



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:07 PM UTC

PDB ID : 3OR1 / pdb_00003or1
Title : Crystal structure of dissimilatory sulfite reductase I (DsrI)
Authors : Hsieh, Y.C.; Liu, M.Y.; Wang, V.C.C.; Chiang, Y.L.; Liu, E.H.; Wu, W.G.;
Chan, S.I.; Chen, C.J.
Deposited on : 2010-09-06
Resolution : 1.76 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

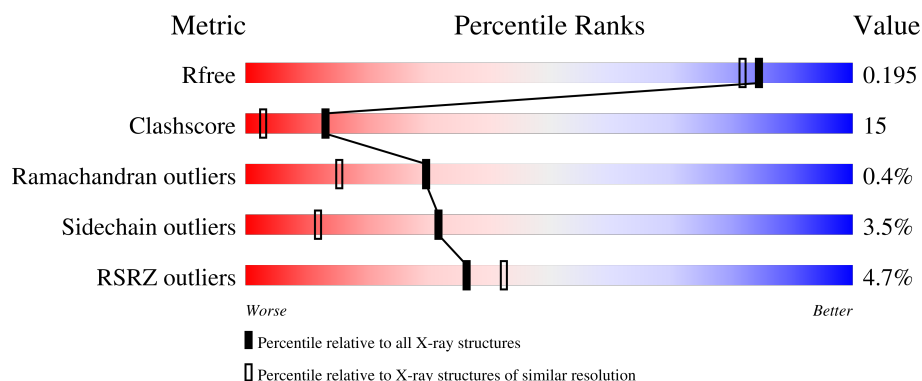
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	437	5% 45% 44% 10% .
1	D	437	2% 67% 27% 5% .
2	B	386	3% 62% 30% 8% .
2	E	386	2% 70% 26% .
3	C	105	23% 59% 34% 5% ..

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Mol	Chain	Length	Quality of chain
3	F	105	12% 68% 23% 8% ..

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	SRM	A	580	X	-	-	-
5	SRM	D	582	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15467 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 Sulfite reductase alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3422	2163	585	646	28			
1	D	435	Total	C	N	O	S	0	0	0
			3422	2163	585	646	28			

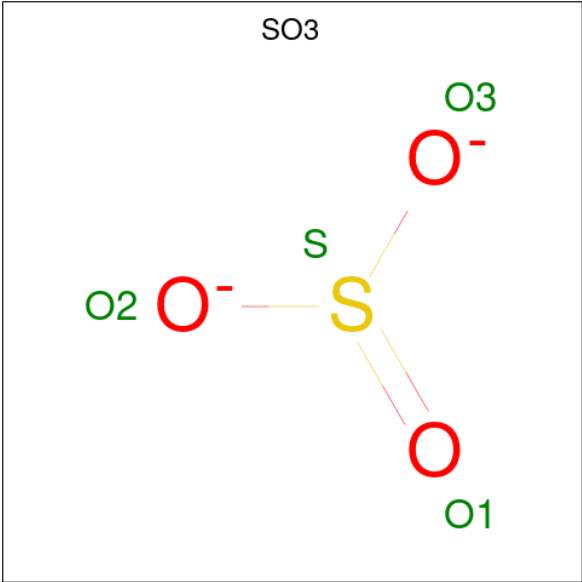
- Molecule 2 is a protein called Sulfite reductase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	385	Total	C	N	O	S	0	0	0
			2999	1912	519	542	26			
2	E	385	Total	C	N	O	S	0	0	0
			2999	1912	519	542	26			

- Molecule 3 is a protein called Sulfite reductase gama.

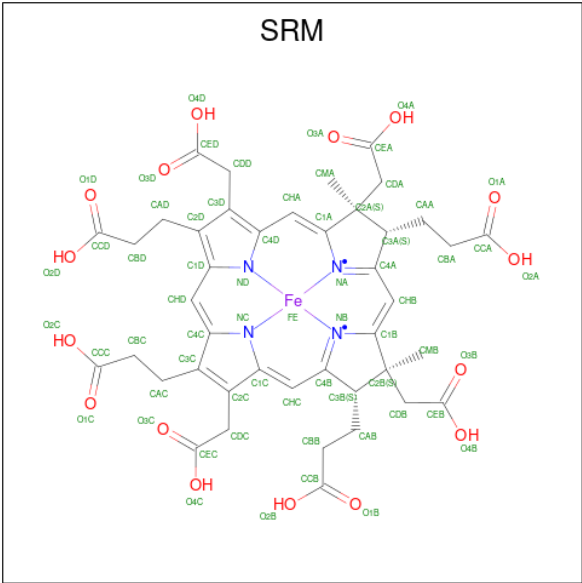
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	104	Total	C	N	O	S	0	0	0
			787	508	125	149	5			
3	F	104	Total	C	N	O	S	0	0	0
			787	508	125	149	5			

- Molecule 4 is SULFITE ION (CCD ID: SO3) (formula: O₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	O	S		0	0
			4	3	1			
4	D	1	Total	O	S		0	0
			4	3	1			

- Molecule 5 is SIROHEME (CCD ID: SRM) (formula: C₄₂H₄₄FeN₄O₁₆).



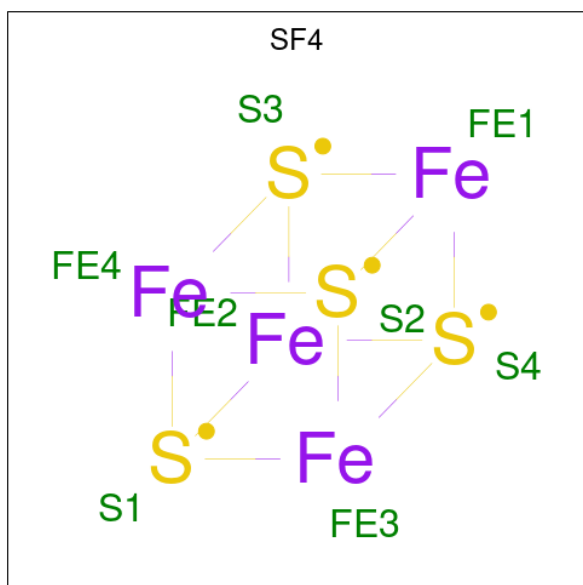
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	B	1	Total	C	N	O		0	0
			62	42	4	16			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	Fe	N	O	
			63	42	1	4	16	
5	E	1	Total	C	N	O		
			62	42	4	16		

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S		
			8	4	4	0	0
6	A	1	Total	Fe	S		
			8	4	4	0	0
6	B	1	Total	Fe	S		
			8	4	4	0	0
6	B	1	Total	Fe	S		
			8	4	4	0	0
6	D	1	Total	Fe	S		
			8	4	4	0	0
6	D	1	Total	Fe	S		
			8	4	4	0	0
6	E	1	Total	Fe	S		
			8	4	4	0	0
6	E	1	Total	Fe	S		
			8	4	4	0	0

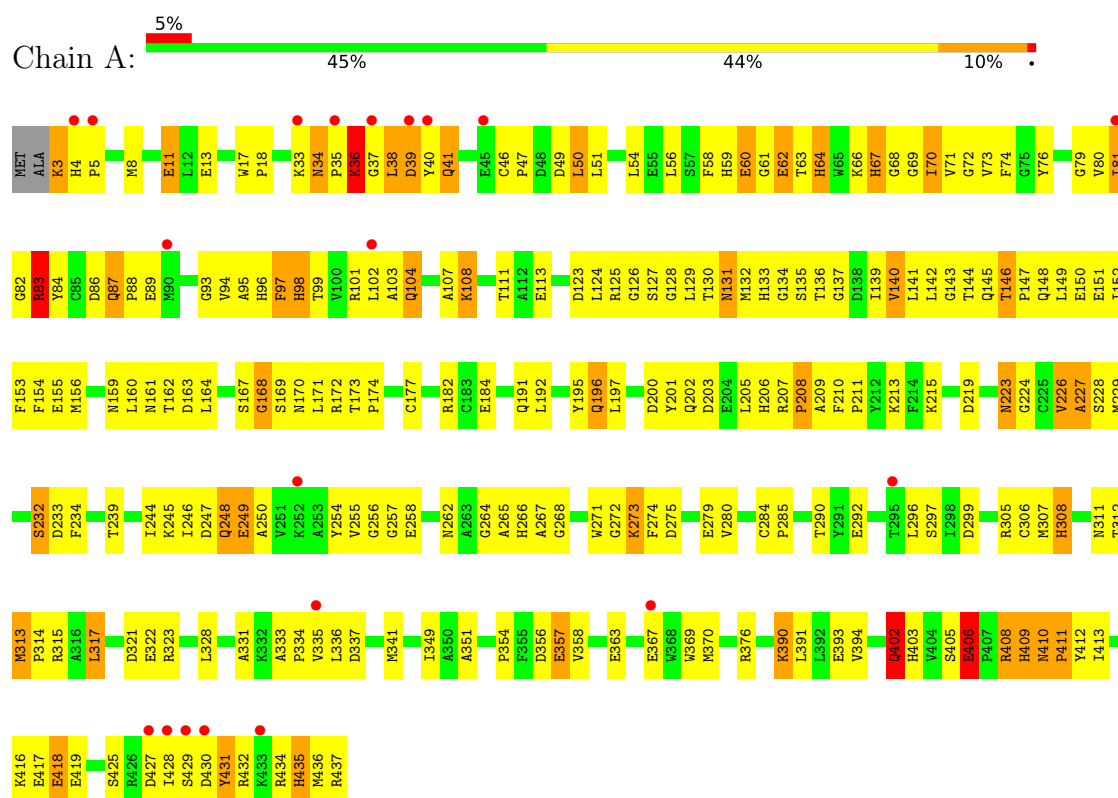
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	164	Total 164	O 164	0	0
7	B	160	Total 160	O 160	0	0
7	C	12	Total 12	O 12	0	0
7	D	220	Total 220	O 220	0	0
7	E	155	Total 155	O 155	0	0
7	F	18	Total 18	O 18	0	0

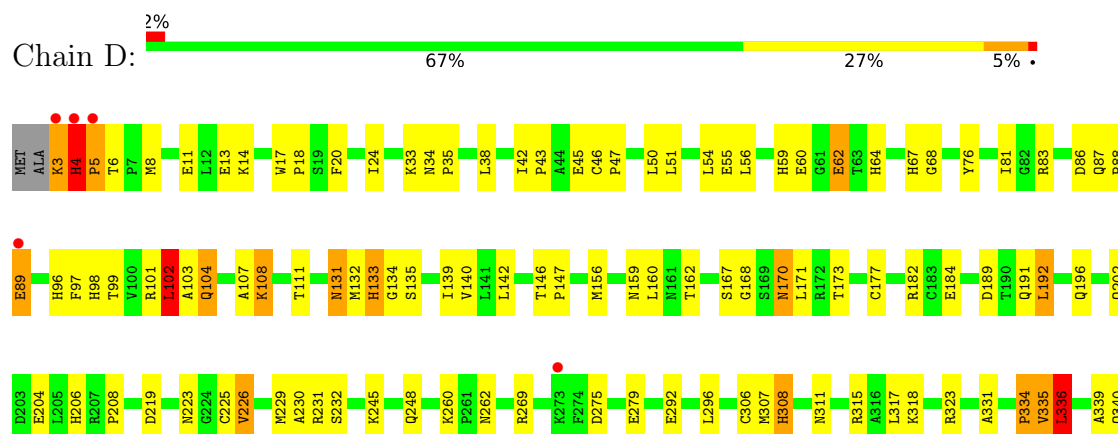
3 Residue-property plots [i](#)

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: Sulfite reductase alpha

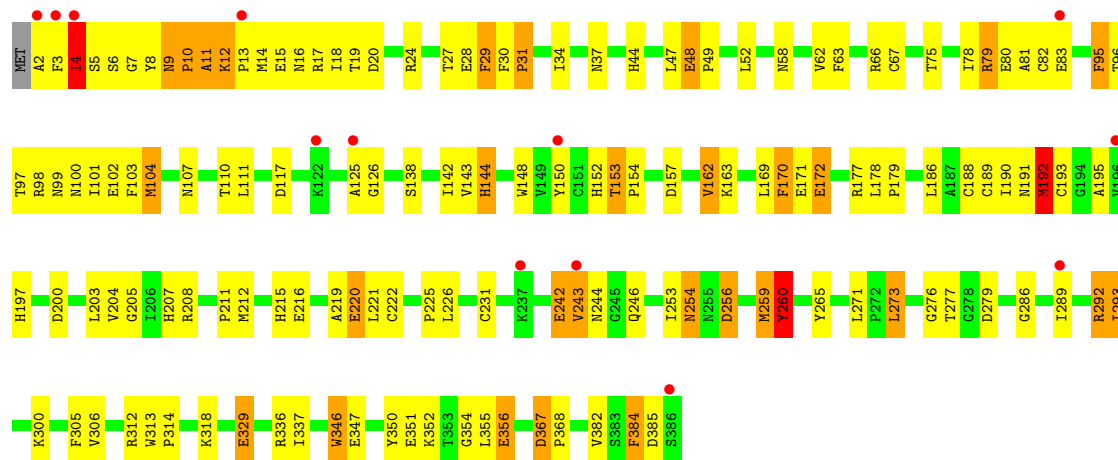


• Molecule 1: Sulfite reductase alpha

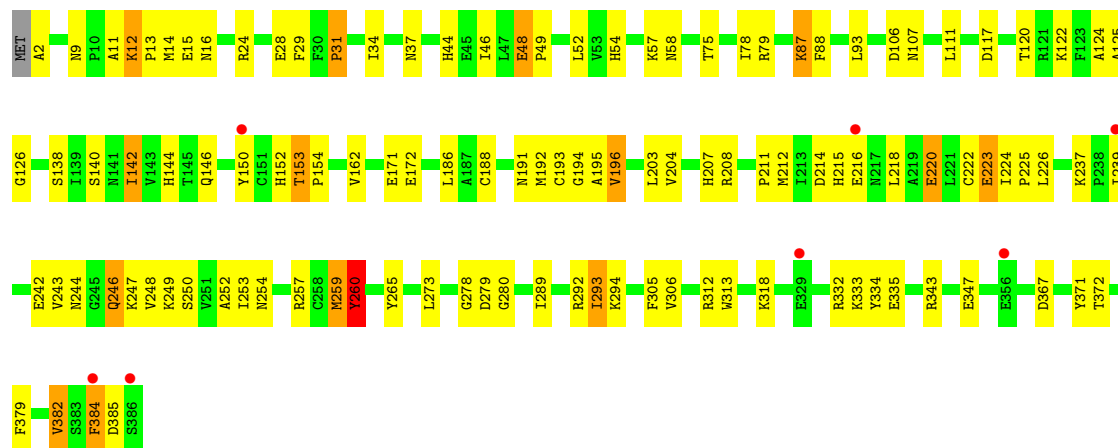




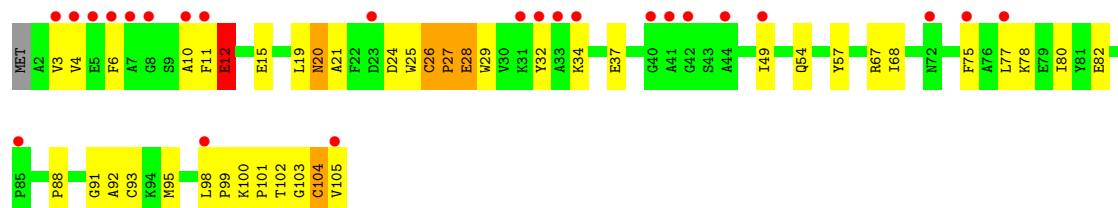
• Molecule 2: Sulfite reductase beta



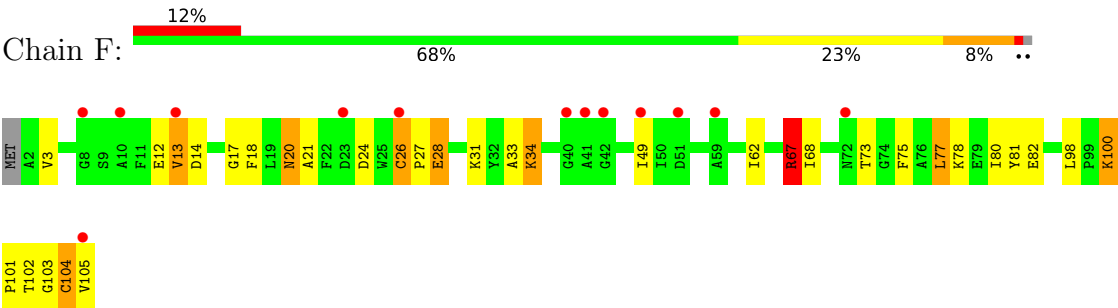
• Molecule 2: Sulfite reductase beta



• Molecule 3: Sulfite reductase gamma



● Molecule 3: Sulfite reductase gama



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.72Å 60.48Å 132.91Å 90.00° 94.30° 90.00°	Depositor
Resolution (Å)	30.00 – 1.76 30.00 – 1.76	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.76) 99.7 (30.00-1.76)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.212 0.192 , 0.195	Depositor DCC
R_{free} test set	10018 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15467	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: SF4, SRM, SO3

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	2.94	292/3512 (8.3%)	1.43	50/4751 (1.1%)
1	D	1.56	84/3512 (2.4%)	1.16	31/4751 (0.7%)
2	B	2.20	158/3076 (5.1%)	1.24	28/4170 (0.7%)
2	E	1.68	94/3076 (3.1%)	1.13	20/4170 (0.5%)
3	C	1.59	17/808 (2.1%)	1.15	4/1090 (0.4%)
3	F	1.83	18/808 (2.2%)	1.21	8/1090 (0.7%)
All	All	2.13	663/14792 (4.5%)	1.24	141/20022 (0.7%)

