



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:42 PM UTC

PDB ID : 3OR2 / pdb_00003or2
Title : Crystal structure of dissimilatory sulfite reductase II (DsrII)
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Chan, S.I.; Chen, C.J.
Deposited on : 2010-09-06
Resolution : 2.05 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

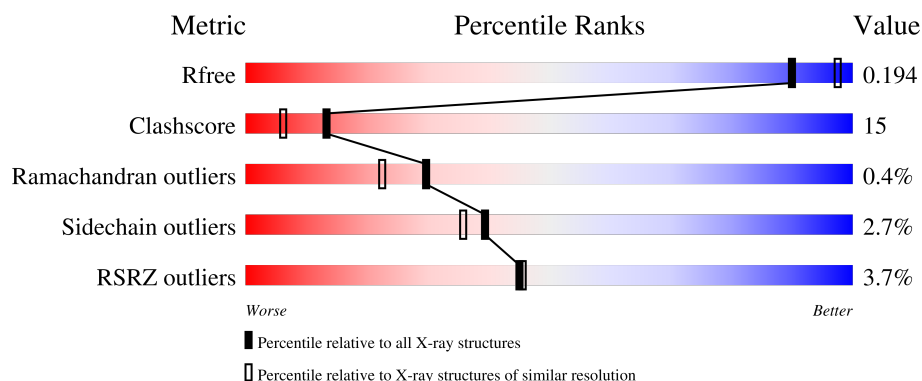
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	435	2% 67% 28% 5%
1	D	435	2% 66% 29% 5%
2	B	385	3% 72% 25% ••
2	E	385	3% 71% 26% •
3	C	104	22% 63% 32% 5%

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Mol	Chain	Length	Quality of chain
3	F	104	

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
4	SF4	B	803	-	-	X	-
5	SO3	A	6573	-	-	X	-
6	SRM	A	582	X	-	-	-
6	SRM	D	584	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15433 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3421	2163	585	645	28			
1	D	435	Total	C	N	O	S	0	0	0
			3421	2163	585	645	28			

- Molecule 2 is a protein called Sulfite reductase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	385	Total	C	N	O	S	3	1	0
			3001	1914	519	541	27			
2	E	385	Total	C	N	O	S	0	0	0
			2998	1912	519	541	26			

- Molecule 3 is a protein called Sulfite reductase subunit gamma.

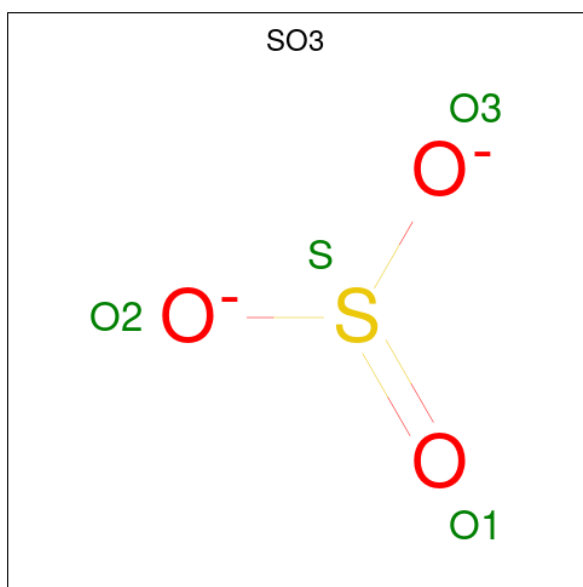
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	104	Total	C	N	O	S	3	1	0
			793	514	126	147	6			
3	F	104	Total	C	N	O	S	0	0	0
			790	512	126	147	5			

