265:PRO:HA	1:F:266:LYS:HB2	1.53	0.90
1:B:105:MET:HB2	1:C:238:PRO:O	1.71	0.90
1:D:152:ILE:HD11	1:D:157:ALA:HB2	1.51	0.90
1:E:105:MET:HA	1:E:105:MET:CE	2.00	0.89
1:E:206:HIS:CD2	1:E:208:GLY:H	1.88	0.89
1:E:108:VAL:HG22	1:F:239:THR:HG21	1.54	0.89
1:B:206:HIS:CD2	1:B:208:GLY:H	1.92	0.88
1:B:104:MET:HE2	1:C:215:THR:HA	1.54	0.88
1:D:117:ARG:HD3	7:D:617:HOH:O	1.72	0.88
1:B:104:MET:HE3	1:C:240:TYR:CD2	2.08	0.88
1:A:246:ASN:ND2	7:A:918:HOH:O	1.93	0.87
1:E:107:PRO:CD	7:E:705:HOH:O	2.19	0.86
1:D:104:MET:HE1	1:E:215:THR:HA	1.57	0.86
1:A:267:GLU:CB	1:A:268:ASN:HB2	2.06	0.86
1:E:127:ARG:CZ	7:E:731:HOH:O	2.21	0.86
1:E:167:ALA:HB2	1:E:173:ALA:HB2	1.57	0.85
1:A:117:ARG:HH12	1:A:154:THR:HA	1.41	0.85
1:F:265:PRO:CA	1:F:266:LYS:HB2	2.06	0.84
1:F:206:HIS:CD2	1:F:208:GLY:N	2.41	0.84
1:B:148:LYS:HB3	1:B:148:LYS:HZ2	1.40	0.84
1:F:231:ASP:OD2	1:F:233:LYS:HG3	1.76	0.84
1:D:206:HIS:HD2	1:D:208:GLY:H	1.23	0.84
1:B:104:MET:N	6:C:474:AZI:N3	2.25	0.84
1:C:230:SER:O	1:C:232:PRO:HD3	1.79	0.82
1:C:244:ASP:N	1:C:247:THR:CG2	2.41	0.82
1:F:244:ASP:H	1:F:247:THR:CG2	1.93	0.81
1:C:267:GLU:CG	1:C:268:ASN:CB	2.59	0.81
1:E:231:ASP:OD2	1:E:232:PRO:N	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:ALA:HB2	1:E:173:ALA:CA	2.12	0.80
1:B:106:GLY:HA2	1:C:181:LEU:HD11	1.63	0.80
1:E:108:VAL:CG2	1:F:239:THR:HG21	2.11	0.79
1:F:211[A]:ASN:HD22	1:F:214:LEU:H	1.30	0.79
1:C:206:HIS:HD2	1:C:208:GLY:N	1.78	0.79
1:C:264:ASP:O	1:C:266:LYS:CG	2.26	0.79
1:C:136:LYS:HG2	1:C:213:PHE:CD2	2.17	0.79
1:C:231:ASP:OD2	1:C:233:LYS:N	2.16	0.78
1:B:231:ASP:OD2	1:B:232:PRO:N	2.16	0.78
1:F:167:ALA:HA	1:F:173:ALA:HB2	1.66	0.78
1:B:265:PRO:CB	1:B:266:LYS:HB2	2.14	0.78
1:B:105:MET:HE3	1:B:106:GLY:N	1.98	0.77
1:B:105:MET:HE3	1:B:106:GLY:H	1.50	0.77
1:A:136:LYS:HD2	1:A:245:ILE:HD11	1.65	0.77
1:C:244:ASP:CG	1:C:247:THR:HG22	2.11	0.76
1:B:146[A]:PRO:HB3	1:B:266:LYS:HG2	1.67	0.76
1:A:105:MET:HE1	1:B:179:GLY:HA2	1.67	0.76
1:A:264:ASP:HB2	1:A:265:PRO:CD	2.15	0.76
1:D:265:PRO:HA	1:D:266:LYS:HB2	1.68	0.76
1:F:244:ASP:H	1:F:247:THR:HG21	1.50	0.76
1:E:167:ALA:HB2	1:E:173:ALA:HA	1.66	0.76
1:B:117:ARG:NH1	1:B:155:GLY:O	2.19	0.76
1:F:230:SER:O	1:F:232:PRO:CD	2.32	0.74
1:B:105:MET:CE	1:C:179:GLY:O	2.35	0.74
1:B:266:LYS:HZ2	1:B:266:LYS:CA	1.92	0.74
1:C:241:LYS:HE3	1:C:243:VAL:HG11	1.70	0.74
1:B:265:PRO:HA	1:B:266:LYS:HD2	1.68	0.74
1:B:107:PRO:CD	7:B:431:HOH:O	2.22	0.74
1:A:104:MET:N	5:B:374:ACT:OXT	2.21	0.74
1:D:145:THR:HB	1:D:146[A]:PRO:HD2	1.67	0.74
1:B:263:GLY:O	1:B:264:ASP:HB3	1.84	0.74
1:B:108:VAL:HG22	1:C:239:THR:HG21	1.68	0.73
1:A:267:GLU:HB2	1:A:268:ASN:CG	2.13	0.73
1:E:265:PRO:HA	1:E:266:LYS:HB2	1.71	0.73
1:C:244:ASP:O	1:C:246:ASN:N	2.22	0.73
1:F:267:GLU:HB2	1:F:268:ASN:CB	2.18	0.73
1:C:267:GLU:CG	1:C:268:ASN:HB3	2.17	0.73
1:F:167:ALA:HA	1:F:173:ALA:CB	2.18	0.73
1:F:206:HIS:HD2	1:F:208:GLY:H	0.84	0.73
1:A:135:ARG:HH11	1:A:135:ARG:HG2	1.52	0.73
1:C:265:PRO:CA	1:C:266:LYS:HB2	2.11	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:MET:HE2	1:E:215:THR:HG23	1.71	0.73
1:B:265:PRO:CA	1:B:266:LYS:HB2	2.20	0.72