All (663) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	ASN	C-O	-19.21	1.15	1.23
1	A	209	ALA	CA-CB	-17.14	1.29	1.54
1	A	146	THR	C-O	-16.68	1.08	1.24
2	B	178	LEU	C-O	-16.61	1.06	1.23
1	A	290	THR	C-O	-16.39	1.04	1.23
1	A	98	HIS	C-O	-16.32	1.03	1.23
1	A	162	THR	C-O	-16.11	1.05	1.24
1	D	335	VAL	C-O	-16.10	1.07	1.24
3	F	102	THR	C-O	-15.84	1.03	1.23
1	A	154	PHE	C-O	-15.48	1.06	1.24
1	D	42	ILE	C-O	-15.48	1.04	1.24
2	B	52	LEU	C-O	-15.45	1.04	1.23
1	A	103	ALA	C-O	-15.30	1.05	1.23
1	D	171	LEU	C-O	-15.14	1.05	1.24
3	C	103	GLY	C-O	-15.07	1.06	1.23
3	F	103	GLY	C-O	-14.96	1.06	1.23
1	A	124	LEU	C-O	-14.89	1.06	1.24
2	E	318	LYS	C-O	-14.10	1.07	1.24
2	B	243	VAL	C-O	-14.10	1.10	1.24
3	F	102	THR	CB-OG1	-14.03	1.21	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	27	THR	C-O	-13.99	1.06	1.24
2	B	3	PHE	C-O	-13.89	1.07	1.23
1	A	141	LEU	C-O	-13.78	1.07	1.23
1	A	246	ILE	C-O	-13.77	1.09	1.24
1	A	131	ASN	C-O	-13.72	1.07	1.24
1	A	317	LEU	C-O	-13.72	1.08	1.24
2	B	356	GLU	C-O	-13.64	1.07	1.24
1	A	393	GLU	C-O	-13.59	1.08	1.24
1	A	431	TYR	C-O	-13.57	1.08	1.24
1	A	144	THR	C-O	-13.55	1.08	1.23
2	E	196	VAL	C-O	-13.54	1.08	1.24
1	A	357	GLU	C-O	-13.46	1.08	1.24
1	A	130	THR	C-O	-13.43	1.06	1.23
1	D	62	GLU	C-O	-13.42	1.08	1.23
1	A	171	LEU	C-O	-13.31	1.07	1.24
1	A	208	PRO	C-O	-13.23	1.06	1.24
1	A	125	ARG	C-O	-13.15	1.06	1.24
2	B	226	LEU	C-O	-13.15	1.08	1.24
2	E	9	ASN	C-O	-13.14	1.09	1.24
1	D	245	LYS	C-O	-13.13	1.07	1.24
1	A	192	LEU	C-O	-13.13	1.08	1.24
2	B	384	PHE	CE1-CZ	-13.06	0.99	1.38
2	B	204	VAL	C-O	-12.98	1.09	1.24
1	A	40	TYR	C-O	-12.98	1.08	1.23
1	D	8	MET	C-O	-12.97	1.09	1.24
1	A	129	LEU	C-O	-12.90	1.08	1.24
2	B	117	ASP	C-O	-12.88	1.09	1.24
1	D	434	ARG	C-O	-12.85	1.07	1.24
1	A	209	ALA	C-O	-12.75	1.07	1.24
1	D	103	ALA	C-O	-12.70	1.08	1.23
1	A	328	LEU	C-O	-12.70	1.08	1.24
1	D	275	ASP	C-O	-12.67	1.09	1.23
2	B	104	MET	C-O	-12.53	1.08	1.24
1	A	210	PHE	C-O	-12.47	1.09	1.23
2	E	220	GLU	CB-CG	-12.46	1.15	1.52
1	A	83	ARG	CD-NE	-12.44	1.28	1.46
2	B	215	HIS	C-O	-12.39	1.09	1.24
1	A	234	PHE	C-O	-12.39	1.09	1.23
1	D	102	LEU	C-O	-12.39	1.09	1.24
1	A	140	VAL	C-O	-12.34	1.10	1.24
1	A	97	PHE	C-O	-12.33	1.09	1.23
1	A	207	ARG	C-O	-12.18	1.15	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	356	ASP	C-O	-12.13	1.09	1.24
1	A	80	VAL	C-O	-12.13	1.11	1.24
1	D	51	LEU	C-O	-12.08	1.09	1.24
1	A	406	GLU	CB-CG	-12.08	1.16	1.52
1	A	155	GLU	C-O	-12.06	1.10	1.24
1	D	432	ARG	CD-NE	-12.06	1.29	1.46
1	A	232	SER	C-O	-12.05	1.09	1.23
2	B	81	ALA	C-O	-12.04	1.10	1.24
1	D	391	LEU	C-O	-11.98	1.09	1.24
2	B	9	ASN	C-O	-11.97	1.12	1.24
2	E	382	VAL	C-O	-11.89	1.09	1.23
1	A	145	GLN	C-O	-11.89	1.09	1.23
1	A	70	ILE	C-O	-11.87	1.10	1.24
1	A	333	ALA	C-O	-11.87	1.08	1.23
1	A	59	HIS	C-O	-11.82	1.10	1.24
2	B	203	LEU	C-O	-11.82	1.10	1.24
2	E	306	VAL	C-O	-11.78	1.09	1.24
1	A	127	SER	C-O	-11.71	1.09	1.24
2	E	93	LEU	C-O	-11.71	1.10	1.23
1	A	264	GLY	C-O	-11.69	1.08	1.24
3	C	102	THR	C-O	-11.67	1.08	1.23
2	B	350	TYR	C-O	-11.62	1.10	1.24
1	A	299	ASP	C-O	-11.59	1.10	1.23
3	F	98	LEU	C-O	-11.57	1.09	1.23
2	B	305	PHE	C-O	-11.51	1.10	1.23
1	A	96	HIS	C-O	-11.47	1.10	1.24
1	A	417	GLU	C-O	-11.46	1.10	1.24
1	A	435	HIS	C-O	-11.46	1.10	1.23
1	A	50	LEU	CG-CD1	-11.45	1.14	1.52
2	E	28	GLU	C-O	-11.43	1.09	1.24
1	A	135	SER	C-O	-11.28	1.09	1.24
1	A	68	GLY	C-O	-11.23	1.06	1.24
1	A	5	PRO	C-O	-11.22	1.11	1.23
1	A	229	MET	CB-CG	-11.15	1.19	1.52
1	A	315	ARG	C-O	-11.12	1.09	1.24
1	D	103	ALA	CA-CB	-11.07	1.35	1.53
1	D	6	THR	C-O	-11.05	1.11	1.23
1	A	174	PRO	C-O	-11.04	1.10	1.23
2	B	8	TYR	C-O	-11.02	1.10	1.23
1	A	35	PRO	C-O	-11.01	1.10	1.24
1	D	269	ARG	C-O	-11.01	1.10	1.23
1	A	250	ALA	C-O	-10.98	1.11	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	384	PHE	CD1-CE1	-10.95	1.05	1.38
2	B	6	SER	C-O	-10.91	1.09	1.24
1	A	84	TYR	C-O	-10.91	1.11	1.24
2	B	306	VAL	CB-CG2	-10.86	1.16	1.52
2	E	125	ALA	CA-CB	-10.85	1.34	1.53
1	A	265	ALA	C-O	-10.84	1.10	1.24
1	D	428	ILE	C-O	-10.83	1.10	1.24
2	B	384	PHE	C-O	-10.82	1.10	1.24
1	A	411	PRO	C-O	-10.81	1.09	1.24
1	A	315	ARG	CZ-NH2	-10.76	1.19	1.33
1	A	406	GLU	C-O	-10.76	1.12	1.24
3	F	67	ARG	CZ-NH2	-10.69	1.19	1.33
1	D	317	LEU	C-O	-10.68	1.12	1.24
1	A	50	LEU	C-O	-10.67	1.11	1.24
1	A	156	MET	C-O	-10.66	1.11	1.24
3	C	67	ARG	C-O	-10.58	1.10	1.24
1	A	408	ARG	C-O	-10.56	1.10	1.23
2	B	82	CYS	C-O	-10.55	1.11	1.24
2	E	111	LEU	C-O	-10.53	1.11	1.24
2	B	18	ILE	C-O	-10.45	1.11	1.24
2	E	220	GLU	C-O	-10.44	1.11	1.24
1	A	268	GLY	C-O	-10.43	1.10	1.23
1	A	101	ARG	C-O	-10.40	1.11	1.24
1	D	335	VAL	CB-CG1	-10.40	1.18	1.52
1	D	408	ARG	C-O	-10.40	1.11	1.23
1	A	173	THR	C-O	-10.30	1.10	1.24
2	E	87	LYS	C-O	-10.29	1.10	1.24
2	E	57	LYS	CG-CD	-10.29	1.21	1.52
2	E	237	LYS	C-O	-10.29	1.14	1.24
1	A	432	ARG	C-O	-10.29	1.10	1.24
2	E	16	ASN	C-O	-10.24	1.06	1.24
2	B	243	VAL	CB-CG2	-10.24	1.18	1.52
1	D	435	HIS	C-O	-10.23	1.09	1.23
1	A	41	GLN	C-O	-10.22	1.10	1.24
1	A	182	ARG	C-O	-10.21	1.11	1.24
2	E	125	ALA	C-O	-10.21	1.10	1.24
2	E	243	VAL	C-O	-10.21	1.13	1.24
1	A	36	LYS	C-O	-10.20	1.10	1.24
2	B	79	ARG	C-O	-10.18	1.12	1.24
2	E	14	MET	SD-CE	-10.15	1.54	1.79
2	B	20	ASP	CG-OD1	-10.13	1.06	1.25
3	F	26	CYS	CB-SG	-10.12	1.47	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	HIS	C-O	-10.11	1.10	1.24
1	A	148	GLN	C-O	-9.99	1.10	1.24
1	A	228	SER	C-O	-9.98	1.12	1.24
2	B	170	PHE	C-O	-9.95	1.12	1.24
1	D	269	ARG	CZ-NH2	-9.93	1.20	1.33
1	A	248	GLN	C-O	-9.93	1.12	1.24
2	B	191	ASN	CG-OD1	-9.90	1.04	1.23
2	B	352	LYS	C-O	-9.90	1.12	1.24
1	A	321	ASP	C-O	-9.88	1.11	1.24
2	B	244	ASN	C-O	-9.86	1.11	1.23
2	B	162	VAL	C-O	-9.83	1.12	1.24
2	B	221	LEU	C-O	-9.83	1.11	1.24
2	E	48	GLU	CB-CG	-9.82	1.23	1.52
1	A	233	ASP	C-O	-9.80	1.11	1.24
2	B	219	ALA	C-O	-9.79	1.11	1.24
2	B	144	HIS	C-O	-9.79	1.12	1.23
1	A	255	VAL	C-O	-9.76	1.12	1.24
2	B	355	LEU	C-O	-9.74	1.11	1.23
2	B	10	PRO	C-O	-9.74	1.10	1.24
2	B	80	GLU	C-O	-9.73	1.12	1.24
2	B	83	GLU	C-O	-9.72	1.12	1.24
1	A	4	HIS	C-O	-9.71	1.10	1.23
2	B	171	GLU	C-O	-9.66	1.11	1.24
2	B	103	PHE	C-O	-9.64	1.12	1.24
2	E	306	VAL	CB-CG2	-9.63	1.20	1.52
2	B	192	MET	SD-CE	-9.59	1.55	1.79
2	B	191	ASN	CG-ND2	-9.56	1.13	1.33
2	E	15	GLU	C-O	-9.49	1.12	1.23
2	B	277	THR	C-O	-9.49	1.11	1.24
1	A	402	GLN	C-O	-9.44	1.11	1.24
1	A	37	GLY	C-O	-9.41	1.13	1.24
1	A	229	MET	C-O	-9.37	1.11	1.24
2	B	83	GLU	C-N	-9.33	1.22	1.33
3	F	100	LYS	C-O	-9.30	1.12	1.24
2	E	28	GLU	CD-OE1	-9.28	1.07	1.25
1	A	150	GLU	C-O	-9.27	1.12	1.24
2	B	11	ALA	CA-CB	-9.24	1.38	1.53
2	E	343	ARG	C-O	-9.21	1.13	1.24
1	A	168	GLY	C-O	-9.20	1.11	1.23
2	E	31	PRO	C-O	-9.18	1.17	1.25
2	E	248	VAL	C-O	-9.17	1.13	1.23
1	A	273	LYS	C-O	-9.17	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	GLU	C-O	-9.16	1.12	1.24
1	A	148	GLN	C-N	-9.15	1.22	1.33
2	B	20	ASP	C-O	-9.12	1.11	1.23
1	A	142	LEU	C-O	-9.09	1.11	1.23
1	A	195	TYR	C-O	-9.09	1.13	1.24
2	E	14	MET	C-O	-9.08	1.12	1.24
2	E	367	ASP	C-O	-9.08	1.16	1.24
2	E	220	GLU	CD-OE2	-9.07	1.08	1.25
1	A	432	ARG	C-N	-9.05	1.21	1.33
1	A	249	GLU	C-O	-9.02	1.13	1.24
1	D	436	MET	C-O	-9.01	1.13	1.23
2	B	177	ARG	C-O	-8.99	1.11	1.24
2	E	223	GLU	C-O	-8.99	1.11	1.23
1	A	434	ARG	C-O	-8.94	1.12	1.24
2	B	143	VAL	C-O	-8.94	1.15	1.24
2	B	66	ARG	CZ-NH2	-8.93	1.21	1.33
1	A	83	ARG	C-O	-8.92	1.12	1.23
2	B	195	ALA	CA-CB	-8.90	1.40	1.53
1	A	160	LEU	CG-CD1	-8.88	1.23	1.52
1	A	174	PRO	CA-C	8.86	1.63	1.52
2	B	28	GLU	CD-OE2	-8.85	1.08	1.25
2	B	97	THR	C-O	-8.85	1.12	1.24
1	A	226	VAL	C-O	-8.83	1.11	1.24
1	A	275	ASP	C-O	-8.82	1.13	1.23
1	A	223	ASN	C-O	-8.82	1.12	1.24
2	B	19	THR	C-O	-8.79	1.12	1.23
2	E	122	LYS	C-O	-8.78	1.12	1.23
1	A	257	GLY	C-O	-8.77	1.11	1.24
2	E	384	PHE	C-O	-8.77	1.13	1.24
1	A	64	HIS	C-O	-8.77	1.11	1.24
1	A	406	GLU	CA-CB	-8.76	1.41	1.54
1	A	201	TYR	C-O	-8.72	1.11	1.24
1	A	254	TYR	C-O	-8.72	1.14	1.24
1	A	71	VAL	C-O	-8.72	1.13	1.23
1	D	318	LYS	C-O	-8.68	1.12	1.23
1	A	102	LEU	C-O	-8.66	1.13	1.24
1	A	250	ALA	CA-CB	-8.64	1.39	1.53
2	E	78	ILE	C-O	-8.63	1.14	1.24
1	A	95	ALA	C-O	-8.62	1.14	1.24
3	F	104	CYS	C-O	-8.62	1.14	1.23
1	A	394	VAL	C-O	-8.62	1.12	1.24
2	B	306	VAL	C-O	-8.61	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	LEU	C-O	-8.58	1.12	1.23
3	F	67	ARG	CD-NE	-8.58	1.34	1.46
1	A	418	GLU	C-O	-8.54	1.13	1.24
1	A	203	ASP	C-O	-8.54	1.13	1.24
1	D	43	PRO	C-O	-8.52	1.13	1.23
1	D	275	ASP	CG-OD2	-8.51	1.09	1.25
2	B	16	ASN	C-O	-8.50	1.11	1.23
2	B	220	GLU	N-CA	-8.50	1.35	1.46
2	B	20	ASP	CG-OD2	-8.49	1.09	1.25
1	A	66	LYS	C-O	-8.48	1.12	1.23
2	B	329	GLU	C-O	-8.48	1.13	1.24
2	B	102	GLU	C-O	-8.47	1.13	1.24
2	E	196	VAL	CB-CG2	-8.47	1.24	1.52
1	A	202	GLN	C-O	-8.45	1.14	1.24
1	D	437	ARG	CD-NE	-8.41	1.34	1.46
1	A	94	VAL	C-O	-8.41	1.05	1.23
1	D	269	ARG	CZ-NH1	-8.40	1.21	1.32
1	A	409	HIS	C-O	-8.38	1.12	1.24
1	A	182	ARG	CZ-NH2	-8.36	1.22	1.33
1	A	137	GLY	C-O	-8.36	1.12	1.23
2	B	191	ASN	C-O	-8.35	1.13	1.24
1	A	70	ILE	CG1-CD1	-8.32	1.19	1.51
2	B	220	GLU	CB-CG	-8.31	1.27	1.52
1	A	403	HIS	C-O	-8.30	1.12	1.24
1	A	356	ASP	CG-OD2	-8.28	1.09	1.25
2	B	78	ILE	C-O	-8.28	1.14	1.24
3	C	80	ILE	CG1-CD1	-8.28	1.19	1.51
2	B	98	ARG	C-O	-8.27	1.12	1.24
1	A	436	MET	C-O	-8.26	1.14	1.23
1	A	196	GLN	C-O	-8.26	1.14	1.24
1	A	58	PHE	CE1-CZ	-8.24	1.14	1.38
1	D	260	LYS	CE-NZ	-8.21	1.24	1.49
1	A	152	ILE	C-O	-8.21	1.14	1.24
1	A	89	GLU	C-O	-8.18	1.14	1.24
2	B	66	ARG	CZ-NH1	-8.18	1.21	1.32
1	D	374	LYS	CD-CE	-8.16	1.27	1.52
2	B	179	PRO	C-O	-8.14	1.14	1.24
3	F	67	ARG	C-O	-8.11	1.14	1.24
2	E	243	VAL	CB-CG2	-8.11	1.25	1.52
2	E	244	ASN	C-O	-8.10	1.13	1.23
2	B	67	CYS	C-O	-8.10	1.13	1.23
3	F	104	CYS	N-CA	-8.09	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	117	ASP	CG-OD1	-8.06	1.10	1.25
1	A	132	MET	C-O	-8.04	1.14	1.23
2	E	120	THR	C-O	-8.04	1.13	1.24
1	A	227	ALA	CA-CB	-8.01	1.41	1.53
2	B	243	VAL	N-CA	-8.01	1.36	1.46
1	A	49	ASP	C-O	-7.99	1.14	1.24
1	A	83	ARG	NE-CZ	-7.99	1.24	1.33
1	A	51	LEU	C-O	-7.95	1.14	1.24
1	A	192	LEU	CG-CD1	-7.94	1.26	1.52
1	A	370	MET	C-O	-7.93	1.14	1.24
3	C	12	GLU	C-O	-7.91	1.14	1.23
1	A	153	PHE	C-O	-7.91	1.14	1.24
2	B	15	GLU	C-O	-7.89	1.14	1.23
1	D	56	LEU	C-O	-7.89	1.14	1.24
2	B	66	ARG	C-O	-7.87	1.14	1.24
1	A	315	ARG	CB-CG	-7.86	1.28	1.52
1	A	79	GLY	C-O	-7.84	1.13	1.24
2	E	117	ASP	C-O	-7.84	1.15	1.24
1	A	163	ASP	C-O	-7.82	1.13	1.23
1	A	34	ASN	CA-CB	-7.80	1.47	1.52
1	D	374	LYS	CG-CD	-7.80	1.29	1.52
1	A	271	TRP	C-O	-7.77	1.13	1.24
1	A	335	VAL	N-CA	-7.76	1.36	1.46
1	A	213	LYS	C-O	-7.74	1.14	1.23
1	A	83	ARG	CZ-NH2	-7.72	1.23	1.33
1	A	123	ASP	C-O	-7.72	1.15	1.24
1	A	143	GLY	C-O	-7.70	1.13	1.23
2	E	126	GLY	C-O	-7.70	1.13	1.23
2	B	178	LEU	CG-CD2	-7.69	1.27	1.52
1	A	87	GLN	C-O	-7.68	1.15	1.23
1	A	437	ARG	CB-CG	-7.67	1.29	1.52
2	B	220	GLU	C-O	-7.66	1.14	1.24
1	A	207	ARG	CA-C	7.63	1.61	1.52
1	A	87	GLN	CG-CD	-7.62	1.32	1.52
2	E	120	THR	CA-CB	-7.61	1.40	1.53
1	D	5	PRO	C-O	-7.61	1.14	1.24
2	E	196	VAL	N-CA	-7.60	1.37	1.46
1	A	410	ASN	C-O	-7.57	1.13	1.23
1	A	248	GLN	CD-NE2	-7.57	1.17	1.33
1	A	148	GLN	CD-OE1	-7.55	1.09	1.23
3	F	67	ARG	CB-CG	-7.55	1.29	1.52
2	E	48	GLU	C-O	-7.52	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	102	GLU	CD-OE1	-7.52	1.11	1.25
1	A	297	SER	C-O	-7.50	1.14	1.23
1	A	200	ASP	C-N	-7.50	1.23	1.33
2	B	351	GLU	C-O	-7.48	1.15	1.24
2	B	117	ASP	N-CA	-7.47	1.37	1.46
1	A	136	THR	CB-CG2	-7.47	1.27	1.52
2	B	276	GLY	C-O	-7.47	1.14	1.23
2	B	27	THR	CB-CG2	-7.45	1.27	1.52
1	A	161	ASN	CG-ND2	-7.43	1.17	1.33
2	E	237	LYS	N-CA	-7.41	1.39	1.45
2	B	170	PHE	N-CA	-7.39	1.37	1.46
1	A	74	PHE	C-O	-7.37	1.14	1.23
2	B	208	ARG	CZ-NH1	-7.37	1.22	1.32
2	E	93	LEU	CG-CD1	-7.36	1.28	1.52
3	C	80	ILE	C-O	-7.35	1.15	1.24
1	D	432	ARG	CZ-NH2	-7.34	1.24	1.33
1	A	437	ARG	C-O	-7.34	1.08	1.23
1	A	58	PHE	C-O	-7.32	1.15	1.24
1	A	151	GLU	C-O	-7.31	1.15	1.24