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



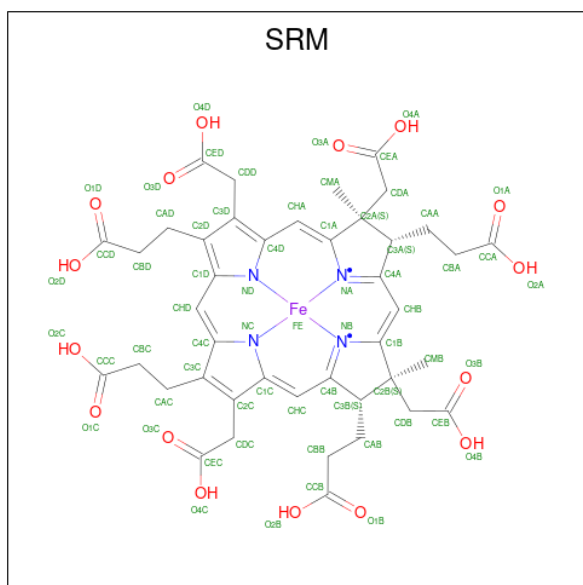
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			7	3	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			7	3	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is SULFITE ION (CCD ID: SO3) (formula: O₃S).



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

- Molecule 6 is SIROHEME (CCD ID: SRM) (formula: $\text{C}_{42}\text{H}_{44}\text{FeN}_4\text{O}_{16}$).

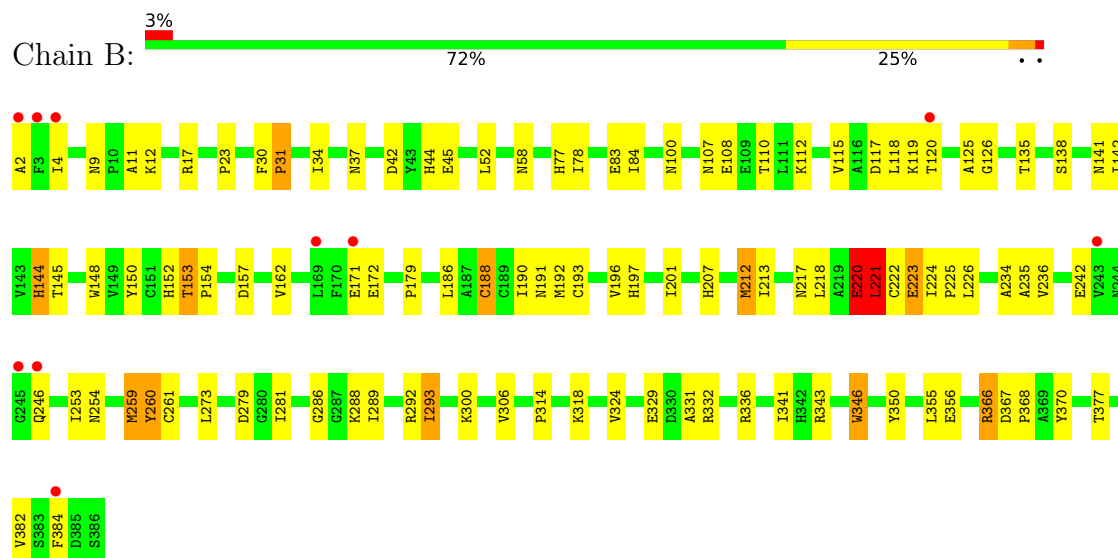


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
6	B	1	Total	C	N	O		0	0
			62	42	4	16			
6	D	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
6	E	1	Total	C	N	O		0	0
			62	42	4	16			

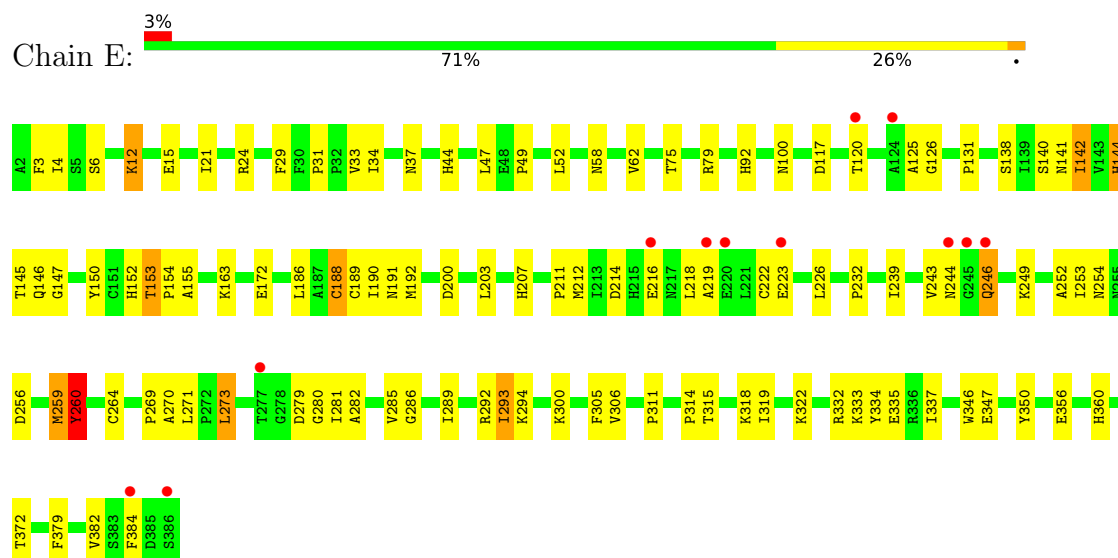
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	157	Total	O	0	0
			157	157		
7	B	139	Total	O	0	0
			139	139		
7	C	8	Total	O	0	0
			8	8		
7	D	212	Total	O	0	0
			212	212		
7	E	149	Total	O	0	0
			149	149		
7	F	16	Total	O	0	0
			16	16		