1:E:104:MET:HE2	1:F:215:THR:HA	1.71	0.72
1:B:156:MET:HA	1:B:156:MET:CE	2.19	0.72
1:C:241:LYS:HE3	1:C:243:VAL:CG1	2.19	0.72
1:D:206:HIS:CD2	1:D:208:GLY:H	2.08	0.71
1:A:135:ARG:HD3	7:A:915:HOH:O	1.89	0.71
1:A:268:ASN:OXT	7:A:905:HOH:O	2.07	0.71
1:F:206:HIS:HE1	7:F:810:HOH:O	1.72	0.71
1:F:265:PRO:CA	1:F:266:LYS:HE2	2.19	0.71
1:A:206:HIS:HD2	1:A:208:GLY:H	1.36	0.71
1:A:246:ASN:HB2	7:A:918:HOH:O	1.91	0.70
1:A:241[A]:LYS:HD3	7:A:910:HOH:O	1.92	0.70
1:C:267:GLU:CG	1:C:268:ASN:HB2	2.20	0.70
1:A:145:THR:HB	1:A:146[A]:PRO:HD2	1.72	0.70
1:D:249:ARG:HH21	1:D:249:ARG:HG3	1.56	0.70
1:E:231:ASP:OD2	1:E:231:ASP:C	2.35	0.70
1:B:139:GLN:HG3	7:B:399:HOH:O	1.91	0.70
1:B:104:MET:CE	1:C:240:TYR:HD2	2.00	0.69
1:C:267:GLU:HB2	1:C:268:ASN:HB2	0.79	0.69
1:F:104:MET:HE2	1:F:104:MET:HA	1.73	0.69
1:F:244:ASP:N	1:F:247:THR:CG2	2.54	0.69
1:B:105:MET:HE3	1:B:105:MET:C	2.17	0.69
1:E:206:HIS:HD2	1:E:208:GLY:N	1.81	0.69
1:E:104:MET:N	6:F:774:AZI:N3	2.40	0.68
1:C:265:PRO:HA	1:C:266:LYS:CG	2.22	0.68
1:F:211[A]:ASN:HD21	1:F:213:PHE:HB3	1.56	0.68
1:B:105:MET:CE	1:B:106:GLY:H	2.06	0.68
1:C:135:ARG:NH2	1:C:139:GLN:OE1	2.26	0.68
1:F:229[A]:SER:HB2	1:F:253:ASP:OD1	1.94	0.68
1:F:267:GLU:CB	1:F:268:ASN:CA	2.52	0.68
1:F:267:GLU:HG3	1:F:268:ASN:HB2	1.75	0.68
1:B:148:LYS:HB3	1:B:148:LYS:NZ	2.07	0.68
1:E:104:MET:HE3	1:F:240:TYR:HD2	1.59	0.68
1:F:266:LYS:HA	1:F:266:LYS:CE	2.23	0.68
1:E:108:VAL:HG22	1:F:239:THR:CG2	2.24	0.67
1:E:265:PRO:CA	1:E:266:LYS:HB2	2.24	0.67
1:B:145:THR:HB	1:B:146[A]:PRO:HD2	1.77	0.67
1:E:145:THR:HB	1:E:146[A]:PRO:HD2	1.77	0.66
1:B:108:VAL:CG2	1:C:239:THR:HG21	2.25	0.66
1:B:105:MET:HG3	1:B:261:LEU:HD21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:MET:HG3	1:B:261:LEU:HD23	1.76	0.66
1:B:266:LYS:NZ	1:B:266:LYS:CA	2.46	0.66
1:F:265:PRO:HA	1:F:266:LYS:CB	2.24	0.65
1:D:264:ASP:HB2	1:D:265:PRO:HD2	1.78	0.65
1:D:250:LEU:HB2	1:D:255:ILE:HD11	1.77	0.65
1:D:152:ILE:HD11	1:D:157:ALA:CB	2.27	0.65
1:B:105:MET:CE	1:B:105:MET:CA	2.49	0.65
1:D:152:ILE:CD1	1:D:157:ALA:HB2	2.27	0.65
1:A:264:ASP:HB2	1:A:265:PRO:HD2	1.79	0.65
1:B:105:MET:HE1	1:C:179:GLY:C	2.22	0.64
1:D:264:ASP:HB2	1:D:265:PRO:CD	2.27	0.64
1:D:267:GLU:HB2	1:D:268:ASN:CG	2.22	0.64
1:C:104:MET:HE3	1:C:104:MET:HA	1.79	0.64
1:B:231:ASP:OD2	1:B:231:ASP:C	2.41	0.64
1:C:266:LYS:HA	1:C:266:LYS:CE	2.16	0.64
1:F:104:MET:HA	1:F:104:MET:CE	2.28	0.63
1:E:255:ILE:O	1:E:259:GLN:HB2	1.97	0.63
1:C:244:ASP:O	1:C:247:THR:CG2	2.46	0.63
1:D:104:MET:CE	1:E:215:THR:HG23	2.29	0.63
1:B:241[A]:LYS:HD2	7:B:411:HOH:O	1.99	0.63
1:B:266:LYS:HA	1:B:266:LYS:HZ3	1.62	0.63
1:D:249:ARG:HG3	1:D:249:ARG:NH2	2.13	0.63
1:E:251:SER:O	1:E:254:ASP:N	2.31	0.62
1:B:105:MET:HE1	1:C:179:GLY:O	2.00	0.62
1:F:266:LYS:HE2	1:F:266:LYS:CA	2.29	0.62
1:B:139:GLN:CG	7:B:399:HOH:O	2.47	0.62
1:C:211[A]:ASN:HD22	1:C:214:LEU:H	1.47	0.62
1:F:244:ASP:O	1:F:247:THR:CG2	2.46	0.62
1:F:265:PRO:HA	1:F:266:LYS:CE	2.26	0.62
1:C:245:ILE:HG23	1:C:245:ILE:O	2.01	0.61
1:B:251:SER:O	1:B:254:ASP:N	2.29	0.61
1:D:104:MET:N	5:E:674:ACT:O	2.33	0.61
1:C:206:HIS:CD2	1:C:208:GLY:N	2.61	0.61