1	A	170	ASN	C-O	-7.30	1.15	1.23
2	B	117	ASP	C-N	-7.30	1.24	1.33
1	D	408	ARG	CZ-NH2	-7.30	1.24	1.33
1	D	393	GLU	C-O	-7.30	1.15	1.24
2	E	343	ARG	CZ-NH2	-7.30	1.24	1.33
1	A	223	ASN	CG-OD1	-7.29	1.09	1.23
2	E	384	PHE	CE1-CZ	-7.29	1.16	1.38
1	A	62	GLU	C-O	-7.28	1.15	1.23
1	A	402	GLN	CD-NE2	-7.28	1.18	1.33
2	E	243	VAL	CA-CB	-7.27	1.44	1.54
1	D	340	GLN	CD-OE1	-7.27	1.09	1.23
1	A	335	VAL	C-O	-7.25	1.16	1.24
1	A	211	PRO	C-O	-7.23	1.15	1.24
1	A	247	ASP	C-O	-7.22	1.15	1.23
2	E	28	GLU	CB-CG	-7.22	1.30	1.52
1	A	328	LEU	CG-CD1	-7.21	1.28	1.52
2	E	385	ASP	N-CA	-7.20	1.36	1.46
1	D	170	ASN	C-O	-7.18	1.16	1.23
2	E	347	GLU	C-O	-7.18	1.15	1.24
1	A	164	LEU	CG-CD1	-7.16	1.28	1.52
2	B	273	LEU	C-O	-7.16	1.15	1.24
1	A	160	LEU	C-O	-7.15	1.14	1.24
2	E	107	ASN	C-O	-7.15	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	14	LYS	C-O	-7.13	1.14	1.23
1	A	39	ASP	C-O	-7.12	1.14	1.23
1	A	164	LEU	C-O	-7.06	1.14	1.23
2	E	220	GLU	CG-CD	-7.06	1.34	1.52
2	B	28	GLU	C-O	-7.02	1.15	1.24
2	E	196	VAL	CA-C	-7.01	1.44	1.52
2	E	257	ARG	C-O	-7.01	1.14	1.24
1	D	147	PRO	C-O	-7.01	1.15	1.24
1	A	36	LYS	CG-CD	-7.00	1.31	1.52
2	B	205	GLY	C-O	-7.00	1.17	1.24
2	B	48	GLU	C-O	-7.00	1.15	1.24
3	C	104	CYS	C-N	-6.99	1.23	1.33
2	E	57	LYS	C-O	-6.98	1.15	1.24
2	E	16	ASN	CG-OD1	-6.97	1.10	1.23
2	E	384	PHE	CG-CD2	-6.96	1.24	1.38
2	B	95	PHE	C-O	-6.95	1.14	1.23
1	D	103	ALA	N-CA	-6.94	1.37	1.46
2	B	79	ARG	CZ-NH2	-6.94	1.24	1.33
2	E	382	VAL	CB-CG2	-6.93	1.29	1.52
2	B	384	PHE	CE2-CZ	-6.91	1.18	1.38
1	A	272	GLY	C-O	-6.89	1.15	1.23
1	A	36	LYS	CB-CG	-6.87	1.31	1.52
1	A	336	LEU	CG-CD2	-6.87	1.29	1.52
1	A	67	HIS	C-O	-6.87	1.15	1.23
1	A	234	PHE	CA-C	6.87	1.61	1.53
2	B	29	PHE	C-O	-6.85	1.14	1.24
2	B	256	ASP	C-O	-6.83	1.15	1.24
3	C	80	ILE	CA-CB	-6.80	1.46	1.54
1	A	58	PHE	CD2-CE2	-6.80	1.18	1.38
1	A	256	GLY	C-O	-6.80	1.15	1.24
2	E	117	ASP	CG-OD2	-6.79	1.12	1.25
2	E	24	ARG	CZ-NH2	-6.74	1.24	1.33
1	A	432	ARG	CZ-NH2	-6.73	1.24	1.33
1	A	72	GLY	C-O	-6.70	1.14	1.23
1	A	131	ASN	N-CA	-6.68	1.38	1.46
2	B	95	PHE	CG-CD1	-6.66	1.24	1.38
1	A	36	LYS	C-N	-6.66	1.26	1.33
1	D	275	ASP	CG-OD1	-6.66	1.12	1.25
1	D	11	GLU	C-O	-6.65	1.15	1.24
2	B	208	ARG	CZ-NH2	-6.62	1.24	1.33
3	F	100	LYS	N-CA	-6.61	1.37	1.45
2	B	143	VAL	N-CA	-6.61	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	226	LEU	CG-CD2	-6.60	1.30	1.52
2	B	80	GLU	CD-OE1	-6.60	1.12	1.25
2	B	82	CYS	C-N	-6.57	1.25	1.33
2	B	220	GLU	CG-CD	-6.57	1.35	1.52
2	E	372	THR	C-O	-6.57	1.15	1.24
1	A	125	ARG	CZ-NH1	-6.57	1.23	1.32
1	A	317	LEU	CG-CD2	-6.55	1.30	1.52
1	D	432	ARG	C-O	-6.55	1.15	1.24
1	A	74	PHE	CE2-CZ	-6.54	1.19	1.38
1	D	56	LEU	CG-CD1	-6.54	1.30	1.52
2	B	384	PHE	CG-CD2	-6.53	1.25	1.38
2	E	384	PHE	CE2-CZ	-6.52	1.19	1.38
3	F	98	LEU	CG-CD1	-6.52	1.31	1.52
2	B	79	ARG	CZ-NH1	-6.52	1.23	1.32
1	D	245	LYS	CD-CE	-6.52	1.32	1.52
1	D	340	GLN	C-O	-6.50	1.16	1.23
1	D	317	LEU	CG-CD2	-6.47	1.31	1.52
3	C	99	PRO	C-O	-6.46	1.16	1.23
2	E	385	ASP	C-O	-6.46	1.15	1.23
2	B	256	ASP	N-CA	-6.45	1.37	1.46
2	B	3	PHE	C-N	-6.44	1.25	1.33
2	B	17	ARG	CZ-NH2	-6.44	1.25	1.33
1	A	61	GLY	C-O	-6.43	1.14	1.23
2	B	367	ASP	C-O	-6.43	1.18	1.24
2	E	194	GLY	N-CA	-6.42	1.38	1.46
2	E	142	ILE	C-O	-6.41	1.17	1.24
2	B	220	GLU	CA-CB	-6.39	1.42	1.53
1	A	93	GLY	C-O	-6.37	1.16	1.23
2	B	111	LEU	C-O	-6.37	1.16	1.24
1	A	126	GLY	C-O	-6.34	1.15	1.23
1	A	232	SER	CB-OG	-6.34	1.29	1.42
2	E	384	PHE	CB-CG	-6.33	1.36	1.50
1	A	437	ARG	N-CA	-6.33	1.34	1.46
2	E	195	ALA	CA-C	6.33	1.60	1.52
1	A	203	ASP	C-N	-6.32	1.24	1.33
1	D	5	PRO	CB-CG	-6.32	1.18	1.49
1	A	160	LEU	CG-CD2	-6.31	1.31	1.52
2	B	14	MET	C-N	-6.31	1.24	1.33
2	B	99	ASN	C-O	-6.31	1.14	1.23
1	A	234	PHE	CE1-CZ	-6.30	1.19	1.38
2	E	24	ARG	CG-CD	-6.28	1.33	1.52
1	A	8	MET	C-O	-6.27	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	ASP	CG-OD1	-6.27	1.13	1.25
1	A	418	GLU	CB-CG	-6.25	1.33	1.52
3	C	26	CYS	C-O	-6.25	1.16	1.24
1	A	59	HIS	CA-C	-6.25	1.45	1.52
2	E	106	ASP	C-O	-6.25	1.15	1.23
2	B	117	ASP	CG-OD1	-6.22	1.13	1.25
2	B	220	GLU	CD-OE1	-6.22	1.13	1.25
2	E	343	ARG	NE-CZ	-6.20	1.26	1.33
1	A	202	GLN	CG-CD	-6.20	1.36	1.52
1	A	356	ASP	CG-OD1	-6.19	1.13	1.25
2	E	203	LEU	C-O	-6.19	1.17	1.24
1	A	58	PHE	CG-CD2	-6.18	1.25	1.38
2	B	104	MET	SD-CE	-6.17	1.64	1.79
2	B	66	ARG	NE-CZ	-6.16	1.26	1.33
1	A	56	LEU	C-O	-6.16	1.17	1.24
1	A	51	LEU	CG-CD2	-6.15	1.32	1.52
1	A	297	SER	N-CA	-6.15	1.38	1.45
2	B	204	VAL	CB-CG1	-6.14	1.32	1.52
1	D	428	ILE	N-CA	-6.14	1.38	1.46
1	A	292	GLU	C-O	-6.12	1.17	1.24
1	A	321	ASP	N-CA	-6.12	1.38	1.46
2	E	140	SER	C-O	-6.12	1.15	1.23
1	A	210	PHE	CG-CD1	-6.12	1.26	1.38
2	B	104	MET	N-CA	-6.11	1.38	1.46
1	D	436	MET	SD-CE	-6.11	1.64	1.79
2	B	5	SER	C-O	-6.09	1.15	1.23
1	A	161	ASN	C-O	-6.09	1.16	1.23
1	A	299	ASP	CG-OD1	-6.09	1.13	1.25
1	D	427	ASP	C-O	-6.09	1.16	1.24
1	A	98	HIS	C-N	-6.09	1.25	1.33
1	A	334	PRO	C-O	-6.09	1.16	1.24
3	C	20	ASN	C-O	-6.08	1.17	1.24
1	A	60	GLU	C-O	-6.08	1.16	1.24
1	A	245	LYS	C-O	-6.05	1.16	1.24
1	A	351	ALA	CA-CB	-6.05	1.44	1.53
3	C	54	GLN	C-O	-6.05	1.17	1.24
1	A	249	GLU	CB-CG	-6.04	1.34	1.52
2	E	124	ALA	CA-CB	-6.04	1.44	1.53
1	A	147	PRO	C-O	-6.03	1.16	1.24
2	B	16	ASN	CG-ND2	-6.03	1.20	1.33
1	A	97	PHE	CG-CD1	-6.01	1.26	1.38
1	A	322	GLU	N-CA	-6.00	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	370	MET	CB-CG	-5.99	1.34	1.52
1	D	340	GLN	N-CA	-5.99	1.38	1.45
2	E	195	ALA	C-O	-5.99	1.15	1.24
1	D	50	LEU	C-O	-5.98	1.17	1.24
1	A	88	PRO	CA-CB	-5.97	1.45	1.53
3	F	80	ILE	C-O	-5.97	1.17	1.24
2	E	124	ALA	C-O	-5.97	1.17	1.24
1	A	321	ASP	CG-OD2	-5.97	1.14	1.25
1	A	425	SER	C-O	-5.96	1.16	1.24
1	D	434	ARG	CZ-NH2	-5.96	1.25	1.33
1	A	192	LEU	C-N	-5.95	1.26	1.33
1	A	247	ASP	CA-C	-5.95	1.45	1.53
2	B	329	GLU	CD-OE1	-5.95	1.14	1.25
2	B	204	VAL	CB-CG2	-5.94	1.32	1.52
1	A	128	GLY	C-O	-5.93	1.15	1.24
1	D	4	HIS	C-O	-5.93	1.11	1.23
2	E	107	ASN	CG-ND2	-5.93	1.20	1.33
3	C	104	CYS	C-O	-5.93	1.15	1.23
1	A	434	ARG	CZ-NH1	-5.93	1.24	1.32
2	B	204	VAL	CA-CB	5.91	1.61	1.54
1	A	41	GLN	C-N	-5.91	1.27	1.33
1	A	49	ASP	CG-OD1	-5.89	1.14	1.25
1	A	297	SER	CB-OG	-5.89	1.30	1.42
1	A	247	ASP	CG-OD1	-5.88	1.14	1.25
1	A	159	ASN	CG-ND2	-5.88	1.21	1.33
2	B	95	PHE	CE1-CZ	-5.87	1.21	1.38
1	D	336	LEU	CG-CD1	-5.86	1.33	1.52
1	A	248	GLN	CB-CG	-5.85	1.34	1.52
1	A	149	LEU	C-N	-5.85	1.26	1.34
1	D	336	LEU	C-O	-5.84	1.11	1.23
1	A	169	SER	C-O	-5.83	1.14	1.23
3	F	26	CYS	N-CA	-5.82	1.40	1.46
1	A	334	PRO	CB-CG	-5.81	1.20	1.49
1	A	369	TRP	C-N	-5.81	1.25	1.34
2	B	18	ILE	N-CA	-5.80	1.39	1.46
1	A	81	ILE	CA-CB	5.79	1.60	1.53
2	E	57	LYS	N-CA	-5.79	1.39	1.46
2	B	216	GLU	C-O	-5.79	1.17	1.24
2	B	143	VAL	CB-CG1	-5.79	1.33	1.52
2	B	47	LEU	C-O	-5.78	1.16	1.24
1	A	49	ASP	CG-OD2	-5.77	1.14	1.25
1	A	408	ARG	CD-NE	-5.77	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	80	GLU	N-CA	-5.76	1.39	1.46
2	B	52	LEU	C-N	-5.76	1.26	1.33
3	F	33	ALA	C-O	5.75	1.31	1.24
1	A	125	ARG	CD-NE	-5.74	1.38	1.46
2	E	16	ASN	CG-ND2	-5.74	1.21	1.33
1	A	201	TYR	CA-C	5.71	1.61	1.52
1	D	11	GLU	CD-OE1	-5.71	1.14	1.25
2	B	66	ARG	CD-NE	-5.71	1.38	1.46
2	B	385	ASP	C-O	-5.70	1.16	1.23
1	A	192	LEU	CG-CD2	-5.69	1.33	1.52
1	D	8	MET	SD-CE	-5.69	1.65	1.79
1	A	406	GLU	CG-CD	-5.68	1.37	1.52
1	A	267	ALA	C-O	-5.68	1.17	1.24
1	D	432	ARG	CA-C	5.67	1.60	1.52
1	A	182	ARG	CZ-NH1	-5.67	1.24	1.32
2	B	292	ARG	C-O	-5.67	1.17	1.24
1	D	101	ARG	CZ-NH1	-5.67	1.24	1.32
1	A	434	ARG	CZ-NH2	-5.66	1.26	1.33
1	A	123	ASP	CG-OD2	-5.65	1.14	1.25
2	E	48	GLU	N-CA	-5.65	1.40	1.46
3	C	27	PRO	C-O	-5.64	1.17	1.24
2	B	350	TYR	CG-CD2	-5.63	1.27	1.39
2	E	371	TYR	C-O	-5.62	1.16	1.24
2	E	384	PHE	CD1-CE1	-5.62	1.21	1.38
1	A	129	LEU	CG-CD2	-5.61	1.34	1.52
2	B	29	PHE	CE1-CZ	-5.61	1.21	1.38
1	A	51	LEU	N-CA	5.58	1.53	1.46
1	A	268	GLY	C-N	-5.58	1.25	1.33
1	A	418	GLU	CA-C	-5.58	1.44	1.52
1	A	73	VAL	C-O	-5.58	1.17	1.24
1	A	250	ALA	C-N	-5.58	1.26	1.33
2	E	48	GLU	CD-OE1	-5.57	1.14	1.25
1	A	299	ASP	CG-OD2	-5.57	1.14	1.25
2	B	178	LEU	CG-CD1	-5.57	1.34	1.52
2	B	203	LEU	CG-CD1	-5.57	1.34	1.52
1	A	38	LEU	CA-C	-5.56	1.45	1.52
1	A	336	LEU	CG-CD1	-5.56	1.34	1.52
2	B	243	VAL	CA-CB	-5.56	1.47	1.54
1	D	5	PRO	CA-CB	-5.56	1.45	1.53
1	D	43	PRO	CB-CG	-5.55	1.21	1.49
1	D	428	ILE	CA-CB	-5.55	1.46	1.54
1	A	127	SER	CB-OG	-5.55	1.31	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	GLN	C-N	-5.54	1.26	1.34
2	B	384	PHE	CB-CG	-5.54	1.38	1.50
1	D	318	LYS	CG-CD	-5.53	1.35	1.52
1	D	432	ARG	NE-CZ	-5.53	1.26	1.33
1	A	202	GLN	CD-OE1	-5.52	1.13	1.23
2	E	9	ASN	CG-OD1	-5.51	1.13	1.23
1	D	334	PRO	C-N	-5.51	1.27	1.33
2	E	57	LYS	CB-CG	-5.50	1.35	1.52
1	D	374	LYS	CA-CB	-5.50	1.44	1.53
1	A	266	HIS	CD2-NE2	-5.49	1.31	1.37
2	B	17	ARG	CZ-NH1	-5.48	1.25	1.32
1	A	152	ILE	N-CA	-5.47	1.40	1.46
2	B	170	PHE	CE2-CZ	-5.44	1.22	1.38
2	B	102	GLU	CD-OE2	-5.43	1.15	1.25
1	A	393	GLU	CD-OE1	-5.43	1.15	1.25
2	B	221	LEU	CG-CD1	-5.42	1.34	1.52
2	B	354	GLY	C-N	-5.42	1.26	1.33
1	A	103	ALA	N-CA	-5.41	1.39	1.46
1	A	89	GLU	CB-CG	-5.39	1.36	1.52
1	A	153	PHE	CA-C	5.39	1.59	1.52
2	E	122	LYS	CD-CE	-5.38	1.36	1.52
2	E	220	GLU	N-CA	-5.38	1.39	1.46
1	A	38	LEU	CA-CB	-5.38	1.44	1.53
1	D	437	ARG	CB-CG	-5.37	1.36	1.52
1	A	159	ASN	CG-OD1	-5.36	1.13	1.23
1	A	182	ARG	CB-CG	-5.36	1.36	1.52
2	B	355	LEU	N-CA	-5.36	1.39	1.46
1	A	196	GLN	CD-NE2	-5.36	1.22	1.33
2	B	208	ARG	CD-NE	-5.35	1.38	1.46
1	A	409	HIS	CA-C	5.35	1.59	1.52
1	D	102	LEU	CB-CG	-5.35	1.42	1.53
2	B	356	GLU	CB-CG	-5.34	1.36	1.52
2	E	248	VAL	CA-CB	-5.33	1.46	1.55
1	A	434	ARG	NE-CZ	-5.33	1.27	1.33
1	A	197	LEU	C-O	-5.33	1.17	1.24
2	B	162	VAL	CB-CG1	-5.33	1.34	1.52
2	B	100	ASN	CG-OD1	-5.32	1.13	1.23
1	A	63	THR	C-N	-5.30	1.26	1.33
2	B	220	GLU	C-N	-5.29	1.26	1.33
2	B	52	LEU	CG-CD2	-5.27	1.35	1.52
2	B	15	GLU	CD-OE2	-5.27	1.15	1.25
2	E	243	VAL	CB-CG1	-5.27	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	244	ASN	C-N	-5.25	1.25	1.33
1	D	102	LEU	CG-CD1	-5.25	1.35	1.52
1	D	269	ARG	CD-NE	-5.25	1.39	1.46
1	A	266	HIS	CA-C	5.24	1.59	1.52
1	A	321	ASP	CG-OD1	-5.24	1.15	1.25
2	B	171	GLU	C-N	-5.23	1.25	1.33
1	A	173	THR	C-N	-5.22	1.27	1.33
2	E	248	VAL	CB-CG2	-5.22	1.35	1.52
2	B	356	GLU	CA-CB	-5.21	1.46	1.53
1	A	315	ARG	CZ-NH1	-5.21	1.25	1.32
1	D	393	GLU	CA-C	-5.21	1.46	1.52
3	C	37	GLU	C-O	-5.20	1.17	1.24
1	A	64	HIS	N-CA	-5.19	1.40	1.46
3	F	100	LYS	CD-CE	-5.19	1.36	1.52
1	D	391	LEU	CG-CD1	-5.19	1.35	1.52
1	D	408	ARG	CZ-NH1	-5.19	1.25	1.32
2	B	100	ASN	C-O	-5.18	1.17	1.23
1	A	233	ASP	CG-OD2	-5.17	1.15	1.25
2	B	95	PHE	CE2-CZ	-5.17	1.23	1.38
2	E	195	ALA	CA-CB	-5.15	1.45	1.53
1	A	228	SER	CB-OG	-5.15	1.31	1.42
2	B	220	GLU	CD-OE2	-5.14	1.15	1.25
2	E	220	GLU	CD-OE1	-5.14	1.15	1.25
1	D	317	LEU	CG-CD1	-5.14	1.35	1.52
1	A	163	ASP	CG-OD1	-5.13	1.15	1.25
3	C	37	GLU	CD-OE1	-5.12	1.15	1.25
1	D	170	ASN	CA-CB	-5.12	1.47	1.53
1	A	155	GLU	CD-OE2	-5.11	1.15	1.25
2	B	48	GLU	CG-CD	-5.11	1.39	1.52
3	C	93	CYS	C-O	-5.10	1.18	1.24
1	A	102	LEU	CG-CD1	-5.09	1.35	1.52
2	B	242	GLU	C-N	-5.09	1.26	1.33
1	D	428	ILE	CG1-CD1	-5.09	1.31	1.51
2	E	257	ARG	N-CA	-5.09	1.39	1.46
1	D	131	ASN	C-O	-5.09	1.18	1.24
1	A	358	VAL	C-O	-5.07	1.18	1.24
2	B	225	PRO	C-N	-5.07	1.27	1.33
1	A	40	TYR	CA-C	-5.07	1.46	1.52
1	A	58	PHE	C-N	-5.07	1.27	1.33
2	B	163	LYS	C-O	-5.06	1.18	1.24
1	A	182	ARG	C-N	-5.05	1.27	1.33
2	B	271	LEU	C-O	-5.05	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	292	GLU	C-O	-5.05	1.17	1.23
2	B	179	PRO	CA-CB	-5.04	1.46	1.53
2	E	9	ASN	C-N	-5.04	1.27	1.33
1	A	60	GLU	CD-OE2	-5.03	1.15	1.25
1	D	50	LEU	N-CA	-5.03	1.40	1.46
1	A	202	GLN	N-CA	-5.03	1.40	1.46
1	D	133	HIS	C-O	-5.03	1.13	1.23
1	A	147	PRO	CA-CB	-5.03	1.46	1.53
1	A	274	PHE	CD1-CE1	-5.02	1.23	1.38
1	A	337	ASP	C-O	-5.01	1.17	1.23
1	A	227	ALA	C-O	-5.01	1.17	1.23
2	B	17	ARG	C-O	-5.01	1.17	1.24
1	D	51	LEU	C-N	-5.01	1.28	1.33