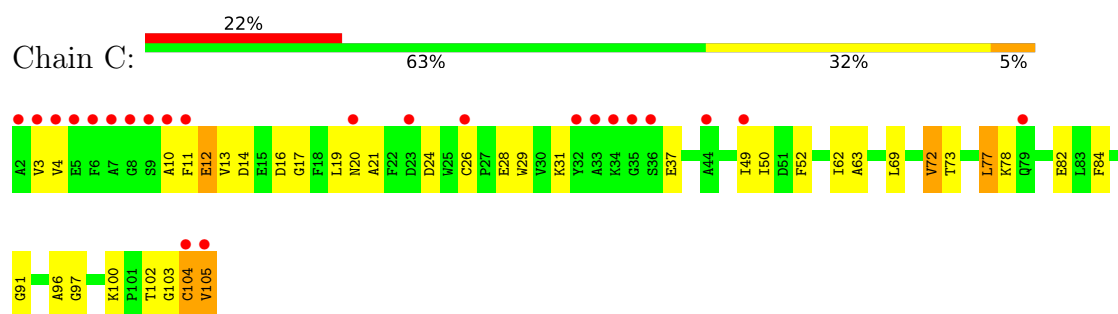
- Molecule 2: Sulfite reductase subunit beta



- Molecule 2: Sulfite reductase subunit beta

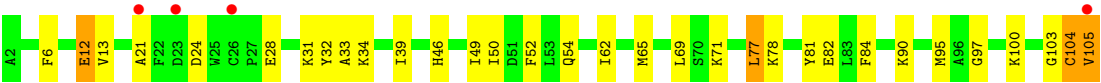


- Molecule 3: Sulfite reductase subunit gamma



- Molecule 3: Sulfite reductase subunit gamma





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.13Å 59.98Å 133.21Å 90.00° 94.24° 90.00°	Depositor
Resolution (Å)	30.00 – 2.05 30.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.05) 97.7 (30.00-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 2.04Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.219 0.193 , 0.194	Depositor DCC
R_{free} test set	5609 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15433	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: SO3, SF4, SRM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.85	29/3511 (0.8%)	1.12	32/4751 (0.7%)
1	D	0.85	20/3511 (0.6%)	1.11	29/4751 (0.6%)
2	B	0.94	35/3081 (1.1%)	1.13	29/4178 (0.7%)
2	E	0.65	9/3075 (0.3%)	1.00	16/4170 (0.4%)
3	C	0.96	11/817 (1.3%)	1.02	7/1101 (0.6%)
3	F	0.78	4/811 (0.5%)	1.02	5/1093 (0.5%)
All	All	0.84	108/14806 (0.7%)	1.08	118/20044 (0.6%)