1:A:246:ASN:CB	7:A:918:HOH:O	2.47	0.61
1:A:135:ARG:HH11	1:A:135:ARG:CG	2.14	0.61
1:B:106:GLY:HA2	1:C:181:LEU:CD1	2.31	0.61
1:B:105:MET:CB	1:C:238:PRO:O	2.46	0.60
1:B:105:MET:HB3	1:C:239:THR:HA	1.83	0.60
1:B:180:ILE:HD12	7:B:419:HOH:O	2.01	0.60
1:E:246:ASN:C	1:E:246:ASN:OD1	2.43	0.60
1:E:246:ASN:O	1:E:247:THR:C	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:THR:N	1:B:265:PRO:HD3	2.16	0.59
1:D:267:GLU:HB2	1:D:268:ASN:HB2	1.84	0.59
1:A:259:GLN:NE2	7:A:886:HOH:O	2.32	0.59
1:C:136:LYS:HG2	1:C:213:PHE:CE2	2.38	0.59
1:A:117:ARG:NH1	1:A:154:THR:CA	2.61	0.59
1:D:250:LEU:HB2	1:D:255:ILE:CD1	2.31	0.59
1:C:266:LYS:O	1:C:267:GLU:O	2.21	0.59
1:F:265:PRO:CB	1:F:266:LYS:HB2	2.32	0.59
1:B:180:ILE:HD13	7:B:386:HOH:O	2.03	0.58
1:B:267:GLU:CG	1:B:268:ASN:HB2	2.26	0.58
1:B:146[A]:PRO:HB3	1:B:266:LYS:CG	2.33	0.58
1:B:265:PRO:HA	1:B:266:LYS:HB2	1.85	0.58
1:E:106:GLY:HA2	1:F:181:LEU:CD1	2.29	0.58
1:F:231:ASP:CG	1:F:233:LYS:HG3	2.27	0.58
1:A:206:HIS:CD2	1:A:208:GLY:H	2.19	0.58
1:F:244:ASP:CG	1:F:247:THR:CG2	2.71	0.58
1:B:146[A]:PRO:HB3	1:B:266:LYS:HD3	1.85	0.57
1:E:265:PRO:C	1:E:266:LYS:HE2	2.29	0.57
1:A:117:ARG:NE	7:A:896:HOH:O	2.38	0.57
1:B:231:ASP:CG	1:B:232:PRO:CD	2.77	0.57
1:C:244:ASP:O	1:C:247:THR:HG23	2.04	0.57
1:F:244:ASP:CA	1:F:247:THR:CG2	2.83	0.57
1:A:105:MET:HE1	1:B:179:GLY:CA	2.34	0.57
1:E:105:MET:CG	1:E:261:LEU:HD21	2.35	0.57
1:F:244:ASP:O	1:F:247:THR:HG22	2.05	0.57
1:A:145:THR:HB	1:A:146[A]:PRO:CD	2.35	0.57
1:D:145:THR:HB	1:D:146[A]:PRO:CD	2.35	0.57
1:D:267:GLU:HB2	1:D:268:ASN:CB	2.35	0.57
1:A:105:MET:HE3	1:B:179:GLY:O	2.05	0.56
1:B:180:ILE:CD1	7:B:419:HOH:O	2.53	0.56
1:E:237:PHE:CD1	1:E:238:PRO:HD2	2.39	0.56
1:A:114:ILE:O	1:A:149:PHE:HA	2.06	0.56
1:C:241:LYS:HD3	7:C:503:HOH:O	2.05	0.56
1:F:211[A]:ASN:ND2	1:F:213:PHE:HB3	2.20	0.56
1:E:256:ARG:O	1:E:260:SER:HB3	2.04	0.56
1:A:113:TYR:C	1:A:114:ILE:HG13	2.30	0.56
1:F:136:LYS:HG2	1:F:213:PHE:HE2	1.61	0.56
1:B:146[A]:PRO:CB	1:B:266:LYS:HG2	2.35	0.56
1:F:136:LYS:HE2	1:F:245:ILE:HD11	0.98	0.56
1:F:207:SER:HB2	1:F:242:TYR:CE2	2.41	0.56
1:A:231:ASP:CG	1:A:233:LYS:HE3	2.29	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:VAL:HG22	1:C:239:THR:CG2	2.37	0.55
1:C:218:HIS:CE1	1:C:228:HIS:CD2	2.93	0.55
1:C:244:ASP:C	1:C:246:ASN:N	2.64	0.55
1:E:105:MET:HG2	1:E:261:LEU:CD2	2.36	0.55
1:C:229[A]:SER:HB2	1:C:253:ASP:OD1	2.06	0.55
1:F:244:ASP:CB	1:F:247:THR:HG22	2.37	0.55
1:B:144:VAL:C	1:B:265:PRO:HD3	2.32	0.55
1:B:145:THR:HB	1:B:146[A]:PRO:CD	2.35	0.55
1:C:244:ASP:OD1	1:C:247:THR:HG22	2.06	0.55
1:E:167:ALA:CB	7:E:710:HOH:O	2.55	0.55
1:A:176:GLY:HA2	1:A:200:ASP:OD1	2.08	0.54
1:F:135:ARG:NH2	1:F:139:GLN:OE1	2.36	0.54
1:F:265:PRO:C	1:F:266:LYS:HE2	2.31	0.54
1:C:267:GLU:HA	7:C:487:HOH:O	2.05	0.54
1:E:121:TYR:CE1	1:E:127:ARG:HG2	2.42	0.54
1:E:180:ILE:HD13	7:E:684:HOH:O	2.07	0.54
1:F:167:ALA:CA	1:F:173:ALA:HB2	2.35	0.54
1:F:217:VAL:HG12	1:F:235:VAL:HG21	1.90	0.54
1:A:267:GLU:CB	1:A:268:ASN:CB	2.73	0.54
1:F:136:LYS:HE3	1:F:245:ILE:CD1	2.10	0.54
1:C:266:LYS:C	1:C:267:GLU:O	2.50	0.54