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ARG	NE-CZ-NH2	-14.37	106.27	119.20
3	F	67	ARG	NE-CZ-NH1	11.36	132.86	121.50
1	D	432	ARG	NE-CZ-NH2	-11.23	109.09	119.20
1	A	315	ARG	NE-CZ-NH2	9.92	128.13	119.20
1	D	269	ARG	NE-CZ-NH2	9.82	128.04	119.20
1	D	437	ARG	NE-CZ-NH2	-9.20	110.92	119.20
3	F	67	ARG	CD-NE-CZ	9.13	137.19	124.40
1	D	405	SER	N-CA-C	-9.04	102.03	113.23
1	A	405	SER	N-CA-C	-8.84	102.63	113.41
3	F	67	ARG	NE-CZ-NH2	-8.73	111.34	119.20
1	A	155	GLU	CA-C-O	7.96	128.99	120.55
1	D	102	LEU	CB-CG-CD1	-7.93	86.89	110.70
3	C	104	CYS	O-C-N	7.83	133.22	122.41
1	D	139	ILE	N-CA-C	-7.80	98.59	108.89
2	E	220	GLU	CB-CA-C	-7.73	97.71	110.85
3	F	104	CYS	CA-C-N	7.71	135.59	121.70
3	F	104	CYS	C-N-CA	7.71	135.59	121.70
1	A	406	GLU	CB-CA-C	-7.64	97.55	109.55
2	E	120	THR	CA-CB-OG1	7.46	120.79	109.60
2	E	2	ALA	CA-C-N	-7.44	112.52	122.42
2	E	2	ALA	C-N-CA	-7.44	112.52	122.42
1	A	127	SER	N-CA-C	7.43	120.43	111.82
1	D	177	CYS	N-CA-C	-7.40	100.98	110.53
2	B	100	ASN	CA-C-O	-7.40	112.99	121.72
2	E	120	THR	OG1-CB-CG2	7.34	123.99	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	ARG	NE-CZ-NH1	-7.30	114.20	121.50
1	D	335	VAL	CA-C-O	-7.29	112.67	121.13
2	B	31	PRO	N-CA-C	-7.28	102.79	110.58
1	A	139	ILE	N-CA-C	-7.21	97.86	108.54
1	D	432	ARG	NE-CZ-NH1	7.17	128.68	121.50
1	A	406	GLU	N-CA-C	7.14	119.80	108.23
1	D	432	ARG	CD-NE-CZ	7.10	134.34	124.40
1	A	256	GLY	N-CA-C	7.04	122.68	114.16
2	B	83	GLU	CA-C-O	6.98	127.95	120.55
2	B	143	VAL	CA-C-O	-6.94	112.55	120.95
2	E	48	GLU	N-CA-C	6.71	114.04	108.07
2	E	191	ASN	N-CA-C	-6.70	104.21	112.38
1	D	142	LEU	N-CA-C	6.66	119.71	107.99
1	D	269	ARG	NE-CZ-NH1	-6.59	114.91	121.50
3	C	104	CYS	CA-C-N	6.42	133.27	121.70
3	C	104	CYS	C-N-CA	6.42	133.27	121.70
1	A	13	GLU	N-CA-C	-6.42	105.49	113.38
1	A	177	CYS	N-CA-C	-6.39	101.53	110.35
1	A	49	ASP	N-CA-C	6.36	119.20	111.82
3	F	102	THR	CA-CB-OG1	6.30	119.04	109.60
2	E	220	GLU	CG-CD-OE2	-6.28	103.95	118.40
1	A	131	ASN	CA-CB-CG	6.28	118.88	112.60
1	D	134	GLY	CA-C-O	-6.26	114.10	122.24
1	D	413	ILE	N-CA-C	6.25	117.79	108.23
1	A	406	GLU	CA-C-N	-6.21	114.25	120.21
1	A	406	GLU	C-N-CA	-6.21	114.25	120.21
2	E	78	ILE	N-CA-CB	6.18	117.37	110.51
2	B	79	ARG	N-CA-C	6.17	118.80	111.33
2	E	260	TYR	N-CA-C	6.17	120.05	111.90
1	A	413	ILE	N-CA-C	6.17	117.66	108.23
3	F	26	CYS	N-CA-CB	-6.13	104.67	111.10
2	B	12	LYS	CA-C-N	6.12	126.30	119.32
2	B	12	LYS	C-N-CA	6.12	126.30	119.32
1	A	201	TYR	N-CA-C	6.11	119.45	112.97
1	A	108	LYS	N-CA-C	6.09	119.83	111.54
1	A	246	ILE	N-CA-C	6.05	116.57	107.80
1	D	4	HIS	CB-CA-C	6.03	121.55	110.10
1	A	83	ARG	NE-CZ-NH1	5.96	127.46	121.50
1	D	108	LYS	N-CA-C	5.96	119.78	111.74
1	D	437	ARG	CD-NE-CZ	5.92	132.68	124.40
2	B	220	GLU	N-CA-C	5.91	118.67	111.82
1	D	269	ARG	CB-CG-CD	5.90	124.87	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	GLY	CA-C-O	-5.89	116.23	121.41
1	A	124	LEU	N-CA-C	5.87	117.47	111.14
2	B	5	SER	CA-CB-OG	5.86	122.81	111.10
2	B	4	ILE	O-C-N	-5.83	116.75	122.99
1	D	4	HIS	N-CA-CB	5.80	120.37	110.50
1	A	341	MET	N-CA-C	-5.79	101.16	110.14
2	B	7	GLY	CA-C-N	5.79	129.06	120.90
2	B	7	GLY	C-N-CA	5.79	129.06	120.90
2	B	52	LEU	O-C-N	-5.78	115.65	123.10
2	B	286	GLY	N-CA-C	5.77	123.56	115.43
1	A	297	SER	N-CA-C	5.76	117.94	109.24
1	A	131	ASN	N-CA-C	5.74	118.25	108.90
2	B	126	GLY	N-CA-C	5.69	121.25	114.48
1	A	313	MET	CA-C-N	5.68	126.94	119.84
1	A	313	MET	C-N-CA	5.68	126.94	119.84
1	D	101	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	A	203	ASP	CA-C-O	5.67	126.50	120.10
2	B	177	ARG	N-CA-C	5.66	120.92	112.94
2	B	222	CYS	N-CA-C	5.65	118.43	109.50
2	B	24	ARG	N-CA-C	-5.65	102.53	110.50
1	A	308	HIS	N-CA-C	5.64	117.11	111.07
1	D	323	ARG	N-CA-C	5.64	119.16	110.42
1	A	83	ARG	CD-NE-CZ	5.63	132.28	124.40
2	E	48	GLU	O-C-N	5.62	127.12	121.56
1	A	334	PRO	CA-N-CD	-5.61	104.15	112.00
2	B	260	TYR	N-CA-C	5.60	119.30	111.90
2	E	57	LYS	O-C-N	5.59	128.76	122.22
2	B	7	GLY	N-CA-C	-5.58	107.84	114.48
1	A	406	GLU	CB-CG-CD	-5.57	103.13	112.60
1	A	356	ASP	OD1-CG-OD2	-5.55	109.57	122.90
1	D	68	GLY	N-CA-C	5.52	121.11	111.78
1	A	134	GLY	CA-C-O	-5.51	115.07	122.24
3	C	102	THR	N-CA-C	5.51	117.79	109.41
1	A	406	GLU	O-C-N	5.51	125.71	121.85
1	A	5	PRO	CA-C-N	-5.50	116.50	123.15
1	A	5	PRO	C-N-CA	-5.50	116.50	123.15
1	A	323	ARG	N-CA-C	5.50	118.66	110.52
1	D	5	PRO	CB-CA-C	-5.49	102.50	111.56
2	E	222	CYS	N-CA-C	5.47	118.38	109.24
1	A	148	GLN	CA-C-O	5.46	126.08	119.31
1	A	84	TYR	CA-C-O	-5.45	114.27	120.32
1	A	248	GLN	N-CA-C	5.42	117.89	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	220	GLU	CG-CD-OE1	5.41	130.85	118.40
2	B	329	GLU	OE1-CD-OE2	-5.37	110.01	122.90
2	E	220	GLU	N-CA-C	5.34	117.18	111.36
1	A	182	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	D	96	HIS	N-CA-C	-5.28	100.80	109.40
2	B	336	ARG	N-CA-C	-5.28	103.43	110.55
2	E	193	CYS	N-CA-C	-5.27	103.18	110.35
1	D	226	VAL	N-CA-C	-5.27	107.16	112.17
1	A	34	ASN	CA-C-N	5.27	124.90	119.05
1	A	34	ASN	C-N-CA	5.27	124.90	119.05
2	B	346	TRP	N-CA-C	5.26	117.09	111.36
1	D	13	GLU	N-CA-C	-5.26	107.03	113.50
1	D	308	HIS	N-CA-C	5.25	117.42	111.11
2	B	30	PHE	CA-C-N	-5.22	115.90	119.66
2	B	30	PHE	C-N-CA	-5.22	115.90	119.66
1	D	341	MET	N-CA-C	-5.21	102.48	110.14
2	E	195	ALA	N-CA-C	5.21	119.38	112.30
1	D	231	ARG	N-CA-C	5.17	119.16	111.87
2	B	193	CYS	N-CA-C	-5.16	102.74	110.23
1	D	260	LYS	N-CA-C	5.16	116.33	109.93
1	D	408	ARG	N-CA-C	5.12	116.89	110.24
1	A	334	PRO	N-CA-C	5.10	122.98	112.47
1	A	224	GLY	CA-C-O	-5.09	113.93	119.88
2	E	194	GLY	N-CA-C	5.07	117.44	111.35
2	E	12	LYS	CA-C-N	5.07	125.35	119.47
2	E	12	LYS	C-N-CA	5.07	125.35	119.47
2	B	384	PHE	N-CA-C	5.07	117.54	111.71
1	A	244	ILE	N-CA-C	-5.06	103.06	109.58
3	F	13	VAL	CB-CA-C	-5.06	103.34	110.82
1	A	72	GLY	N-CA-C	5.05	117.41	110.69
2	B	231	CYS	N-CA-C	5.02	116.22	109.24
1	A	155	GLU	O-C-N	-5.02	116.80	122.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3422	0	3275	104	0
1	D	3422	0	3275	119	0
2	B	2999	0	2963	87	0
2	E	2999	0	2963	83	0
3	C	787	0	758	48	0
3	F	787	0	758	47	0
4	A	4	0	0	0	0
4	D	4	0	0	0	0
5	A	63	0	33	12	0
5	B	62	0	35	9	0
5	D	63	0	35	10	0
5	E	62	0	34	5	0
6	A	16	0	0	0	0
6	B	16	0	0	0	0
6	D	16	0	0	0	0
6	E	16	0	0	0	0
7	A	164	0	0	10	0
7	B	160	0	0	4	0
7	C	12	0	0	1	0
7	D	220	0	0	8	0
7	E	155	0	0	3	0
7	F	18	0	0	0	0
All	All	15467	0	14129	430	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 15.