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	D	0	1

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	230	ALA	CA-CB	-20.28	1.21	1.53
2	B	220	GLU	CB-CG	-12.67	1.14	1.52
2	E	141	ASN	C-N	-10.49	1.20	1.33
2	E	282	ALA	C-N	-10.24	1.20	1.33
1	A	245	LYS	C-N	-9.59	1.21	1.33
2	B	212	MET	C-N	-9.59	1.21	1.33
1	D	309	CYS	C-N	-9.32	1.22	1.33
1	D	298	ILE	C-N	-9.30	1.21	1.33
2	B	235	ALA	C-O	-9.27	1.12	1.24
1	A	390	LYS	C-O	-9.24	1.13	1.24
2	E	3	PHE	C-N	-9.23	1.21	1.33
2	E	49	PRO	C-O	-9.19	1.12	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	ALA	C-N	-8.96	1.22	1.33
1	A	381	GLU	C-O	-8.89	1.12	1.24
3	F	71	LYS	C-O	-8.88	1.13	1.24
1	D	87	GLN	C-O	-8.86	1.12	1.24
1	D	249	GLU	CA-C	8.58	1.63	1.52
1	D	360	GLU	CD-OE1	-8.56	1.09	1.25
2	B	273	LEU	C-O	-8.45	1.13	1.24
1	A	298	ILE	C-N	-8.38	1.23	1.33
2	B	17	ARG	C-N	-8.36	1.21	1.33
1	A	355	PHE	C-N	-8.35	1.23	1.33
2	E	322	LYS	C-N	-8.28	1.23	1.33
2	B	222	CYS	CA-C	-8.25	1.42	1.52
3	C	73	THR	C-O	-8.10	1.13	1.24
2	B	356	GLU	C-N	-8.07	1.21	1.33
1	A	36	LYS	CB-CG	-7.96	1.28	1.52
2	B	118	LEU	C-N	-7.96	1.23	1.33
2	B	220	GLU	N-CA	-7.95	1.36	1.46
2	B	144	HIS	C-N	-7.93	1.22	1.33
1	A	87	GLN	C-N	-7.85	1.23	1.34
1	D	348	PHE	C-N	-7.81	1.24	1.33
2	E	4	ILE	C-N	-7.74	1.22	1.33
1	A	436	MET	C-O	-7.62	1.14	1.23
3	F	97	GLY	C-N	-7.57	1.22	1.33
1	A	341	MET	CG-SD	-7.53	1.61	1.80
1	A	357	GLU	C-O	-7.43	1.15	1.24
2	B	220	GLU	CA-C	-7.42	1.42	1.52
3	F	13	VAL	C-N	-7.40	1.20	1.33
2	B	83	GLU	C-N	-7.35	1.25	1.33
1	D	151	GLU	C-N	-7.34	1.24	1.33
1	A	341	MET	CA-C	7.32	1.63	1.53
2	B	213	ILE	C-N	-7.23	1.24	1.33
3	C	31	LYS	C-O	-7.18	1.15	1.24
2	B	223	GLU	C-O	-7.13	1.13	1.23
1	A	334	PRO	C-O	-6.96	1.15	1.24
2	B	220	GLU	C-O	-6.94	1.15	1.24
3	C	102	THR	C-O	-6.89	1.15	1.23
3	C	72	VAL	C-O	-6.88	1.16	1.24
2	B	220	GLU	CD-OE1	-6.88	1.12	1.25
2	B	221	LEU	CB-CG	-6.85	1.39	1.53
2	B	221	LEU	CG-CD2	-6.82	1.30	1.52
3	C	72	VAL	N-CA	-6.80	1.38	1.46
1	A	341	MET	CA-CB	-6.75	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	213	LYS	CA-C	6.62	1.61	1.52
1	D	292	GLU	C-N	6.61	1.43	1.33
3	C	72	VAL	CA-CB	-6.60	1.45	1.54
1	A	334	PRO	CA-C	6.52	1.61	1.52
1	D	360	GLU	CD-OE2	-6.51	1.12	1.25
1	A	357	GLU	CA-C	6.39	1.61	1.52
1	D	154	PHE	C-N	6.37	1.42	1.33
2	B	221	LEU	CG-CD1	-6.33	1.31	1.52
1	A	169	SER	C-O	-6.24	1.13	1.23
3	C	105	VAL	C-OXT	6.21	1.35	1.23
1	D	87	GLN	CB-CG	-6.20	1.33	1.52
2	B	366	ARG	C-N	6.14	1.46	1.33
1	A	86	ASP	C-N	-6.14	1.25	1.33
1	A	24	ILE	C-N	-6.12	1.25	1.33
1	D	87	GLN	CD-NE2	-6.10	1.20	1.33
2	B	84	ILE	C-N	6.00	1.41	1.33
2	B	341	ILE	C-N	-6.00	1.26	1.33
1	A	408	ARG	C-O	-5.99	1.16	1.23
2	B	188[A]	CYS	CA-C	5.98	1.60	1.52
2	B	188[B]	CYS	CA-C	5.98	1.60	1.52
1	A	408	ARG	CA-C	5.95	1.60	1.52
2	E	126	GLY	C-O	-5.95	1.15	1.23
2	B	324	VAL	C-N	-5.90	1.26	1.33
1	A	35	PRO	CA-CB	-5.85	1.45	1.53
1	A	334	PRO	CB-CG	-5.85	1.20	1.49
2	B	78	ILE	C-N	5.83	1.41	1.33
2	B	222	CYS	C-N	-5.77	1.25	1.33
1	A	408	ARG	CD-NE	-5.75	1.38	1.46
3	F	12	GLU	C-N	5.70	1.41	1.33
2	B	223	GLU	CD-OE2	-5.56	1.14	1.25
1	A	390	LYS	CG-CD	-5.50	1.35	1.52
2	B	221	LEU	C-O	-5.41	1.17	1.24
1	D	336	LEU	CG-CD2	-5.39	1.34	1.52
1	A	318	LYS	C-N	-5.39	1.24	1.33
2	E	49	PRO	N-CD	-5.39	1.40	1.47
2	B	220	GLU	CG-CD	-5.38	1.38	1.52
3	C	97	GLY	C-N	-5.38	1.23	1.33
2	B	273	LEU	CG-CD2	-5.37	1.34	1.52
1	D	275	ASP	C-N	-5.30	1.27	1.34
1	D	249	GLU	C-N	-5.29	1.26	1.33
2	E	33	VAL	C-N	5.28	1.40	1.33
1	D	230	ALA	CA-C	5.24	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	334	PRO	CA-CB	-5.18	1.46	1.53
3	C	73	THR	N-CA	-5.18	1.39	1.46
1	A	340	GLN	N-CA	-5.15	1.39	1.46
3	C	104[A]	CYS	CB-SG	5.15	1.98	1.81
3	C	104[B]	CYS	CB-SG	5.15	1.98	1.81
1	A	407	PRO	C-N	-5.07	1.26	1.33
1	A	319	ILE	C-N	5.06	1.41	1.33
1	D	393	GLU	CD-OE1	-5.06	1.15	1.25
2	B	77	HIS	C-N	-5.06	1.27	1.33
2	B	201	ILE	C-N	-5.05	1.27	1.33
2	B	234	ALA	C-N	-5.02	1.27	1.33
2	B	221	LEU	CA-CB	-5.01	1.44	1.53