1:C:266:LYS:HE2	1:C:266:LYS:CA	2.29	0.54
1:B:246:ASN:O	1:B:246:ASN:CG	2.50	0.53
1:B:267:GLU:HG2	1:B:268:ASN:CG	2.33	0.53
1:E:105:MET:HB2	1:F:238:PRO:O	2.07	0.53
1:D:114:ILE:O	1:D:149:PHE:HA	2.09	0.53
1:E:167:ALA:CB	1:E:173:ALA:HA	2.35	0.53
1:E:211[A]:ASN:HD22	1:E:214:LEU:H	1.54	0.53
1:C:244:ASP:O	1:C:247:THR:HG22	2.09	0.53
1:F:185:PHE:N	1:F:185:PHE:CD1	2.76	0.53
1:A:117:ARG:HD3	7:A:896:HOH:O	2.09	0.53
1:F:167:ALA:CA	1:F:173:ALA:CB	2.85	0.53
1:D:259:GLN:NE2	7:D:593:HOH:O	2.38	0.53
1:E:105:MET:HB3	1:F:239:THR:HA	1.91	0.53
1:C:104:MET:HA	1:C:104:MET:CE	2.38	0.52
1:E:266:LYS:HE2	1:E:266:LYS:N	2.24	0.52
1:B:104:MET:HE2	1:C:215:THR:CA	2.34	0.52
1:F:218:HIS:CE1	1:F:228:HIS:NE2	2.77	0.52
1:A:114:ILE:CD1	1:A:147:LEU:HD22	2.38	0.52
1:A:213:PHE:O	1:A:217:VAL:HG23	2.10	0.52
1:C:264:ASP:C	1:C:266:LYS:HG2	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:PHE:CG	1:E:238:PRO:HD2	2.45	0.52
1:E:105:MET:CE	1:F:179:GLY:O	2.57	0.52
1:F:110[A]:ARG:HG3	1:F:110[A]:ARG:HH11	1.74	0.52
1:D:136:LYS:HD2	1:D:245:ILE:HD11	1.92	0.52
1:E:125:MET:HG3	1:E:203:TRP:O	2.10	0.52
1:C:136:LYS:CD	1:C:245:ILE:HD11	2.29	0.51
1:F:244:ASP:O	1:F:247:THR:HG23	2.10	0.51
1:B:162:VAL:HB	1:B:196:HIS:CD2	2.46	0.51
1:B:237:PHE:CG	1:B:238:PRO:HD2	2.45	0.51
1:D:105:MET:HE3	1:D:105:MET:C	2.36	0.51
1:F:147:LEU:HD21	1:F:262:TYR:CD2	2.46	0.51
1:C:244:ASP:CA	1:C:247:THR:CG2	2.89	0.51
1:D:250:LEU:HB3	1:D:255:ILE:HD13	1.93	0.51
1:E:244:ASP:OD1	1:E:247:THR:HB	2.10	0.51
1:F:244:ASP:CA	1:F:247:THR:HG22	2.41	0.50
1:C:265:PRO:HA	1:C:266:LYS:HG2	1.92	0.50
1:A:105:MET:CE	1:B:179:GLY:C	2.85	0.50
1:D:250:LEU:CB	1:D:255:ILE:HD13	2.41	0.50
1:B:127:ARG:HG2	1:B:127:ARG:HH11	1.76	0.50
1:E:167:ALA:HB1	7:E:710:HOH:O	2.11	0.50
1:B:152:ILE:HD11	1:B:157:ALA:HB2	1.94	0.50
1:C:211[A]:ASN:HD21	1:C:213:PHE:HB3	1.77	0.50
1:A:248:PHE:O	1:A:249:ARG:HG2	2.12	0.50
1:C:237:PHE:CD1	1:C:238:PRO:HD2	2.46	0.50
1:B:106:GLY:HA3	7:B:431:HOH:O	2.11	0.50
1:B:220:ILE:O	1:B:224:LEU:HG	2.12	0.50
1:B:237:PHE:CD1	1:B:238:PRO:HD2	2.47	0.49
1:D:211[A]:ASN:HD22	1:D:214:LEU:H	1.59	0.49
1:B:266:LYS:H	1:B:267:GLU:HB3	1.77	0.49
1:F:207:SER:O	1:F:207:SER:OG	2.29	0.49
1:A:135:ARG:HG2	1:A:135:ARG:NH1	2.22	0.49
1:F:191:ILE:HD12	7:F:804:HOH:O	2.13	0.49
1:C:244:ASP:N	1:C:247:THR:HG23	2.25	0.49
1:E:105:MET:CG	1:E:261:LEU:CD2	2.91	0.49
1:F:136:LYS:HG2	1:F:213:PHE:CD2	2.42	0.49
1:F:217:VAL:CG1	1:F:235:VAL:HG21	2.42	0.49
1:E:108:VAL:HG21	1:F:239:THR:HG21	1.95	0.49
1:E:267:GLU:O	1:E:267:GLU:HG2	2.11	0.49
1:B:146[A]:PRO:HB3	1:B:266:LYS:CD	2.43	0.49
1:B:229[A]:SER:HB3	1:B:234:ALA:HB3	1.95	0.49
1:B:267:GLU:HG2	1:B:268:ASN:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ASP:C	1:C:233:LYS:N	2.70	0.48
1:A:117:ARG:CD	7:A:896:HOH:O	2.61	0.48
1:A:244:ASP:OD2	1:A:246:ASN:N	2.46	0.48
1:E:104:MET:HG2	1:F:215:THR:HG23	1.94	0.48
1:F:267:GLU:HB2	1:F:268:ASN:HB2	1.94	0.48
1:F:110[A]:ARG:HG3	1:F:110[A]:ARG:NH1	2.28	0.48
1:C:145:THR:HB	1:C:146[A]:PRO:CD	2.44	0.48
1:D:250:LEU:CB	1:D:255:ILE:CD1	2.91	0.48
1:D:201:GLU:HA	1:D:201:GLU:OE1	2.13	0.48
1:C:104:MET:CE	1:C:104:MET:CA	2.92	0.48