All (430) 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)
5:A:580:SRM:HHA	3:C:104:CYS:SG	1.36	1.62
5:D:582:SRM:HHA	3:F:104:CYS:SG	1.47	1.51
5:A:580:SRM:CHA	3:C:104:CYS:SG	2.10	1.39
7:A:6631:HOH:O	3:C:105:VAL:CG2	1.75	1.34
5:D:582:SRM:CHA	3:F:104:CYS:SG	2.20	1.29
1:A:427:ASP:OD2	1:A:429:SER:HB3	1.38	1.24
1:D:3:LYS:HA	1:D:4:HIS:HB3	1.14	1.12
1:A:3:LYS:O	1:A:3:LYS:HG3	1.41	1.07
1:D:167:SER:HB2	3:F:105:VAL:HG21	1.33	1.06
2:E:382:VAL:CG2	2:E:384:PHE:HD1	1.68	1.06
3:F:13:VAL:HG11	3:F:17:GLY:HA2	1.40	1.04
5:B:581:SRM:HBA1	5:B:581:SRM:HMA3	1.38	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:VAL:HG22	3:C:12:GLU:OE2	1.61	0.99
7:A:6631:HOH:O	3:C:105:VAL:HG21	1.39	0.99
1:D:3:LYS:O	1:D:3:LYS:HD3	1.63	0.98
7:D:6726:HOH:O	3:F:105:VAL:HG23	1.63	0.97
2:E:196:VAL:HG11	2:E:204:VAL:HG22	1.47	0.97
1:A:39:ASP:OD1	2:B:2:ALA:HA	1.65	0.96
1:D:3:LYS:CA	1:D:4:HIS:HB3	1.97	0.94
2:B:382:VAL:CG2	2:B:384:PHE:HD1	1.80	0.94
1:A:70:ILE:HG12	3:C:100:LYS:HD2	1.49	0.94
5:E:583:SRM:HBA1	5:E:583:SRM:HMA3	1.48	0.93
3:C:26:CYS:SG	3:C:28:GLU:HG2	2.10	0.91
2:B:382:VAL:HG23	2:B:384:PHE:HD1	1.34	0.91
2:E:196:VAL:HG11	2:E:204:VAL:CG2	2.01	0.90
2:E:382:VAL:HG23	2:E:384:PHE:HD1	1.36	0.90
1:D:104:GLN:H	1:D:104:GLN:HE21	1.20	0.89
3:C:3:VAL:CG2	3:C:12:GLU:OE2	2.21	0.88
1:A:69:GLY:O	1:A:70:ILE:HD13	1.74	0.86
1:D:97:PHE:O	2:E:150:TYR:HE1	1.59	0.86
2:E:382:VAL:HG21	2:E:384:PHE:HD1	1.40	0.85
1:D:34:ASN:HD21	1:D:38:LEU:H	1.23	0.85
1:A:97:PHE:O	2:B:150:TYR:CE1	2.30	0.84
1:A:104:GLN:H	1:A:104:GLN:HE21	1.25	0.83
1:A:97:PHE:O	2:B:150:TYR:HE1	1.61	0.83
1:D:104:GLN:H	1:D:104:GLN:NE2	1.77	0.82
5:B:581:SRM:HBA1	5:B:581:SRM:CMA	2.10	0.81
7:D:6726:HOH:O	3:F:105:VAL:CG2	2.21	0.80
7:A:6631:HOH:O	3:C:105:VAL:HG23	1.52	0.80
1:D:3:LYS:HA	1:D:4:HIS:CB	2.02	0.80
1:D:402:GLN:H	1:D:402:GLN:HE21	1.29	0.80
1:D:3:LYS:O	1:D:3:LYS:CG	2.30	0.80
3:F:26:CYS:SG	3:F:28:GLU:OE2	2.41	0.79
1:D:3:LYS:O	1:D:3:LYS:CD	2.30	0.79
2:B:382:VAL:CG2	2:B:384:PHE:CD1	2.65	0.79
1:D:97:PHE:O	2:E:150:TYR:CE1	2.36	0.79
3:C:105:VAL:OXT	3:C:105:VAL:HG12	1.82	0.78
2:B:37:ASN:HD21	2:B:58:ASN:HD21	1.29	0.78
1:A:69:GLY:C	1:A:70:ILE:HD13	2.09	0.78
2:E:37:ASN:HD21	2:E:58:ASN:HD21	1.28	0.78
1:D:170:ASN:ND2	1:D:208:PRO:HG3	1.99	0.78
1:A:104:GLN:H	1:A:104:GLN:NE2	1.82	0.77
1:D:131:ASN:HB2	1:D:140:VAL:HB	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:LYS:HB2	1:D:419:GLU:HG3	1.66	0.77
2:E:382:VAL:CG2	2:E:384:PHE:CD1	2.61	0.77
1:A:34:ASN:HD21	1:A:38:LEU:H	1.32	0.76
2:E:382:VAL:HG23	2:E:384:PHE:CD1	2.20	0.76
3:F:28:GLU:HA	3:F:31:LYS:HE2	1.67	0.76
2:E:382:VAL:HG21	2:E:384:PHE:CD1	2.21	0.76
3:C:49:ILE:HD11	3:C:75:PHE:HD1	1.50	0.75
1:D:308:HIS:HD2	2:E:292:ARG:HE	1.35	0.75
1:A:427:ASP:CG	1:A:429:SER:HB3	2.12	0.74
2:B:9:ASN:C	2:B:9:ASN:HD22	1.93	0.74
3:F:13:VAL:HG11	3:F:17:GLY:CA	2.15	0.74
2:E:208:ARG:HD2	2:E:305:PHE:CE1	2.23	0.73
1:D:262:ASN:ND2	2:E:292:ARG:HH22	1.86	0.73
3:F:13:VAL:HG12	3:F:14:ASP:N	2.02	0.73
1:D:5:PRO:HG2	1:D:5:PRO:O	1.88	0.72
1:A:83:ARG:CD	2:B:150:TYR:O	2.38	0.72
2:B:382:VAL:HG21	2:B:384:PHE:CD1	2.24	0.72
1:D:402:GLN:H	1:D:402:GLN:NE2	1.88	0.72
1:D:408:ARG:HH11	1:D:410:ASN:HD21	1.38	0.71
1:D:156:MET:HE3	1:D:162:THR:HB	1.71	0.71
1:A:402:GLN:H	1:A:402:GLN:HE21	1.37	0.71
1:A:46:CYS:HB3	1:A:47:PRO:HD3	1.72	0.71
1:D:104:GLN:HE22	1:D:173:THR:HG21	1.54	0.71
1:A:83:ARG:HD3	2:B:150:TYR:O	1.91	0.70
1:A:3:LYS:O	1:A:3:LYS:CG	2.30	0.70
3:C:49:ILE:HD11	3:C:75:PHE:CD1	2.26	0.70
1:A:167:SER:HB2	3:C:105:VAL:HG21	1.73	0.70
1:A:308:HIS:HD2	2:B:292:ARG:HE	1.37	0.70
1:D:184:GLU:OE1	2:E:44:HIS:HD2	1.75	0.69
5:D:582:SRM:O1A	2:E:150:TYR:HD2	1.74	0.69
1:D:81:ILE:CD1	3:F:105:VAL:HG22	2.22	0.69
1:A:427:ASP:OD2	1:A:429:SER:CB	2.29	0.69
1:A:70:ILE:HG12	3:C:100:LYS:CD	2.23	0.69
3:F:105:VAL:OXT	3:F:105:VAL:HG12	1.91	0.69
1:D:83:ARG:H	1:D:98:HIS:HD2	1.40	0.69
1:D:104:GLN:HE21	1:D:104:GLN:N	1.90	0.69
1:A:285:PRO:HG3	2:B:293:ILE:HA	1.75	0.68
3:F:26:CYS:SG	3:F:28:GLU:HG2	2.33	0.68
1:A:427:ASP:OD2	1:A:430:ASP:OD1	2.12	0.67
1:A:83:ARG:H	1:A:98:HIS:HD2	1.40	0.67
1:A:248:GLN:HE22	1:A:296:LEU:H	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:LYS:O	1:D:3:LYS:HG3	1.93	0.67
1:D:170:ASN:HD22	1:D:208:PRO:HG3	1.60	0.67
1:D:223:ASN:HD21	1:D:311:ASN:HD21	1.40	0.67
5:B:581:SRM:HBA1	5:B:581:SRM:C1A	2.24	0.66
2:E:293:ILE:HG22	2:E:294:LYS:HD2	1.78	0.66
1:A:167:SER:OG	3:C:105:VAL:HG11	1.95	0.66
3:F:13:VAL:CG1	3:F:17:GLY:HA2	2.23	0.66
2:E:208:ARG:HD3	2:E:278:GLY:O	1.96	0.66
2:E:224:ILE:HB	2:E:225:PRO:HD3	1.78	0.66
5:B:581:SRM:HMA3	5:B:581:SRM:CBA	2.13	0.65
1:D:418:GLU:CD	1:D:418:GLU:H	2.03	0.65
2:B:9:ASN:ND2	2:B:11:ALA:H	1.94	0.65
1:A:408:ARG:HH11	1:A:410:ASN:HD21	1.44	0.65
2:B:4:ILE:HG13	2:B:4:ILE:O	1.95	0.65
1:A:411:PRO:HG3	2:E:192:MET:CE	2.26	0.64
5:D:582:SRM:HMA2	3:F:104:CYS:SG	2.38	0.64
2:B:11:ALA:C	2:B:13:PRO:HD3	2.22	0.63
1:D:376:ARG:HB3	1:D:376:ARG:NH1	2.14	0.63
3:C:3:VAL:HG22	3:C:12:GLU:HG3	1.81	0.63
1:D:46:CYS:HB3	1:D:47:PRO:HD3	1.81	0.63
2:E:239:ILE:HG12	2:E:252:ALA:HB2	1.79	0.63
1:D:45:GLU:CD	1:D:45:GLU:H	2.08	0.62
5:B:581:SRM:C1A	5:B:581:SRM:CBA	2.76	0.62
1:A:104:GLN:HE21	1:A:104:GLN:N	1.97	0.62
1:D:3:LYS:HE2	1:D:4:HIS:ND1	2.14	0.62
1:A:36:LYS:HB2	7:A:6638:HOH:O	1.99	0.61
1:A:223:ASN:HD21	1:A:311:ASN:HD21	1.48	0.61
1:A:402:GLN:H	1:A:402:GLN:NE2	1.97	0.61
1:D:3:LYS:HD3	1:D:3:LYS:C	2.24	0.61
3:F:3:VAL:HG22	3:F:12:GLU:HG2	1.82	0.61
2:B:142:ILE:O	2:B:144:HIS:HD2	1.84	0.61
3:F:78:LYS:O	3:F:82:GLU:HG3	2.00	0.61
2:B:207:HIS:HD2	2:B:279:ASP:OD1	1.83	0.61
3:C:78:LYS:O	3:C:82:GLU:HG3	2.01	0.61
5:A:580:SRM:C1A	3:C:104:CYS:SG	2.84	0.61
2:B:107:ASN:ND2	2:B:110:THR:H	1.99	0.60
3:C:26:CYS:HB2	3:C:27:PRO:CD	2.31	0.60
5:D:582:SRM:C1A	3:F:104:CYS:SG	2.88	0.60
2:B:9:ASN:C	2:B:9:ASN:ND2	2.56	0.60
2:E:247:LYS:HZ3	2:E:247:LYS:HB3	1.65	0.60
1:A:410:ASN:HD22	1:A:412:TYR:H	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:HIS:HD2	1:D:86:ASP:OD2	1.85	0.59
5:B:581:SRM:HBA2	5:B:581:SRM:NA	2.17	0.59
3:F:13:VAL:CG1	3:F:17:GLY:CA	2.79	0.59
2:B:367:ASP:N	2:B:368:PRO:HD2	2.18	0.59
1:D:230:ALA:HB2	2:E:289:ILE:HD13	1.84	0.59
1:A:206:HIS:HD2	7:A:6580:HOH:O	1.85	0.58
3:C:3:VAL:HG22	3:C:12:GLU:CD	2.27	0.58
1:D:167:SER:OG	3:F:105:VAL:HG11	2.03	0.58
1:D:196:GLN:HE22	1:D:354:PRO:HA	1.68	0.58
1:A:411:PRO:HG3	2:E:192:MET:HE2	1.85	0.58
2:B:382:VAL:HG23	2:B:384:PHE:CD1	2.26	0.58
1:D:248:GLN:HE22	1:D:296:LEU:H	1.50	0.58
1:A:62:GLU:OE1	1:D:435:HIS:HE1	1.86	0.58
2:B:75:THR:O	2:B:79:ARG:HG3	2.04	0.58
2:E:37:ASN:ND2	2:E:58:ASN:HD21	2.01	0.58
1:A:98:HIS:HA	2:B:150:TYR:OH	2.03	0.58
1:D:34:ASN:ND2	1:D:38:LEU:H	1.97	0.57
1:D:98:HIS:HE1	1:D:146:THR:OG1	1.86	0.57
1:D:363:GLU:O	1:D:367:GLU:HG3	2.04	0.57
3:F:67:ARG:HG3	3:F:68:ILE:N	2.20	0.57
1:A:50:LEU:C	1:A:50:LEU:HD13	2.29	0.57
7:B:949:HOH:O	1:D:432:ARG:HD3	2.04	0.57
3:F:13:VAL:CG1	3:F:17:GLY:C	2.77	0.57
1:D:416:LYS:HB3	1:D:418:GLU:OE2	2.03	0.57
2:B:186:LEU:C	2:B:186:LEU:HD23	2.29	0.57
3:F:49:ILE:HD11	3:F:75:PHE:HD1	1.69	0.57
1:A:108:LYS:HD3	1:A:133:HIS:CE1	2.40	0.57
2:B:300:LYS:HB3	1:D:407:PRO:HG2	1.87	0.57
1:A:313:MET:HE3	1:A:317:LEU:HD11	1.87	0.56
2:B:48:GLU:HB3	2:B:49:PRO:CD	2.35	0.56
3:F:13:VAL:HG12	3:F:14:ASP:H	1.70	0.56
1:A:131:ASN:HB2	1:A:140:VAL:HB	1.86	0.56
2:B:153:THR:N	2:B:154:PRO:CD	2.67	0.56
5:D:582:SRM:O1A	2:E:150:TYR:CD2	2.57	0.56
3:C:3:VAL:HG21	3:C:12:GLU:OE2	2.05	0.56
1:A:184:GLU:OE1	2:B:44:HIS:HD2	1.87	0.56
2:E:247:LYS:HB3	2:E:247:LYS:NZ	2.22	0.55
2:B:200:ASP:HB3	2:B:337:ILE:HD12	1.87	0.55
3:C:4:VAL:O	3:C:10:ALA:HA	2.06	0.55
1:A:33:LYS:HG3	7:A:6734:HOH:O	2.07	0.55
1:A:81:ILE:CD1	3:C:105:VAL:HG22	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ARG:NH2	2:E:379:PHE:O	2.39	0.54
5:A:580:SRM:O1A	2:B:150:TYR:HD2	1.91	0.54
1:A:227:ALA:CB	2:B:289:ILE:HD13	2.37	0.54
1:A:376:ARG:HB3	1:A:376:ARG:NH1	2.21	0.54
1:D:308:HIS:CD2	2:E:292:ARG:HE	2.21	0.54
3:F:21:ALA:HB3	3:F:24:ASP:OD2	2.06	0.54
1:D:206:HIS:HD2	7:D:6634:HOH:O	1.90	0.54
1:D:229:MET:HB3	2:E:289:ILE:HD11	1.90	0.54
1:A:83:ARG:HD2	2:B:150:TYR:O	2.07	0.54
2:E:239:ILE:HD12	2:E:239:ILE:C	2.33	0.54
3:C:91:GLY:O	3:C:95:MET:HG3	2.07	0.54
3:F:49:ILE:HD13	3:F:73:THR:HG21	1.90	0.54
1:A:435:HIS:HE1	1:D:62:GLU:OE1	1.91	0.53
1:D:306:CYS:O	1:D:307:MET:HB2	2.08	0.53
2:B:192:MET:HE2	2:B:197:HIS:HB3	1.90	0.53
7:A:6604:HOH:O	2:B:125:ALA:HB3	2.07	0.53
5:B:581:SRM:CMA	5:B:581:SRM:CBA	2.66	0.53
1:D:376:ARG:HB3	1:D:376:ARG:HH11	1.74	0.53
2:B:37:ASN:ND2	2:B:58:ASN:HD21	2.03	0.53
1:A:227:ALA:HB1	2:B:289:ILE:HD13	1.90	0.53
1:A:306:CYS:O	1:A:307:MET:HB2	2.09	0.53
5:A:580:SRM:HMA2	3:C:104:CYS:SG	2.49	0.53
1:D:334:PRO:HD2	7:E:841:HOH:O	2.09	0.53
3:F:13:VAL:HG13	3:F:18:PHE:O	2.09	0.53
1:D:390:LYS:O	1:D:390:LYS:HD3	2.08	0.52
1:D:159:ASN:C	1:D:160:LEU:HD12	2.34	0.52
3:F:13:VAL:CG1	3:F:14:ASP:N	2.72	0.52
3:C:11:PHE:HE2	3:C:26:CYS:HG	1.58	0.52
2:B:300:LYS:CB	1:D:407:PRO:HG2	2.40	0.52
2:E:146:GLN:HE21	2:E:150:TYR:HB3	1.74	0.52
1:D:410:ASN:HD22	1:D:412:TYR:H	1.57	0.52
5:D:582:SRM:HHB	5:D:582:SRM:HBA1	1.91	0.52
2:E:48:GLU:HB2	2:E:49:PRO:CD	2.40	0.52
2:E:280:GLY:HA3	2:E:305:PHE:CE1	2.45	0.52
1:A:349:ILE:HD11	1:A:357:GLU:HB3	1.92	0.52
1:A:70:ILE:HG13	3:C:101:PRO:HD2	1.92	0.52
1:A:280:VAL:HG11	1:A:313:MET:HE2	1.92	0.52
2:E:153:THR:N	2:E:154:PRO:CD	2.72	0.52
3:C:3:VAL:HG22	3:C:12:GLU:CG	2.40	0.52
2:E:220:GLU:HB3	3:F:20:ASN:O	2.10	0.51
2:B:254:ASN:HD21	2:B:256:ASP:HB2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:ASN:C	2:B:254:ASN:HD22	2.18	0.51
5:E:583:SRM:HBA2	5:E:583:SRM:NA	2.25	0.51
1:D:334:PRO:HG2	2:E:192:MET:CE	2.40	0.51
1:A:67:HIS:HE1	2:B:265:TYR:O	1.93	0.51
3:C:21:ALA:HB3	3:C:24:ASP:OD2	2.11	0.51
1:D:168:GLY:HA2	3:F:105:VAL:HB	1.93	0.51
1:A:67:HIS:CE1	2:B:265:TYR:O	2.64	0.50
2:B:243:VAL:O	2:B:243:VAL:HG23	2.11	0.50
3:C:25:TRP:CE3	3:C:26:CYS:HA	2.45	0.50
1:D:34:ASN:N	1:D:35:PRO:HD3	2.26	0.50
1:D:55:GLU:OE2	1:D:59:HIS:HE1	1.94	0.50
1:D:429:SER:O	1:D:433:LYS:HG3	2.12	0.50
2:E:186:LEU:C	2:E:186:LEU:HD23	2.36	0.50
2:B:12:LYS:N	2:B:13:PRO:HD3	2.27	0.50
2:B:211:PRO:HB3	2:B:273:LEU:HB3	1.94	0.50
1:D:189:ASP:CG	1:D:192:LEU:HB2	2.37	0.50
1:A:111:THR:HG23	2:B:29:PHE:HD2	1.75	0.50
1:A:262:ASN:ND2	2:B:292:ARG:HH22	2.09	0.50
1:D:170:ASN:HB3	1:D:208:PRO:HA	1.93	0.50
2:E:211:PRO:HG2	2:E:253:ILE:CD1	2.42	0.50
1:A:390:LYS:O	1:A:390:LYS:HD3	2.11	0.49
1:D:160:LEU:HD12	1:D:160:LEU:N	2.26	0.49
2:B:9:ASN:HD22	2:B:10:PRO:N	2.09	0.49
1:D:3:LYS:CD	1:D:3:LYS:C	2.82	0.49
2:B:212:MET:HE1	1:D:431:TYR:CD2	2.47	0.49
3:F:49:ILE:HD11	3:F:75:PHE:CD1	2.47	0.49
3:F:77:LEU:HD22	3:F:81:TYR:CD1	2.47	0.49
1:D:279:GLU:O	1:D:308:HIS:HE1	1.96	0.49
5:D:582:SRM:HMA2	3:F:104:CYS:CB	2.43	0.49
2:E:242:GLU:HA	2:E:246:GLN:O	2.12	0.49
1:D:87:GLN:N	1:D:88:PRO:HD3	2.27	0.49
5:A:580:SRM:HMA2	3:C:104:CYS:CB	2.43	0.48
1:D:45:GLU:CD	1:D:45:GLU:N	2.71	0.48
1:D:168:GLY:N	3:F:105:VAL:HB	2.28	0.48
2:E:293:ILE:HG22	2:E:294:LYS:CD	2.42	0.48
1:A:67:HIS:HA	2:B:152:HIS:CD2	2.48	0.48
1:D:99:THR:HG23	1:D:140:VAL:HG13	1.96	0.48
1:D:170:ASN:HB2	1:D:204:GLU:O	2.13	0.48
2:B:153:THR:N	2:B:154:PRO:HD2	2.29	0.48
2:B:314:PRO:O	2:B:318:LYS:HG2	2.13	0.48
5:B:581:SRM:CBA	5:B:581:SRM:NA	2.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:PHE:CD2	3:C:32:TYR:HB2	2.48	0.48
1:A:60:GLU:OE1	1:A:64:HIS:HE1	1.96	0.48
2:B:138:SER:HB2	2:B:172:GLU:O	2.14	0.48
3:C:12:GLU:HB3	3:C:20:ASN:HD22	1.78	0.48
1:D:67:HIS:HD2	7:D:6692:HOH:O	1.94	0.48
1:A:196:GLN:HE22	1:A:354:PRO:HA	1.78	0.48
1:A:313:MET:HE3	1:A:317:LEU:CD1	2.44	0.48
1:A:285:PRO:CG	2:B:293:ILE:HA	2.44	0.48
2:E:215:HIS:HD2	2:E:250:SER:OG	1.97	0.48
2:E:207:HIS:HD2	2:E:279:ASP:OD1	1.97	0.47
2:B:31:PRO:HG2	2:B:34:ILE:CG1	2.44	0.47
1:D:3:LYS:HE2	1:D:3:LYS:HB2	1.78	0.47
1:D:81:ILE:HD12	3:F:105:VAL:HG22	1.96	0.47
2:B:152:HIS:C	2:B:154:PRO:HD2	2.39	0.47
1:A:168:GLY:HA2	3:C:105:VAL:HB	1.96	0.47
1:A:312:THR:C	1:A:314:PRO:HD3	2.39	0.47
1:A:431:TYR:CD2	2:E:212:MET:HE1	2.49	0.47
1:D:107:ALA:HB3	1:D:191:GLN:HE21	1.78	0.47
1:A:17:TRP:CD2	1:A:18:PRO:HD2	2.49	0.47
1:A:239:THR:OG1	1:A:305:ARG:HD2	2.14	0.47
5:A:580:SRM:C4D	3:C:104:CYS:SG	2.92	0.47
2:B:9:ASN:HD21	2:B:11:ALA:HB3	1.80	0.47
2:E:254:ASN:C	2:E:254:ASN:HD22	2.21	0.47
5:A:580:SRM:O1A	2:B:150:TYR:CD2	2.68	0.46
3:F:13:VAL:HG13	3:F:17:GLY:C	2.39	0.46
1:A:83:ARG:H	1:A:98:HIS:CD2	2.28	0.46
1:D:98:HIS:HA	2:E:150:TYR:OH	2.16	0.46
2:E:152:HIS:C	2:E:154:PRO:HD2	2.40	0.46
2:E:171:GLU:HG3	7:E:934:HOH:O	2.15	0.46
3:F:26:CYS:SG	3:F:28:GLU:CG	3.02	0.46
1:A:107:ALA:HB3	1:A:191:GLN:HE21	1.81	0.46
1:A:167:SER:CB	3:C:105:VAL:HG11	2.46	0.46
2:B:242:GLU:HA	2:B:246:GLN:O	2.16	0.46
2:E:142:ILE:O	2:E:144:HIS:HD2	1.98	0.46
5:E:583:SRM:C1A	5:E:583:SRM:CBA	2.93	0.46
1:D:104:GLN:NE2	1:D:104:GLN:N	2.54	0.46
2:E:211:PRO:HB3	2:E:273:LEU:HB3	1.97	0.46
1:A:363:GLU:O	1:A:367:GLU:HG3	2.14	0.46
3:C:105:VAL:OXT	3:C:105:VAL:CG1	2.55	0.46
1:A:313:MET:N	1:A:314:PRO:HD3	2.31	0.46
2:B:144:HIS:CG	2:B:162:VAL:HG21	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:PHE:CE2	3:C:29:TRP:HB2	2.51	0.46
1:A:279:GLU:O	1:A:308:HIS:HE1	1.99	0.46
1:D:76:TYR:CD1	1:D:206:HIS:HB3	2.51	0.46
1:D:168:GLY:CA	3:F:105:VAL:HB	2.46	0.46
1:A:406:GLU:HG3	7:A:6681:HOH:O	2.16	0.45
2:B:172:GLU:OE1	2:B:172:GLU:HA	2.14	0.45
2:B:382:VAL:HG22	1:D:402:GLN:OE1	2.16	0.45
1:D:20:PHE:O	1:D:24:ILE:HG13	2.16	0.45
1:D:334:PRO:HG2	2:E:192:MET:HE1	1.98	0.45
7:D:6726:HOH:O	3:F:105:VAL:HG21	2.03	0.45
1:A:427:ASP:CG	1:A:429:SER:H	2.25	0.45
2:B:96:THR:HB	5:B:581:SRM:HAB1	1.98	0.45
1:A:113:GLU:HG3	7:A:6608:HOH:O	2.16	0.45
5:A:580:SRM:HDD1	3:C:104:CYS:SG	2.57	0.45
1:D:371:GLU:HG2	7:D:6743:HOH:O	2.15	0.45
1:A:97:PHE:O	2:B:150:TYR:CZ	2.68	0.45
1:A:416:LYS:HB2	1:A:419:GLU:HG3	1.97	0.45
1:D:34:ASN:HD21	1:D:38:LEU:N	2.02	0.45
3:F:26:CYS:SG	3:F:28:GLU:CD	2.99	0.45
2:B:62:VAL:O	2:B:62:VAL:HG13	2.17	0.45
1:D:104:GLN:HE22	1:D:173:THR:CG2	2.25	0.45
2:E:214:ASP:OD1	2:E:216:GLU:HG2	2.17	0.45
2:E:259:MET:C	2:E:260:TYR:CG	2.93	0.45
1:A:232:SER:O	1:A:331:ALA:HB3	2.15	0.45
3:F:26:CYS:SG	3:F:27:PRO:N	2.89	0.45
2:B:48:GLU:HB3	2:B:49:PRO:HD2	1.99	0.45
1:D:102:LEU:HD21	1:D:156:MET:HE2	1.98	0.45
2:B:63:PHE:O	2:B:104:MET:HA	2.17	0.44
2:B:211:PRO:HG2	2:B:253:ILE:CD1	2.47	0.44
1:D:225:CYS:HA	5:E:583:SRM:C1C	2.48	0.44
1:A:64:HIS:HD2	1:A:86:ASP:OD1	2.00	0.44
1:A:98:HIS:HE1	1:A:146:THR:OG1	2.01	0.44
1:A:60:GLU:OE1	1:A:64:HIS:CE1	2.70	0.44
1:D:170:ASN:HD22	1:D:208:PRO:CG	2.29	0.44
2:B:312:ARG:O	2:B:313:TRP:C	2.60	0.44
2:E:223:GLU:HB3	3:F:62:ILE:HG22	1.99	0.44
2:E:333:LYS:O	2:E:334:TYR:HB2	2.18	0.44
1:D:390:LYS:HD3	1:D:390:LYS:C	2.43	0.44
3:C:57:TYR:CD1	3:C:98:LEU:HD22	2.53	0.43
7:D:6620:HOH:O	2:E:44:HIS:HE1	2.00	0.43
3:F:100:LYS:HG3	3:F:101:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ASP:OD1	1:D:226:VAL:HG12	2.18	0.43
2:E:138:SER:HB2	2:E:172:GLU:O	2.18	0.43
2:E:75:THR:O	2:E:79:ARG:HG3	2.18	0.43
2:E:208:ARG:HD2	2:E:305:PHE:CD1	2.53	0.43
3:F:13:VAL:HG13	3:F:18:PHE:N	2.34	0.43
2:B:346:TRP:CE2	1:D:407:PRO:HD2	2.53	0.43
1:D:308:HIS:HD2	2:E:292:ARG:NE	2.10	0.43
2:E:48:GLU:HB2	2:E:49:PRO:HD2	2.00	0.43
1:A:41:GLN:NE2	2:B:4:ILE:HG23	2.34	0.43
3:C:4:VAL:HG11	3:C:32:TYR:CE2	2.54	0.43
1:D:232:SER:O	1:D:331:ALA:HB3	2.18	0.43
1:A:86:ASP:OD1	1:A:87:GLN:HG2	2.17	0.43
1:A:83:ARG:NH1	5:A:580:SRM:O1A	2.52	0.43
1:A:308:HIS:CD2	2:B:292:ARG:HE	2.25	0.43
1:D:334:PRO:HG3	1:D:339:ALA:HB2	2.00	0.43
2:B:148:TRP:CE3	2:B:157:ASP:HB2	2.53	0.43
2:B:347:GLU:HG2	7:B:814:HOH:O	2.17	0.43
1:D:67:HIS:CE1	2:E:265:TYR:O	2.72	0.43
2:E:12:LYS:N	2:E:13:PRO:HD3	2.34	0.43
1:D:67:HIS:HE1	2:E:265:TYR:O	2.01	0.43
1:D:86:ASP:C	1:D:88:PRO:HD3	2.44	0.43
2:E:218:LEU:C	2:E:218:LEU:HD23	2.44	0.43
2:B:259:MET:C	2:B:260:TYR:CG	2.94	0.42
1:D:135:SER:HB2	5:D:582:SRM:HHC	2.01	0.42
2:E:312:ARG:O	2:E:313:TRP:C	2.61	0.42
1:A:76:TYR:CD1	1:A:206:HIS:HB3	2.55	0.42
3:C:19:LEU:HD21	3:C:29:TRP:CE3	2.54	0.42
1:D:17:TRP:CD2	1:D:18:PRO:HD2	2.53	0.42
2:B:44:HIS:HE1	7:B:837:HOH:O	2.03	0.42
1:D:89:GLU:CD	1:D:89:GLU:H	2.26	0.42
1:D:156:MET:SD	1:D:160:LEU:HD22	2.60	0.42
1:D:335:VAL:HA	1:D:336:LEU:HA	1.85	0.42
3:F:77:LEU:HD22	3:F:81:TYR:CE1	2.55	0.42
2:B:367:ASP:N	2:B:368:PRO:CD	2.82	0.42
3:C:11:PHE:HB3	3:C:19:LEU:CD2	2.49	0.42
1:D:416:LYS:HB2	1:D:419:GLU:CG	2.44	0.42
2:E:11:ALA:C	2:E:13:PRO:HD3	2.45	0.42
2:E:246:GLN:OE1	2:E:246:GLN:HA	2.18	0.42
5:E:583:SRM:HBA2	5:E:583:SRM:C1A	2.50	0.42
1:A:81:ILE:HD11	3:C:105:VAL:HG22	2.00	0.42
2:B:384:PHE:CD1	2:B:384:PHE:N	2.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:ARG:HD3	2:E:54:HIS:CE1	2.54	0.42
2:E:87:LYS:HD3	2:E:88:PHE:CE1	2.55	0.42
1:A:219:ASP:OD1	1:A:226:VAL:HG12	2.20	0.41
1:A:428:ILE:HD13	2:E:214:ASP:HB2	2.02	0.41
5:D:582:SRM:CCA	2:E:150:TYR:HD2	2.32	0.41
2:E:211:PRO:HG2	2:E:253:ILE:HD13	2.01	0.41
2:E:332:ARG:O	2:E:335:GLU:HB2	2.20	0.41
1:A:411:PRO:HG3	2:E:192:MET:HE1	2.00	0.41
1:D:376:ARG:HH11	1:D:376:ARG:CB	2.33	0.41
2:E:223:GLU:HB2	2:E:226:LEU:HD12	2.01	0.41
5:A:580:SRM:CCA	2:B:150:TYR:HD2	2.34	0.41
2:B:31:PRO:HG2	2:B:34:ILE:HG12	2.01	0.41
1:D:111:THR:HG23	2:E:29:PHE:HD2	1.84	0.41
1:D:202:GLN:OE1	1:D:206:HIS:HE1	2.04	0.41
1:A:284:CYS:HA	1:A:285:PRO:HD3	1.92	0.41
2:B:190:ILE:C	2:B:190:ILE:HD12	2.45	0.41
1:A:428:ILE:CD1	2:E:214:ASP:HB2	2.50	0.41
1:D:83:ARG:H	1:D:98:HIS:CD2	2.29	0.41
2:B:95:PHE:CE2	2:B:101:ILE:HG12	2.56	0.41
1:A:11:GLU:O	1:A:11:GLU:HG3	2.20	0.41
3:C:68:ILE:HD12	7:C:514:HOH:O	2.19	0.41
1:D:132:MET:HA	1:D:133:HIS:HA	1.88	0.41
3:F:13:VAL:HG11	3:F:17:GLY:C	2.43	0.41
1:A:99:THR:N	2:B:150:TYR:OH	2.53	0.41
7:B:949:HOH:O	1:D:437:ARG:HD2	2.20	0.41
1:D:102:LEU:HA	1:D:102:LEU:HD12	1.80	0.41
2:E:239:ILE:HD12	2:E:239:ILE:O	2.20	0.41
1:A:172:ARG:HB2	1:A:215:LYS:HG2	2.03	0.41
1:A:409:HIS:HD2	7:A:6614:HOH:O	2.04	0.41
2:B:254:ASN:C	2:B:254:ASN:ND2	2.79	0.41
1:D:60:GLU:OE1	1:D:64:HIS:CE1	2.74	0.41
1:D:108:LYS:HD3	1:D:133:HIS:CE1	2.56	0.41
1:D:408:ARG:HH11	1:D:410:ASN:ND2	2.13	0.41
1:D:409:HIS:HD2	7:D:6621:HOH:O	2.03	0.41
2:E:46:ILE:HG12	2:E:52:LEU:HD22	2.03	0.41
2:E:207:HIS:HE1	7:E:954:HOH:O	2.03	0.41
2:B:313:TRP:N	2:B:314:PRO:HD3	2.35	0.41
1:A:376:ARG:HB3	1:A:376:ARG:HH11	1.85	0.40
2:B:169:LEU:O	2:B:170:PHE:C	2.64	0.40
1:A:205:LEU:HD23	1:A:205:LEU:C	2.46	0.40
3:C:57:TYR:CG	3:C:98:LEU:HD22	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:144:HIS:CG	2:E:162:VAL:HG21	2.56	0.40
1:A:390:LYS:HD3	1:A:390:LYS:C	2.47	0.40
1:A:410:ASN:ND2	1:A:410:ASN:C	2.79	0.40
2:B:259:MET:C	2:B:260:TYR:CD1	2.99	0.40
2:E:31:PRO:HG2	2:E:34:ILE:CG1	2.51	0.40
3:F:13:VAL:CG1	3:F:14:ASP:H	2.34	0.40
5:A:580:SRM:CDD	3:C:104:CYS:SG	3.09	0.40
3:C:88:PRO:O	3:C:92:ALA:HB3	2.22	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	433/437 (99%)	418 (96%)	15 (4%)	0	100	100
1	D	433/437 (99%)	422 (98%)	10 (2%)	1 (0%)	43	27
2	B	383/386 (99%)	365 (95%)	16 (4%)	2 (0%)	24	11
2	E	383/386 (99%)	369 (96%)	12 (3%)	2 (0%)	24	11
3	C	102/105 (97%)	98 (96%)	3 (3%)	1 (1%)	12	3
3	F	102/105 (97%)	99 (97%)	2 (2%)	1 (1%)	12	3
All	All	1836/1856 (99%)	1771 (96%)	58 (3%)	7 (0%)	30	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	4	HIS
3	C	34	LYS
3	F	34	LYS
2	E	293	ILE