1:F:234:ALA:C	1:F:236:MET:N	2.71	0.48
1:E:116:TYR:HA	1:E:159:ILE:O	2.15	0.47
1:F:266:LYS:HE2	1:F:266:LYS:HA	1.88	0.47
1:C:172:HIS:O	1:C:183[A]:HIS:HE1	1.96	0.47
1:E:105:MET:CB	1:F:238:PRO:O	2.62	0.47
1:F:122:THR:HB	1:F:163:PHE:CD2	2.49	0.47
1:F:244:ASP:O	1:F:247:THR:N	2.48	0.47
1:B:110[A]:ARG:HH11	1:C:241:LYS:HB2	1.79	0.47
1:B:137:ALA:HA	1:B:217:VAL:HG22	1.97	0.47
1:E:105:MET:HE3	1:E:105:MET:CA	2.22	0.47
1:B:105:MET:CG	1:B:261:LEU:HD23	2.45	0.47
1:D:148:LYS:HA	1:D:148:LYS:HD2	1.64	0.47
1:D:176:GLY:HA2	1:D:200:ASP:OD1	2.14	0.47
1:B:124:ASP:OD1	1:B:202:PHE:HA	2.15	0.47
1:C:231:ASP:OD2	1:C:233:LYS:CB	2.63	0.47
1:A:105:MET:HE1	1:B:179:GLY:C	2.40	0.47
1:B:110[A]:ARG:NH1	1:C:241:LYS:HB2	2.29	0.47
1:D:231:ASP:OD2	1:D:233:LYS:HD3	2.15	0.47
1:F:136:LYS:CE	1:F:245:ILE:CG1	2.91	0.46
1:F:231:ASP:CG	1:F:233:LYS:H	2.24	0.46
1:F:229[A]:SER:OG	1:F:234:ALA:CB	2.63	0.46
1:E:118:ILE:HA	1:E:161:VAL:HB	1.96	0.46
1:B:105:MET:HE1	1:C:180:ILE:HA	1.98	0.46
1:F:206:HIS:CD2	1:F:207:SER:N	2.84	0.46
1:C:136:LYS:CE	1:C:245:ILE:CG1	2.89	0.46
1:F:127:ARG:HG3	7:F:800:HOH:O	2.15	0.46
1:F:244:ASP:N	1:F:247:THR:HG23	2.29	0.46
1:E:105:MET:CE	1:F:179:GLY:C	2.89	0.46
1:F:171:ASP:HB2	1:F:172:HIS:CD2	2.51	0.46
1:F:136:LYS:CD	1:F:245:ILE:HD11	2.31	0.46
1:F:191:ILE:O	1:F:192:GLY:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:ASP:O	1:F:246:ASN:N	2.49	0.46
1:C:265:PRO:CA	1:C:266:LYS:HG2	2.47	0.45
1:E:231:ASP:HA	1:E:232:PRO:HD3	1.73	0.45
1:E:267:GLU:HB2	1:E:268:ASN:HB2	1.98	0.45
1:B:265:PRO:HA	1:B:266:LYS:CB	2.46	0.45
1:D:123:PRO:HD2	1:D:199:GLU:CD	2.41	0.45
1:B:105:MET:CG	1:B:261:LEU:CD2	2.84	0.45
1:D:113:TYR:C	1:D:114:ILE:HG13	2.41	0.45
1:F:156:MET:HE2	1:F:156:MET:HB2	1.64	0.45
1:A:243:VAL:O	1:A:243:VAL:HG23	2.16	0.45
1:B:241[A]:LYS:NZ	7:B:411:HOH:O	2.27	0.45
1:C:145:THR:HA	1:C:265:PRO:HD3	1.98	0.45
1:D:181:LEU:O	1:D:182:ALA:HB2	2.16	0.45
1:A:231:ASP:HA	1:A:232:PRO:HD3	1.82	0.45
1:B:259:GLN:HG2	1:B:263:GLY:C	2.42	0.45
1:C:251:SER:O	1:C:254:ASP:N	2.46	0.45
1:B:265:PRO:CA	1:B:266:LYS:CB	2.93	0.45
1:B:231:ASP:HA	1:B:232:PRO:HD3	1.76	0.45
1:C:244:ASP:C	1:C:246:ASN:H	2.25	0.45
1:B:211[A]:ASN:HD22	1:B:214:LEU:H	1.64	0.44
1:C:244:ASP:CG	1:C:247:THR:CG2	2.87	0.44
1:C:256:ARG:O	1:C:260:SER:OG	2.34	0.44
1:D:135:ARG:HH21	1:D:136:LYS:HA	1.82	0.44
1:E:251:SER:O	1:E:252:ALA:C	2.59	0.44
1:B:152:ILE:HD12	1:B:154:THR:O	2.16	0.44
1:A:245:ILE:HG21	1:A:245:ILE:HD13	1.68	0.44
1:D:104:MET:HE2	1:D:104:MET:HB2	1.27	0.44
1:F:218:HIS:CE1	1:F:228:HIS:CD2	3.05	0.44
1:A:182:ALA:HB1	1:A:196:HIS:O	2.18	0.44
1:A:105:MET:CE	1:B:179:GLY:HA2	2.44	0.44
1:F:267:GLU:CG	1:F:268:ASN:HB2	2.46	0.44
1:A:136:LYS:HE2	1:A:245:ILE:HG12	1.99	0.44
1:E:159:ILE:HG23	1:E:193:GLY:O	2.18	0.44
1:B:259:GLN:HG2	1:B:264:ASP:N	2.33	0.43
1:E:105:MET:HG3	1:E:261:LEU:HD21	1.99	0.43
1:F:264:ASP:HA	1:F:265:PRO:HD2	1.74	0.43
1:B:255:ILE:O	1:B:259:GLN:HB2	2.18	0.43
1:C:136:LYS:CG	1:C:213:PHE:CE2	3.01	0.43
1:B:259:GLN:HG2	1:B:264:ASP:HB2	2.00	0.43
1:B:168:HIS:CE1	1:B:174:PHE:CD2	3.07	0.43
1:E:105:MET:HE3	1:F:179:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ILE:HG21	1:C:191:ILE:HD13	1.64	0.43
1:C:198:ASP:OD2	1:C:200:ASP:HB2	2.19	0.43
1:C:255:ILE:HD12	1:C:255:ILE:HA	1.77	0.43
1:C:206:HIS:CD2	1:C:207:SER:N	2.87	0.43
1:A:251:SER:HB2	7:A:893:HOH:O	2.18	0.43
1:F:121:TYR:CG	1:F:127:ARG:HG2	2.53	0.43
1:B:265:PRO:HA	1:B:266:LYS:CD	2.42	0.43
1:E:265:PRO:CB	1:E:266:LYS:HB2	2.49	0.43
1:A:123:PRO:HD2	1:A:199:GLU:CD	2.43	0.42
1:A:184:ALA:HA	1:A:194:ASP:O	2.19	0.42
1:F:191:ILE:CD1	7:F:804:HOH:O	2.67	0.42
1:B:105:MET:CE	1:C:179:GLY:C	2.89	0.42
1:C:126:ASN:O	1:C:129:ASP:HB2	2.18	0.42
1:D:152:ILE:HD11	1:D:157:ALA:CA	2.49	0.42
1:F:264:ASP:O	1:F:266:LYS:CE	2.67	0.42
1:B:160:LEU:HA	1:B:160:LEU:HD12	1.67	0.42
1:F:234:ALA:C	1:F:236:MET:H	2.27	0.42
1:C:231:ASP:O	1:C:234:ALA:N	2.39	0.42
1:F:235:VAL:HG12	1:F:254:ASP:OD1	2.20	0.42
1:D:231:ASP:HA	1:D:232:PRO:HD3	1.88	0.42
1:F:251:SER:O	1:F:254:ASP:N	2.51	0.42
1:C:251:SER:O	1:C:254:ASP:HB2	2.19	0.42
1:C:255:ILE:N	1:C:255:ILE:HD13	2.34	0.42
1:F:151:LYS:HD2	7:F:794:HOH:O	2.18	0.42
1:A:177:LYS:N	1:A:200:ASP:HB3	2.35	0.42
1:B:105:MET:CE	1:B:106:GLY:N	2.73	0.42
1:C:109:TRP:HB3	1:C:111:LYS:HB2	2.01	0.42
1:E:180:ILE:CD1	7:E:706:HOH:O	2.68	0.42
1:A:114:ILE:HD12	1:A:147:LEU:HD22	2.01	0.41
1:B:229[A]:SER:HB3	1:B:234:ALA:CB	2.50	0.41
1:D:214:LEU:HD11	1:D:243:VAL:H	1.85	0.41
1:E:267:GLU:CB	1:E:268:ASN:HB2	2.50	0.41
1:A:199:GLU:O	1:A:199:GLU:HG3	2.19	0.41
1:D:108:VAL:HG12	1:D:261:LEU:HD13	2.02	0.41
1:B:229[A]:SER:CB	1:B:234:ALA:CB	2.99	0.41
1:D:160:LEU:HA	1:D:160:LEU:HD12	1.60	0.41
1:A:136:LYS:HD3	1:A:213:PHE:CE2	2.55	0.41
1:E:105:MET:HE1	1:F:180:ILE:HG13	2.02	0.41
1:F:198:ASP:HB3	1:F:201:GLU:HG2	2.02	0.41
1:E:167:ALA:CB	1:E:173:ALA:HB2	2.38	0.41
1:E:231:ASP:O	1:E:234:ALA:N	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:MET:HB3	1:C:104:MET:HE2	1.82	0.41
1:A:152:ILE:HD11	1:A:157:ALA:HB2	2.03	0.41
1:B:258:ILE:HG23	1:B:259:GLN:N	2.35	0.41
1:C:128:GLU:H	1:C:128:GLU:HG2	1.66	0.41
1:D:123:PRO:HD2	1:D:199:GLU:OE2	2.20	0.41
1:D:148:LYS:HD3	7:D:602:HOH:O	2.21	0.41
1:E:248:PHE:O	1:E:249:ARG:HD3	2.21	0.41
1:F:226:LEU:HD23	1:F:226:LEU:HA	1.82	0.41
1:F:240:TYR:CD1	1:F:240:TYR:C	2.99	0.41
1:A:190:GLY:C	1:A:192:GLY:N	2.80	0.40
1:B:258:ILE:CG2	1:B:259:GLN:N	2.84	0.40
1:C:119:ASN:HB2	1:C:160:LEU:HD11	2.03	0.40
1:B:114:ILE:HB	1:B:149:PHE:CD1	2.56	0.40
1:C:245:ILE:O	1:C:245:ILE:CG2	2.68	0.40
1:A:208:GLY:O	1:A:209:GLY:C	2.64	0.40
1:B:231:ASP:O	1:B:234:ALA:HB3	2.22	0.40
1:D:199:GLU:O	1:D:199:GLU:HG3	2.22	0.40
1:B:265:PRO:CA	1:B:266:LYS:HD2	2.44	0.40
1:E:152:ILE:HD12	1:E:154:THR:O	2.21	0.40
1:F:108:VAL:HG23	1:F:262:TYR:CZ	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LYS:NZ	1:E:249:ARG:NH1[1_554]	2.07	0.13

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	163/165 (99%)	155 (95%)	6 (4%)	2 (1%)	10 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	163/165 (99%)	153 (94%)	7 (4%)	3 (2%)	6	2
1	C	163/165 (99%)	152 (93%)	7 (4%)	4 (2%)	4	1
1	D	163/165 (99%)	158 (97%)	3 (2%)	2 (1%)	10	5
1	E	163/165 (99%)	153 (94%)	7 (4%)	3 (2%)	6	2