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Mol	Chain	Res	Type
2	E	153	THR
2	B	153	THR
2	B	293	ILE

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	364/365 (100%)	350 (96%)	14 (4%)	29	10
1	D	364/365 (100%)	350 (96%)	14 (4%)	29	10
2	B	324/325 (100%)	313 (97%)	11 (3%)	32	13
2	E	324/325 (100%)	319 (98%)	5 (2%)	57	41
3	C	79/80 (99%)	75 (95%)	4 (5%)	21	5
3	F	79/80 (99%)	74 (94%)	5 (6%)	16	3
All	All	1534/1540 (100%)	1481 (96%)	53 (4%)	32	12

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	36	LYS
1	A	54	LEU
1	A	83	ARG
1	A	104	GLN
1	A	208	PRO
1	A	249	GLU
1	A	258	GLU
1	A	273	LYS
1	A	390	LYS
1	A	391	LEU
1	A	402	GLN
1	A	406	GLU
1	A	418	GLU
2	B	4	ILE

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Mol	Chain	Res	Type
2	B	172	GLU
2	B	188	CYS
2	B	189	CYS
2	B	192	MET
2	B	220	GLU
2	B	254	ASN
2	B	259	MET
2	B	260	TYR
2	B	329	GLU
2	B	356	GLU
3	C	12	GLU
3	C	15	GLU
3	C	28	GLU
3	C	77	LEU
1	D	3	LYS
1	D	4	HIS
1	D	33	LYS
1	D	54	LEU
1	D	89	GLU
1	D	102	LEU
1	D	104	GLN
1	D	192	LEU
1	D	315	ARG
1	D	336	LEU
1	D	390	LYS
1	D	402	GLN
1	D	418	GLU
1	D	432	ARG
2	E	188	CYS
2	E	246	GLN
2	E	249	LYS
2	E	259	MET
2	E	260	TYR
3	F	20	ASN
3	F	28	GLU
3	F	34	LYS
3	F	67	ARG
3	F	77	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	34	ASN
1	A	64	HIS
1	A	67	HIS
1	A	98	HIS
1	A	104	GLN
1	A	161	ASN
1	A	196	GLN
1	A	206	HIS
1	A	248	GLN
1	A	262	ASN
1	A	308	HIS
1	A	311	ASN
1	A	375	ASN
1	A	402	GLN
1	A	410	ASN
1	A	435	HIS
2	B	9	ASN
2	B	37	ASN
2	B	44	HIS
2	B	107	ASN
2	B	144	HIS
2	B	191	ASN
2	B	207	HIS
2	B	215	HIS
2	B	254	ASN
2	B	263	ASN
2	B	360	HIS
1	D	30	ASN
1	D	34	ASN
1	D	64	HIS
1	D	67	HIS
1	D	98	HIS
1	D	104	GLN
1	D	161	ASN
1	D	170	ASN
1	D	196	GLN
1	D	206	HIS
1	D	248	GLN
1	D	262	ASN
1	D	308	HIS
1	D	311	ASN
1	D	375	ASN

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Mol	Chain	Res	Type
1	D	402	GLN
1	D	409	HIS
1	D	410	ASN
1	D	435	HIS
2	E	37	ASN
2	E	44	HIS
2	E	92	HIS
2	E	144	HIS
2	E	146	GLN
2	E	191	ASN
2	E	207	HIS
2	E	215	HIS
2	E	254	ASN
2	E	263	ASN
3	F	47	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO3	D	6576	5	1,3,3	1.27	0	0,3,3	-	-
5	SRM	D	582	4,2	68,70,70	2.29	15 (22%)	86,112,112	1.85	19 (22%)
6	SF4	D	808	1	0,12,12	-	-	-	-	-
5	SRM	A	580	4,2	68,70,70	2.70	15 (22%)	86,112,112	2.25	21 (24%)
5	SRM	B	581	-	54,66,70	2.26	9 (16%)	56,98,112	2.71	16 (28%)
6	SF4	B	801	2	0,12,12	-	-	-	-	-
6	SF4	E	805	2	0,12,12	-	-	-	-	-
6	SF4	B	802	2	0,12,12	-	-	-	-	-
6	SF4	E	806	2	0,12,12	-	-	-	-	-
6	SF4	A	804	1	0,12,12	-	-	-	-	-
5	SRM	E	583	-	54,66,70	2.24	14 (25%)	56,98,112	2.47	15 (26%)
6	SF4	A	803	1	0,12,12	-	-	-	-	-
6	SF4	D	807	1	0,12,12	-	-	-	-	-
4	SO3	A	6575	5	1,3,3	0.48	0	0,3,3	-	-

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
5	SRM	D	582	4,2	1/1/19/23	16/38/126/126	-
6	SF4	D	808	1	-	-	0/6/5/5
5	SRM	A	580	4,2	1/1/19/23	16/38/126/126	-
5	SRM	B	581	-	-	10/38/94/126	0/4/4/8
6	SF4	B	801	2	-	-	0/6/5/5
6	SF4	E	805	2	-	-	0/6/5/5
6	SF4	B	802	2	-	-	0/6/5/5
6	SF4	E	806	2	-	-	0/6/5/5
6	SF4	A	804	1	-	-	0/6/5/5
5	SRM	E	583	-	-	8/38/94/126	0/4/4/8
6	SF4	A	803	1	-	-	0/6/5/5
6	SF4	D	807	1	-	-	0/6/5/5

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	580	SRM	O1B-CCB	10.21	1.55	1.22
5	A	580	SRM	C4B-NB	8.12	1.41	1.35
5	A	580	SRM	CBB-CCB	-7.68	1.32	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	582	SRM	O1B-CCB	7.54	1.46	1.22
5	D	582	SRM	C4B-NB	7.29	1.40	1.35
5	A	580	SRM	O2B-CCB	6.90	1.53	1.30
5	B	581	SRM	O1A-CCA	6.89	1.44	1.22
5	B	581	SRM	C1D-C2D	6.69	1.46	1.39
5	E	583	SRM	O2A-CCA	-6.61	1.09	1.30
5	E	583	SRM	C1D-C2D	6.54	1.46	1.39
5	D	582	SRM	O2B-CCB	6.42	1.52	1.30
5	B	581	SRM	O2A-CCA	6.40	1.52	1.30
5	E	583	SRM	CAA-CBA	-5.47	1.36	1.52
5	A	580	SRM	FE-NA	5.12	2.10	1.94
5	A	580	SRM	FE-NC	5.08	2.11	1.95
5	D	582	SRM	FE-NC	5.04	2.11	1.95
5	A	580	SRM	FE-NB	4.98	2.10	1.94
5	D	582	SRM	FE-NA	4.88	2.09	1.94
5	B	581	SRM	CMB-C2B	4.68	1.61	1.54
5	B	581	SRM	C1C-C2C	4.68	1.44	1.39
5	D	582	SRM	FE-NB	4.58	2.09	1.94
5	E	583	SRM	C4C-C3C	4.54	1.44	1.39
5	E	583	SRM	C1C-C2C	4.52	1.44	1.39
5	A	580	SRM	CMB-C2B	4.43	1.61	1.54
5	E	583	SRM	CMB-C2B	4.30	1.61	1.54
5	D	582	SRM	CMB-C2B	4.18	1.61	1.54
5	D	582	SRM	FE-ND	4.12	2.08	1.95
5	A	580	SRM	FE-ND	4.08	2.08	1.95
5	B	581	SRM	C4C-C3C	3.81	1.43	1.39
5	E	583	SRM	CAA-C3A	-3.68	1.48	1.54
5	A	580	SRM	C3B-C4B	3.65	1.59	1.51
5	B	581	SRM	C4D-C3D	3.31	1.43	1.39
5	D	582	SRM	C3B-C4B	3.14	1.58	1.51
5	B	581	SRM	CAA-C3A	-2.73	1.50	1.54
5	D	582	SRM	CDD-C3D	2.71	1.55	1.51
5	A	580	SRM	CDD-C3D	2.68	1.55	1.51
5	A	580	SRM	CAA-C3A	-2.51	1.48	1.54
5	E	583	SRM	C4D-C3D	2.51	1.42	1.39
5	E	583	SRM	C4B-C3B	2.46	1.56	1.51
5	E	583	SRM	CMA-C2A	2.43	1.58	1.54
5	D	582	SRM	CAA-C3A	-2.43	1.48	1.54
5	A	580	SRM	CAB-C3B	-2.39	1.49	1.54
5	D	582	SRM	C4D-ND	-2.39	1.35	1.39
5	E	583	SRM	CAB-C3B	2.38	1.57	1.54
5	E	583	SRM	C2A-C1A	2.32	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	580	SRM	C4D-ND	-2.19	1.35	1.39
5	B	581	SRM	CAB-C3B	2.19	1.57	1.54
5	D	582	SRM	CAB-CBB	-2.14	1.46	1.52
5	D	582	SRM	C4C-NC	-2.13	1.35	1.39
5	D	582	SRM	CAB-C3B	-2.07	1.49	1.54
5	A	580	SRM	CMA-C2A	2.05	1.57	1.54
5	E	583	SRM	O2C-CCC	-2.02	1.24	1.30
5	E	583	SRM	O4D-CED	-2.02	1.24	1.30