1	F	163/165 (99%)	151 (93%)	8 (5%)	4 (2%)	4	1
All	All	978/990 (99%)	922 (94%)	38 (4%)	18 (2%)	6	2

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	LYS
1	B	266	LYS
1	C	245	ILE
1	C	266	LYS
1	C	267	GLU
1	D	266	LYS
1	E	247	THR
1	E	266	LYS
1	F	267	GLU
1	B	264	ASP
1	B	267	GLU
1	C	247	THR
1	E	246	ASN
1	F	245	ILE
1	F	266	LYS
1	A	106	GLY
1	D	106	GLY
1	F	193	GLY

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	134/134 (100%)	122 (91%)	12 (9%)	9	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	134/134 (100%)	117 (87%)	17 (13%)	4	1
1	C	134/134 (100%)	116 (87%)	18 (13%)	4	1
1	D	134/134 (100%)	119 (89%)	15 (11%)	6	2
1	E	134/134 (100%)	115 (86%)	19 (14%)	3	1
1	F	134/134 (100%)	117 (87%)	17 (13%)	4	1
All	All	804/804 (100%)	706 (88%)	98 (12%)	5	2

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110[A]	ARG
1	A	122	THR
1	A	127	ARG
1	A	128	GLU
1	A	135	ARG
1	A	156	MET
1	A	165	ARG
1	A	171	ASP
1	A	241[A]	LYS
1	A	247	THR
1	A	256	ARG
1	A	266	LYS
1	B	104	MET
1	B	105	MET
1	B	119	ASN
1	B	122	THR
1	B	136	LYS
1	B	154	THR
1	B	156	MET
1	B	233	LYS
1	B	235	VAL
1	B	239	THR
1	B	241[A]	LYS
1	B	255	ILE
1	B	256	ARG
1	B	259	GLN
1	B	260	SER
1	B	266	LYS
1	B	267	GLU
1	C	104	MET

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Mol	Chain	Res	Type
1	C	105	MET
1	C	135	ARG
1	C	136	LYS
1	C	150	SER
1	C	156	MET
1	C	165	ARG
1	C	177	LYS
1	C	189	SER
1	C	191	ILE
1	C	219	GLU
1	C	229[A]	SER
1	C	230	SER
1	C	241	LYS
1	C	245	ILE
1	C	247	THR
1	C	255	ILE
1	C	260	SER
1	D	104	MET
1	D	105	MET
1	D	110[A]	ARG
1	D	122	THR
1	D	127	ARG
1	D	135	ARG
1	D	136	LYS
1	D	139	GLN
1	D	152	ILE
1	D	156	MET
1	D	191	ILE
1	D	241[A]	LYS
1	D	247	THR
1	D	255	ILE
1	D	266	LYS
1	E	119	ASN
1	E	122	THR
1	E	136	LYS
1	E	142[A]	SER
1	E	154	THR
1	E	187	PRO
1	E	189	SER
1	E	233	LYS
1	E	235	VAL
1	E	239	THR

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Mol	Chain	Res	Type
1	E	241[A]	LYS
1	E	244	ASP
1	E	247	THR
1	E	249	ARG
1	E	255	ILE
1	E	256	ARG
1	E	260	SER
1	E	266	LYS
1	E	267	GLU
1	F	104	MET
1	F	105	MET
1	F	135	ARG
1	F	156	MET
1	F	165	ARG
1	F	207	SER
1	F	229[A]	SER
1	F	233	LYS
1	F	239	THR
1	F	241[A]	LYS
1	F	244	ASP
1	F	245	ILE
1	F	247	THR
1	F	255	ILE
1	F	260	SER
1	F	266	LYS
1	F	267	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	139	GLN
1	A	206	HIS
1	A	211[A]	ASN
1	A	259	GLN
1	B	172	HIS
1	B	206	HIS
1	B	211[A]	ASN
1	B	259	GLN
1	C	119	ASN
1	C	120	ASN
1	C	126	ASN

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Mol	Chain	Res	Type
1	C	172	HIS
1	C	206	HIS
1	C	211[A]	ASN
1	C	259	GLN
1	D	143	ASN
1	D	206	HIS
1	D	211[A]	ASN
1	D	259	GLN
1	E	172	HIS
1	E	206	HIS
1	E	211[A]	ASN
1	E	259	GLN
1	F	119	ASN
1	F	172	HIS
1	F	206	HIS
1	F	211[A]	ASN
1	F	259	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 36 ligands modelled in this entry, 30 are monoatomic - leaving 6 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	ACT	E	674	2	3,3,3	2.14	1 (33%)	3,3,3	0.89	0
6	AZI	C	474	2	2,2,2	2.38	2 (100%)	0,1,1	-	-
4	HAE	A	874	2	4,4,4	1.20	0	2,4,4	4.42	2 (100%)
6	AZI	F	774	2	2,2,2	2.34	2 (100%)	0,1,1	-	-