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	583	SRM	CAA-CBA-CCA	9.44	137.67	112.49
5	B	581	SRM	CAA-C3A-C2A	-9.40	88.33	114.19
5	B	581	SRM	O2A-CCA-O1A	-8.90	100.45	123.33
5	A	580	SRM	O2B-CCB-O1B	-8.62	101.16	123.33
5	A	580	SRM	CAB-CBB-CCB	8.22	134.41	112.49
5	B	581	SRM	CAA-CBA-CCA	7.46	132.38	112.49
5	A	580	SRM	C2A-C1A-CHA	6.53	129.41	123.54
5	D	582	SRM	C2A-C1A-CHA	6.41	129.30	123.54
5	E	583	SRM	CBA-CAA-C3A	6.20	132.22	114.65
5	A	580	SRM	CAB-C3B-C4B	-5.67	101.29	111.19
5	E	583	SRM	CBD-CAD-C2D	-5.28	103.66	112.54
5	B	581	SRM	CBD-CAD-C2D	-5.09	103.98	112.54
5	E	583	SRM	CAA-C3A-C2A	-4.98	100.49	114.19
5	B	581	SRM	O2A-CCA-CBA	4.87	129.38	114.00
5	D	582	SRM	CAB-C3B-C4B	-4.54	103.26	111.19
5	D	582	SRM	C4D-CHA-C1A	4.38	133.94	125.87
5	E	583	SRM	CMA-C2A-C3A	4.33	119.91	112.07
5	D	582	SRM	CAB-CBB-CCB	4.31	123.99	112.49
5	A	580	SRM	C4D-CHA-C1A	4.24	133.68	125.87
5	E	583	SRM	C2C-C1C-NC	-4.12	106.45	109.43
5	E	583	SRM	C2C-CDC-CEC	4.04	118.88	114.20
5	B	581	SRM	C2C-CDC-CEC	4.03	118.86	114.20
5	A	580	SRM	C2C-C1C-NC	-3.87	106.59	110.32
5	B	581	SRM	C2C-C1C-NC	-3.87	106.64	109.43
5	A	580	SRM	CBB-CAB-C3B	3.75	125.29	114.65
5	D	582	SRM	C2C-C1C-NC	-3.73	106.73	110.32
5	D	582	SRM	C1A-NA-C4A	3.72	109.93	105.34
5	B	581	SRM	CMA-C2A-C3A	3.71	118.79	112.07
5	A	580	SRM	C1A-NA-C4A	3.53	109.69	105.34
5	E	583	SRM	CDB-C2B-C1B	-3.51	104.19	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	583	SRM	CMB-C2B-C3B	3.43	118.27	112.07
5	D	582	SRM	O2B-CCB-CBB	3.40	124.75	114.00
5	A	580	SRM	O1B-CCB-CBB	3.39	133.85	123.09
5	B	581	SRM	CMB-C2B-C3B	3.24	117.93	112.07
5	D	582	SRM	O2B-CCB-O1B	-3.14	115.26	123.33
5	A	580	SRM	CMB-C2B-C3B	3.06	117.69	112.05
5	A	580	SRM	C4B-NB-C1B	2.98	109.02	105.34
5	E	583	SRM	O2A-CCA-O1A	-2.97	115.70	123.33
5	D	582	SRM	C4B-NB-C1B	2.91	108.93	105.34
5	D	582	SRM	CMB-C2B-C3B	2.90	117.40	112.05
5	B	581	SRM	CDB-C2B-C1B	-2.86	105.30	110.16
5	E	583	SRM	CAB-C3B-C2B	-2.86	106.31	114.19
5	E	583	SRM	CDA-C2A-C1A	2.78	114.89	110.16
5	B	581	SRM	CAB-C3B-C2B	-2.56	107.13	114.19
5	A	580	SRM	C4A-CHB-C1B	2.55	129.59	125.84
5	B	581	SRM	CMA-C2A-C1A	-2.47	103.94	109.77
5	D	582	SRM	C4A-CHB-C1B	2.38	129.34	125.84
5	E	583	SRM	O2A-CCA-CBA	2.34	121.41	114.00
5	D	582	SRM	CAA-C3A-C4A	2.31	115.22	111.19
5	D	582	SRM	C1D-C2D-C3D	-2.30	104.40	106.81
5	A	580	SRM	CDA-C2A-C1A	2.29	114.20	107.11
5	A	580	SRM	CAA-C3A-C4A	2.26	115.13	111.19
5	D	582	SRM	C4D-ND-C1D	2.24	109.47	105.82
5	A	580	SRM	CMA-C2A-CDA	2.23	114.53	110.74
5	D	582	SRM	CDA-C2A-C1A	2.23	114.00	107.11
5	B	581	SRM	O1A-CCA-CBA	2.22	130.13	123.09
5	B	581	SRM	CBA-CAA-C3A	2.22	120.93	114.65
5	A	580	SRM	C4D-ND-C1D	2.21	109.43	105.82
5	D	582	SRM	CMA-C2A-CDA	2.20	114.47	110.74
5	B	581	SRM	O2D-CCD-CBD	2.18	120.89	114.00
5	A	580	SRM	C1C-C2C-C3C	2.15	109.24	106.84
5	A	580	SRM	C3D-C4D-ND	-2.13	107.79	110.15
5	A	580	SRM	O2B-CCB-CBB	2.12	120.70	114.00
5	B	581	SRM	O3B-CEB-CDB	-2.11	116.97	122.95
5	A	580	SRM	O3B-CEB-CDB	-2.09	117.03	122.95
5	D	582	SRM	O3B-CEB-CDB	-2.09	117.03	122.95
5	A	580	SRM	C1D-C2D-C3D	-2.08	104.62	106.81
5	D	582	SRM	C3D-C4D-ND	-2.08	107.85	110.15
5	E	583	SRM	CBC-CAC-C3C	2.07	116.02	112.54
5	E	583	SRM	O3B-CEB-CDB	-2.06	117.12	122.95
5	D	582	SRM	C1C-C2C-C3C	2.01	109.08	106.84

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	580	SRM	NC
5	D	582	SRM	NC

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	580	SRM	C1A-C2A-CDA-CEA
5	A	580	SRM	CMA-C2A-CDA-CEA
5	A	580	SRM	C3A-C2A-CDA-CEA
5	D	582	SRM	C1A-C2A-CDA-CEA
5	D	582	SRM	CMA-C2A-CDA-CEA
5	D	582	SRM	C3A-C2A-CDA-CEA
5	D	582	SRM	C3B-CAB-CBB-CCB
5	A	580	SRM	C3B-CAB-CBB-CCB
5	E	583	SRM	C3C-CAC-CBC-CCC
5	A	580	SRM	C4A-C3A-CAA-CBA
5	B	581	SRM	C3C-CAC-CBC-CCC
5	A	580	SRM	C2A-CDA-CEA-O4A
5	B	581	SRM	C2B-CDB-CEB-O3B
5	B	581	SRM	C2B-CDB-CEB-O4B
5	D	582	SRM	C2A-CDA-CEA-O3A
5	D	582	SRM	C2A-CDA-CEA-O4A
5	E	583	SRM	C2B-CDB-CEB-O3B
5	E	583	SRM	C2B-CDB-CEB-O4B
5	B	581	SRM	C4A-C3A-CAA-CBA
5	D	582	SRM	C4A-C3A-CAA-CBA
5	A	580	SRM	C2A-C3A-CAA-CBA
5	A	580	SRM	C2A-CDA-CEA-O3A
5	E	583	SRM	C2A-C3A-CAA-CBA
5	D	582	SRM	C3D-CDD-CED-O4D
5	D	582	SRM	CAA-CBA-CCA-O1A
5	D	582	SRM	CAA-CBA-CCA-O2A
5	A	580	SRM	CAA-CBA-CCA-O2A
5	D	582	SRM	CAB-CBB-CCB-O1B
5	A	580	SRM	CAA-CBA-CCA-O1A
5	A	580	SRM	CAC-CBC-CCC-O2C
5	D	582	SRM	CAC-CBC-CCC-O2C
5	A	580	SRM	CAC-CBC-CCC-O1C
5	B	581	SRM	CAC-CBC-CCC-O2C
5	D	582	SRM	CAC-CBC-CCC-O1C
5	B	581	SRM	CAA-CBA-CCA-O2A
5	A	580	SRM	CAB-CBB-CCB-O2B
5	D	582	SRM	CAB-CBB-CCB-O2B

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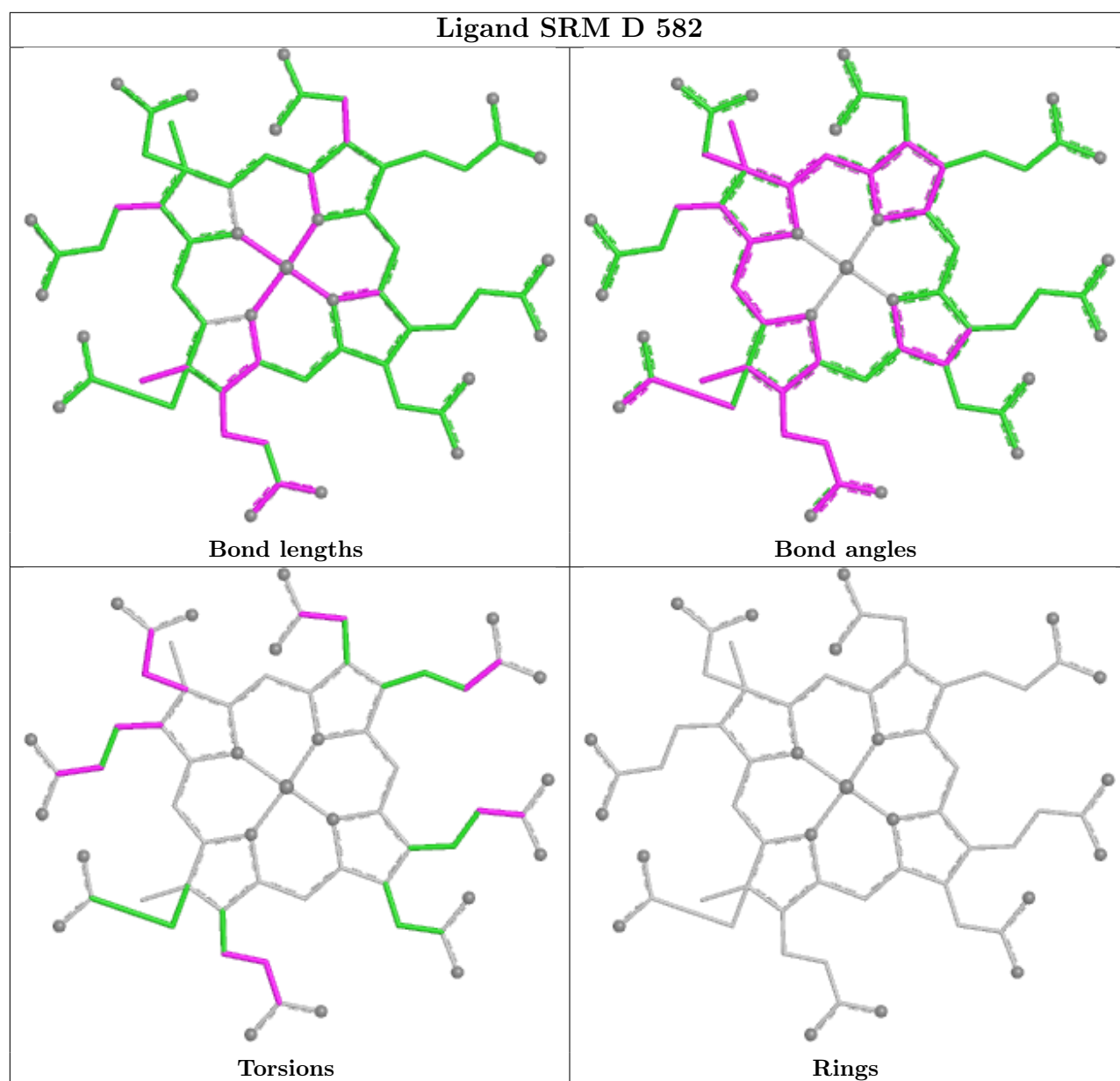
Mol	Chain	Res	Type	Atoms
5	A	580	SRM	CAB-CBB-CCB-O1B
5	E	583	SRM	CAB-CBB-CCB-O1B
5	E	583	SRM	CAC-CBC-CCC-O2C
5	B	581	SRM	CAB-CBB-CCB-O1B
5	A	580	SRM	CAD-CBD-CCD-O2D
5	B	581	SRM	CAC-CBC-CCC-O1C
5	E	583	SRM	CAB-CBB-CCB-O2B
5	B	581	SRM	CAB-CBB-CCB-O2B
5	B	581	SRM	CAA-CBA-CCA-O1A
5	D	582	SRM	C3D-CDD-CED-O3D
5	E	583	SRM	CAC-CBC-CCC-O1C
5	A	580	SRM	CAD-CBD-CCD-O1D
5	D	582	SRM	CAD-CBD-CCD-O2D

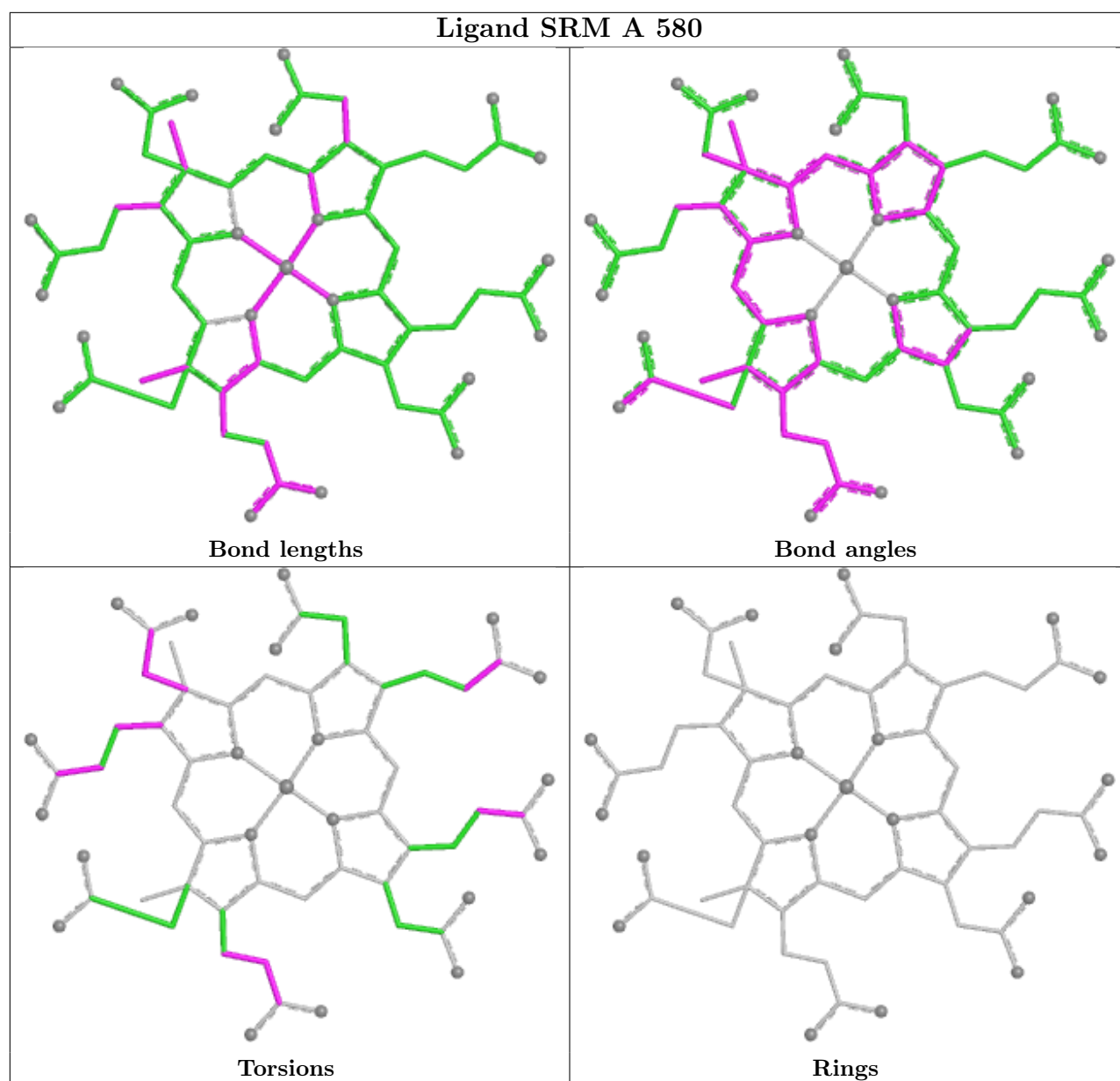
There are no ring outliers.

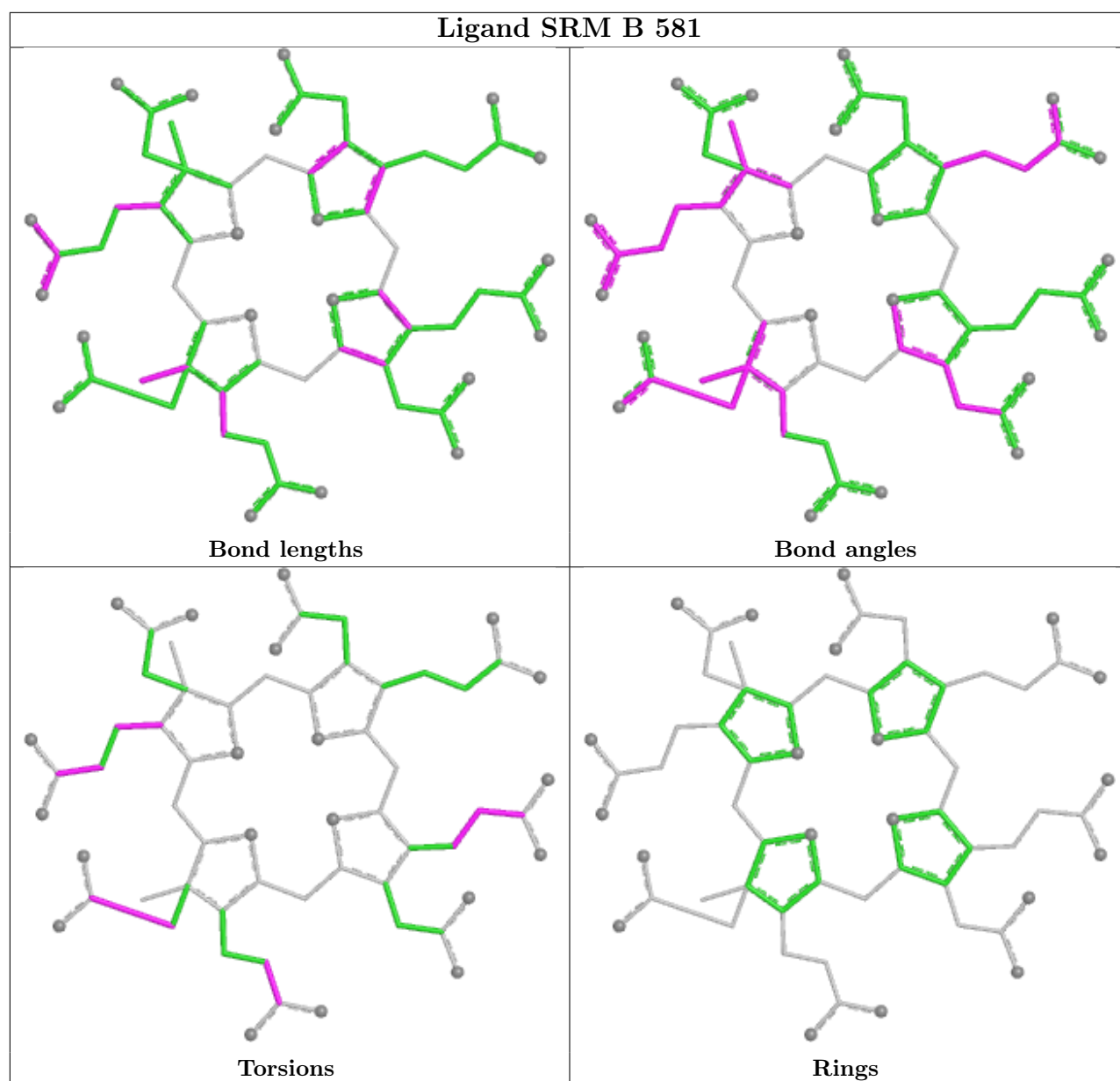
4 monomers are involved in 36 short contacts:

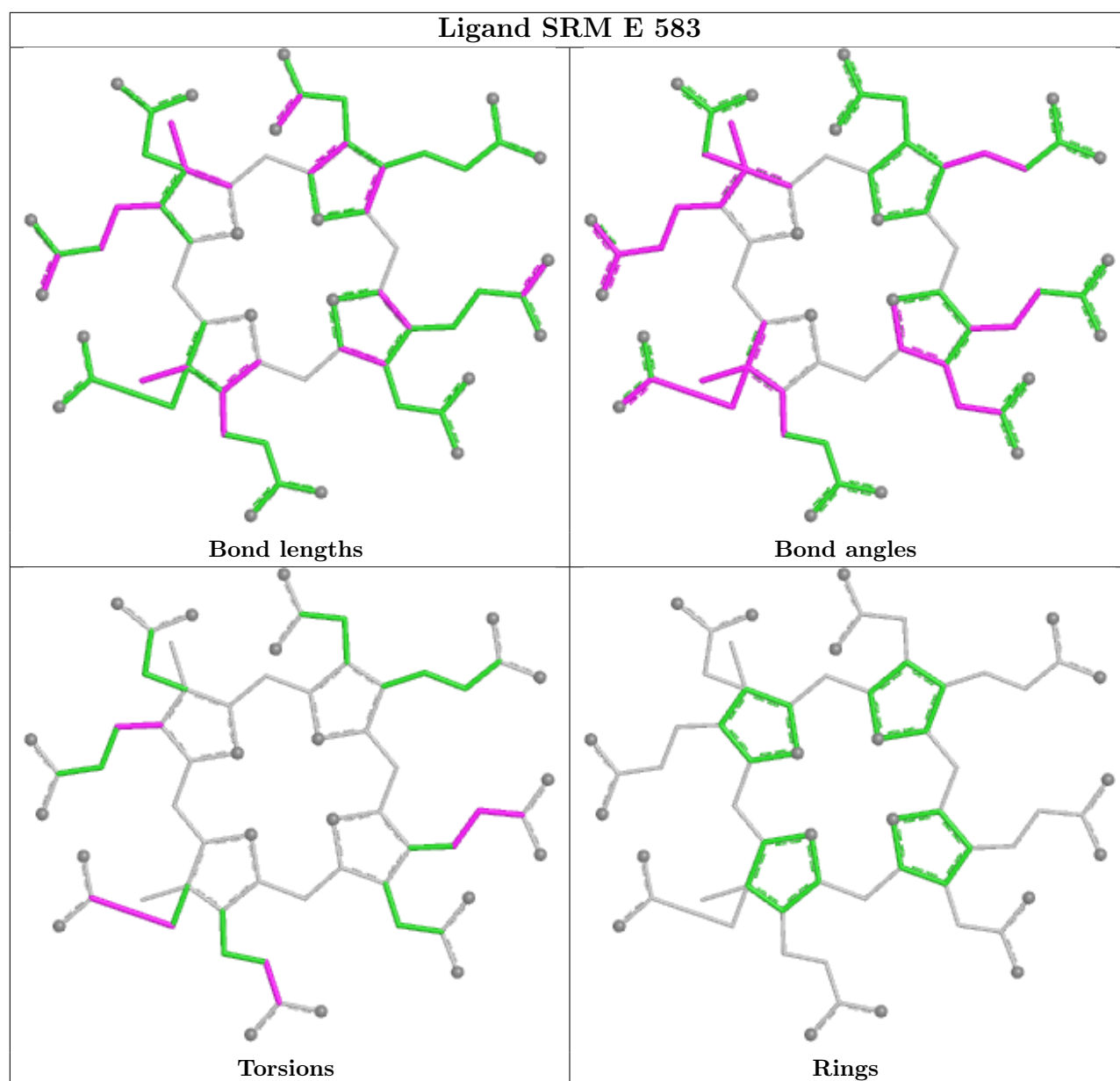
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	582	SRM	10	0
5	A	580	SRM	12	0
5	B	581	SRM	9	0
5	E	583	SRM	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	435/437 (99%)	0.45	20 (4%) 37 43	14, 23, 44, 74	0
1	D	435/437 (99%)	0.01	10 (2%) 61 67	13, 19, 38, 73	0
2	B	385/386 (99%)	0.34	13 (3%) 48 54	15, 23, 40, 59	0
2	E	385/386 (99%)	0.10	7 (1%) 67 74	13, 21, 36, 78	0
3	C	104/105 (99%)	1.37	24 (23%) 2 2	22, 33, 64, 79	0
3	F	104/105 (99%)	0.86	13 (12%) 8 9	22, 29, 47, 66	0
All	All	1848/1856 (99%)	0.33	87 (4%) 36 42	13, 23, 44, 79	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	105	VAL	8.7
3	F	105	VAL	6.9
3	C	72	ASN	5.1
3	C	4	VAL	5.0
2	B	2	ALA	4.7
2	E	386	SER	4.6
3	C	3	VAL	4.5
1	D	3	LYS	4.2
3	C	11	PHE	4.0
1	D	4	HIS	3.7
2	B	196	VAL	3.5
1	D	425	SER	3.5
3	C	40	GLY	3.5
1	D	89	GLU	3.4
1	A	429	SER	3.4
3	C	6	PHE	3.3
3	C	33	ALA	3.3
2	B	4	ILE	3.2
3	C	8	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	10	ALA	3.1
3	C	44	ALA	3.1
3	F	26	CYS	3.1
1	A	5	PRO	3.0
1	A	4	HIS	3.0
2	E	216	GLU	3.0
1	A	430	ASP	3.0
2	E	329	GLU	3.0
3	F	13	VAL	2.9
3	F	42	GLY	2.9
1	A	433	LYS	2.9
1	D	416	LYS	2.9
3	C	5	GLU	2.9
3	F	72	ASN	2.8
1	A	37	GLY	2.8
2	B	3	PHE	2.7
2	B	289	ILE	2.7
2	B	386	SER	2.7
1	A	33	LYS	2.7
1	D	433	LYS	2.7
2	E	239	ILE	2.7
2	B	150	TYR	2.6
3	C	31	LYS	2.6
3	C	77	LEU	2.6
1	A	427	ASP	2.6
2	B	122	LYS	2.6
3	C	7	ALA	2.6
3	F	41	ALA	2.6
3	C	34	LYS	2.5
1	A	367	GLU	2.5
3	C	41	ALA	2.5
2	E	356	GLU	2.4
1	A	40	TYR	2.4
3	C	98	LEU	2.4
3	F	59	ALA	2.4
3	C	42	GLY	2.3
3	F	8	GLY	2.3
2	B	13	PRO	2.3
1	A	45	GLU	2.3
2	E	384	PHE	2.3
1	A	428	ILE	2.3
3	C	23	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	243	VAL	2.3
1	A	295	THR	2.2
1	D	367	GLU	2.2
2	B	237	LYS	2.2
3	C	75	PHE	2.2
3	C	85	PRO	2.2
2	B	125	ALA	2.2
1	A	39	ASP	2.2
3	F	23	ASP	2.2
2	E	150	TYR	2.2
1	D	5	PRO	2.2
3	F	10	ALA	2.2
3	F	40	GLY	2.2
1	A	90	MET	2.1
2	B	83	GLU	2.1
3	C	32	TYR	2.1
3	C	49	ILE	2.1
1	A	335	VAL	2.1
1	D	273	LYS	2.1
1	A	102	LEU	2.1
3	F	51	ASP	2.1
1	D	430	ASP	2.1
1	A	252	LYS	2.1
1	A	81	ILE	2.1
1	A	35	PRO	2.0
3	F	49	ILE	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](#)

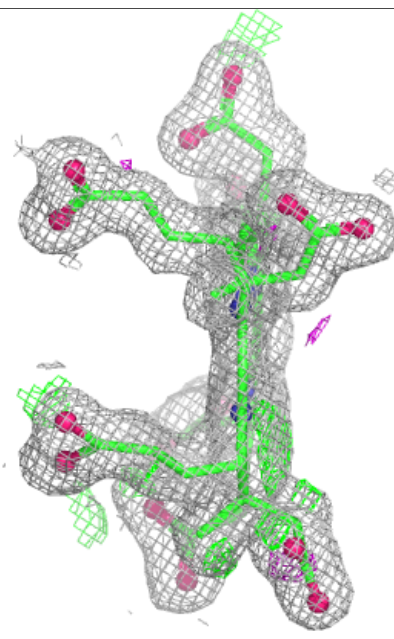
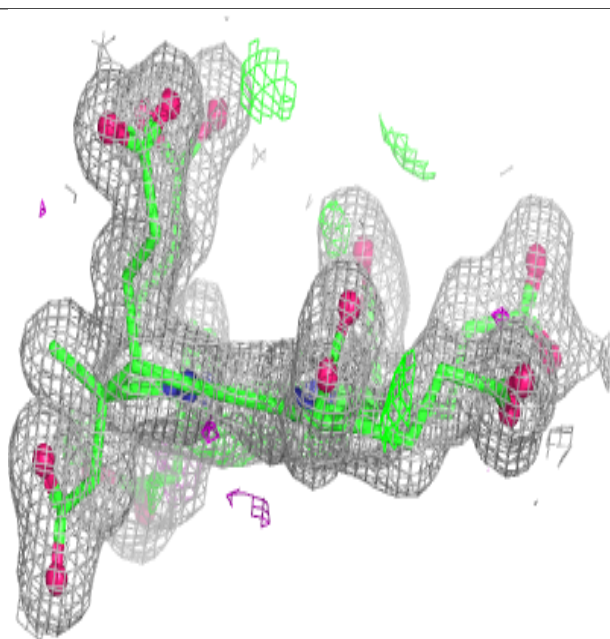
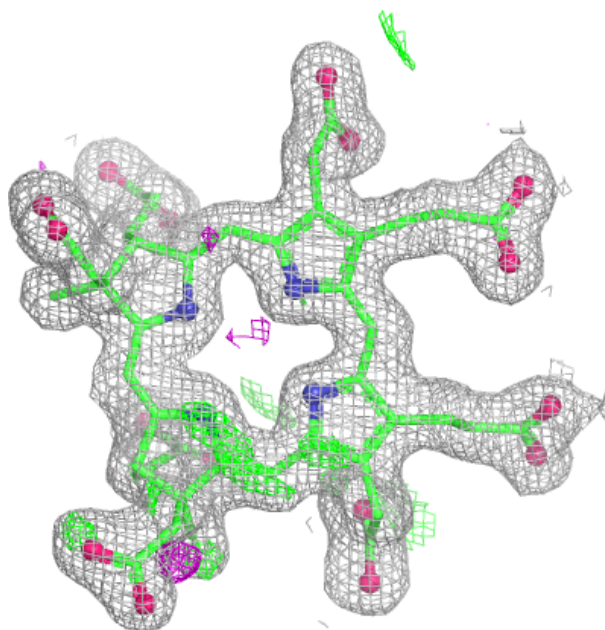
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SRM	B	581	62/63	0.91	0.09	19,21,24,25	0
4	SO3	A	6575	4/4	0.92	0.12	39,40,40,40	0
4	SO3	D	6576	4/4	0.93	0.12	34,35,36,36	0
5	SRM	E	583	62/63	0.93	0.08	14,17,20,23	0
5	SRM	D	582	63/63	0.94	0.10	18,21,28,31	0
5	SRM	A	580	63/63	0.94	0.11	20,24,31,33	0
6	SF4	A	803	8/8	0.94	0.09	22,23,25,26	0
6	SF4	A	804	8/8	0.95	0.08	17,20,23,23	0
6	SF4	B	801	8/8	0.95	0.07	17,23,24,24	0
6	SF4	D	807	8/8	0.95	0.07	17,21,22,22	0
6	SF4	D	808	8/8	0.95	0.08	13,18,21,22	0
6	SF4	E	805	8/8	0.95	0.08	18,21,24,24	0
6	SF4	E	806	8/8	0.95	0.08	22,23,25,25	0
6	SF4	B	802	8/8	0.97	0.06	21,22,22,24	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

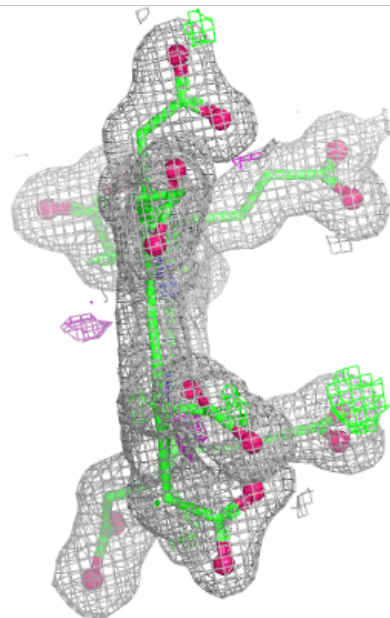
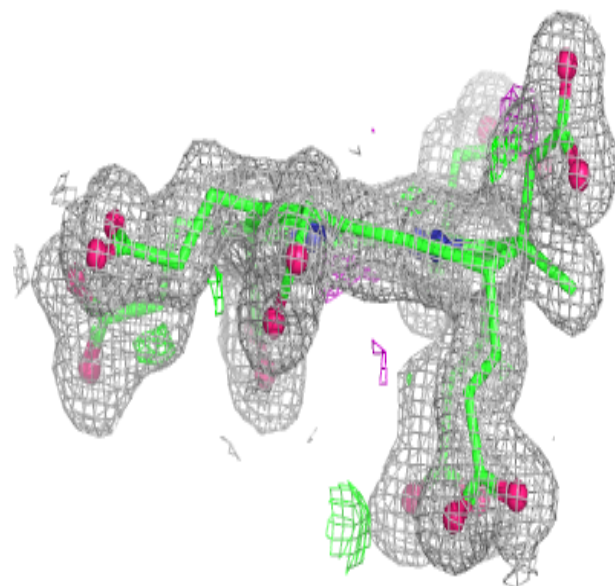
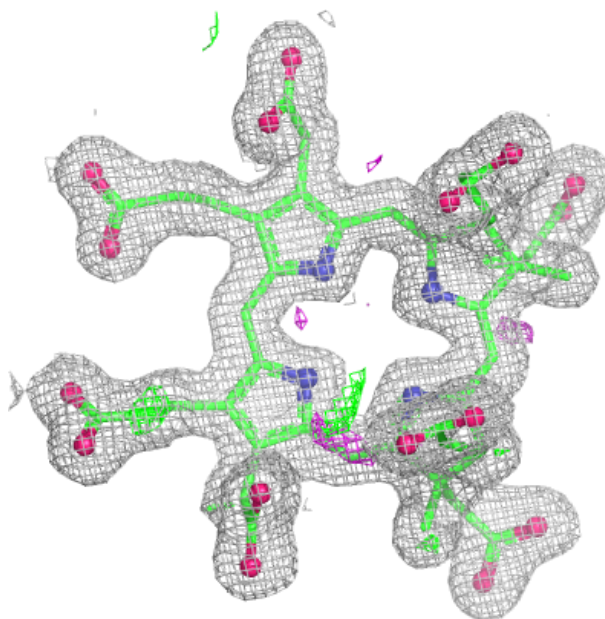
Electron density around SRM B 581:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



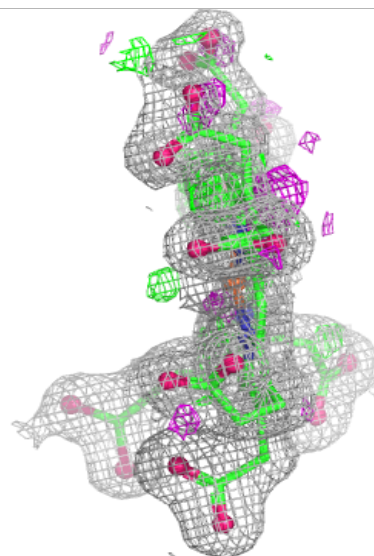
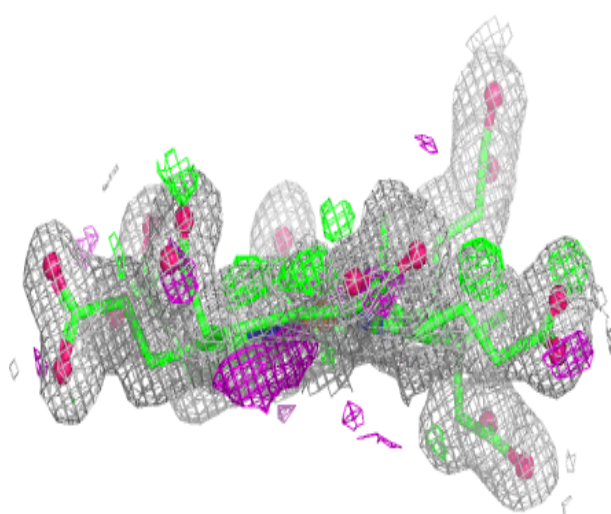
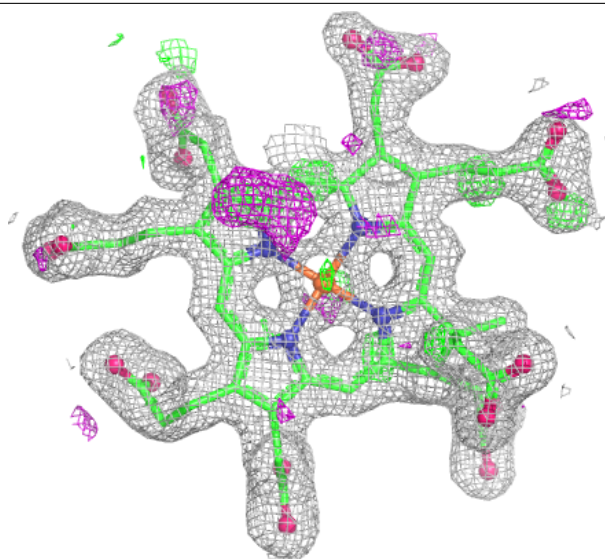
Electron density around SRM E 583:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



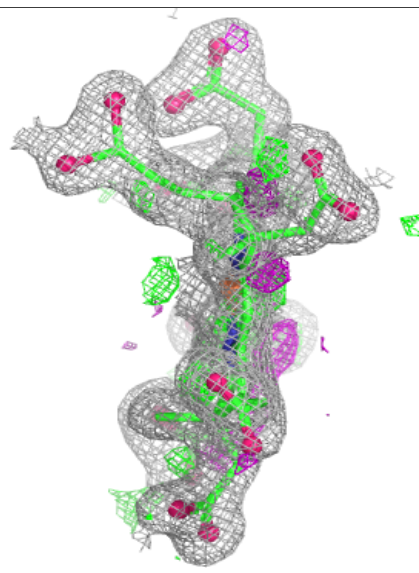
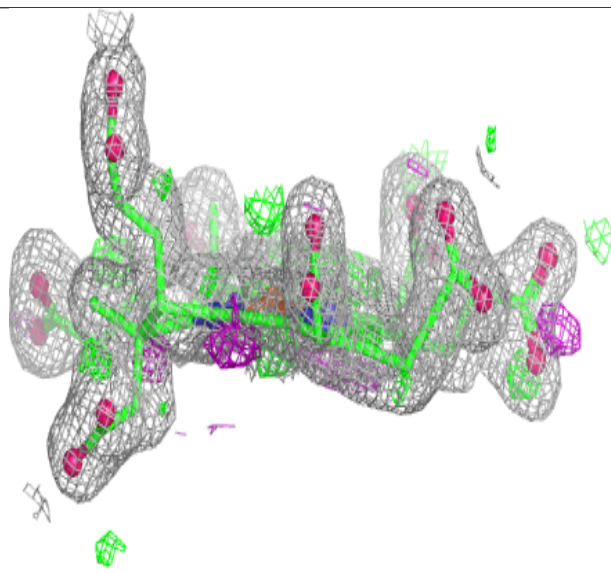
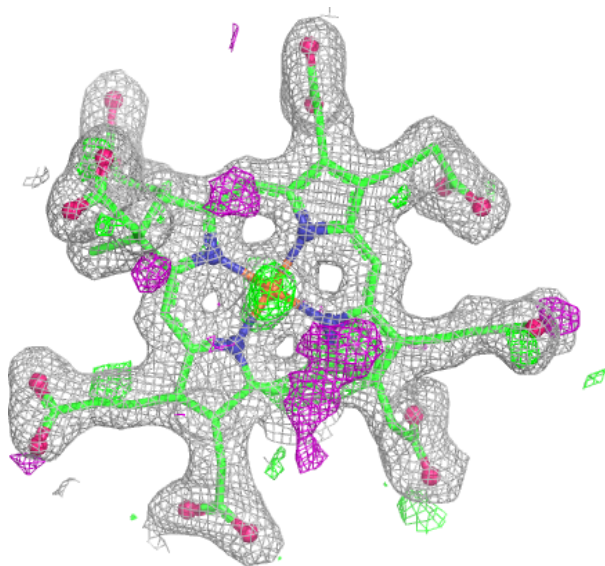
Electron density around SRM D 582:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SRM A 580:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.