4	HAE	D	574	2	4,4,4	1.35	1 (25%)	2,4,4	5.88	2 (100%)
5	ACT	B	374	2	3,3,3	1.84	1 (33%)	3,3,3	5.32	3 (100%)

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
4	HAE	A	874	2	-	0/1/2/2	-
4	HAE	D	574	2	-	0/1/2/2	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	674	ACT	O-C	3.03	1.35	1.22
6	F	774	AZI	N1-N2	-2.59	1.17	1.23
5	B	374	ACT	OXT-C	-2.56	1.19	1.30
6	C	474	AZI	N1-N2	-2.49	1.18	1.23
6	C	474	AZI	N3-N2	-2.26	1.18	1.23
4	D	574	HAE	C2-N	2.19	1.36	1.33
6	F	774	AZI	N3-N2	-2.06	1.18	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	374	ACT	OXT-C-O	-7.67	93.56	122.03
4	D	574	HAE	C1-C2-N	5.93	125.96	116.10
4	D	574	HAE	O2-C2-C1	-5.84	111.66	122.05
4	A	874	HAE	C1-C2-N	4.99	124.39	116.10
5	B	374	ACT	OXT-C-CH3	4.46	133.73	115.05
4	A	874	HAE	O2-C2-C1	-3.77	115.34	122.05
5	B	374	ACT	O-C-CH3	2.46	132.62	122.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	674	ACT	1	0
6	C	474	AZI	1	0
6	F	774	AZI	1	0
5	B	374	ACT	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	165/165 (100%)	-1.19	0 100 100	18, 36, 52, 62	9 (5%)
1	B	165/165 (100%)	-1.19	0 100 100	11, 30, 51, 82	9 (5%)
1	C	165/165 (100%)	-1.15	0 100 100	13, 34, 56, 86	8 (4%)
1	D	165/165 (100%)	-1.19	0 100 100	17, 36, 52, 66	9 (5%)
1	E	165/165 (100%)	-1.22	0 100 100	11, 30, 52, 89	9 (5%)
1	F	165/165 (100%)	-1.13	0 100 100	14, 34, 56, 82	9 (5%)
All	All	990/990 (100%)	-1.18	0 100 100	11, 34, 54, 89	53 (5%)

There are no RSRZ outliers to report.

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	AZI	C	474	3/3	0.98	0.05	29,29,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	873	1/1	0.99	0.03	47,47,47,47	0
3	CA	B	372	1/1	0.99	0.03	35,35,35,35	0
3	CA	D	572	1/1	0.99	0.02	40,40,40,40	0
3	CA	D	573	1/1	0.99	0.03	51,51,51,51	0
3	CA	E	672	1/1	0.99	0.03	32,32,32,32	0
3	CA	A	872	1/1	0.99	0.02	39,39,39,39	0
6	AZI	F	774	3/3	0.99	0.03	29,29,44,48	0
2	ZN	E	669	1/1	1.00	0.01	33,33,33,33	0
2	ZN	E	670	1/1	1.00	0.01	30,30,30,30	0
2	ZN	F	769	1/1	1.00	0.02	33,33,33,33	0
2	ZN	F	770	1/1	1.00	0.01	33,33,33,33	0
3	CA	A	871	1/1	1.00	0.01	44,44,44,44	0
2	ZN	A	869	1/1	1.00	0.01	29,29,29,29	0
2	ZN	A	870	1/1	1.00	0.01	43,43,43,43	0
3	CA	B	371	1/1	1.00	0.01	26,26,26,26	0
2	ZN	B	369	1/1	1.00	0.01	34,34,34,34	0
3	CA	B	373	1/1	1.00	0.01	28,28,28,28	0
3	CA	C	471	1/1	1.00	0.02	28,28,28,28	0
3	CA	C	472	1/1	1.00	0.01	31,31,31,31	0
3	CA	C	473	1/1	1.00	0.01	38,38,38,38	0
3	CA	D	571	1/1	1.00	0.01	43,43,43,43	0
2	ZN	B	370	1/1	1.00	0.01	29,29,29,29	0
2	ZN	C	469	1/1	1.00	0.02	32,32,32,32	0
3	CA	E	671	1/1	1.00	0.01	27,27,27,27	0
2	ZN	C	470	1/1	1.00	0.01	33,33,33,33	0
3	CA	E	673	1/1	1.00	0.01	30,30,30,30	0
3	CA	F	771	1/1	1.00	0.02	29,29,29,29	0
3	CA	F	772	1/1	1.00	0.02	30,30,30,30	0
3	CA	F	773	1/1	1.00	0.01	37,37,37,37	0
4	HAE	A	874	5/5	1.00	0.06	27,34,38,43	0
4	HAE	D	574	5/5	1.00	0.04	28,34,42,43	0
5	ACT	B	374	4/4	1.00	0.04	33,35,37,40	0
5	ACT	E	674	4/4	1.00	0.04	28,33,36,36	0
2	ZN	D	569	1/1	1.00	0.01	28,28,28,28	0
2	ZN	D	570	1/1	1.00	0.01	42,42,42,42	0

6.5 Other polymers

There are no such residues in this entry.