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	228	SER	O-C-N	-10.54	111.12	122.09
1	A	405	SER	N-CA-C	-10.53	100.55	113.50
1	A	341	MET	CG-SD-CE	-10.48	77.83	100.90
1	D	134	GLY	N-CA-C	-9.48	100.40	112.54
2	B	221	LEU	N-CA-C	9.35	124.50	113.18
2	B	355	LEU	O-C-N	-9.25	112.21	123.04
1	A	42	ILE	CA-C-N	8.95	129.51	119.93
1	A	42	ILE	C-N-CA	8.95	129.51	119.93
1	D	405	SER	N-CA-C	-8.62	102.54	113.23
1	A	139	ILE	N-CA-C	-8.49	97.68	108.89
1	D	177	CYS	N-CA-C	-8.39	99.70	110.53
2	B	355	LEU	CA-C-N	8.37	132.67	120.95
2	B	355	LEU	C-N-CA	8.37	132.67	120.95
1	A	117	ALA	CA-C-N	8.31	131.03	120.56
1	A	117	ALA	C-N-CA	8.31	131.03	120.56
1	A	134	GLY	N-CA-C	-8.22	101.23	112.25
2	E	31	PRO	N-CA-C	-7.80	101.18	110.70
3	C	104[A]	CYS	CB-CA-C	-7.74	98.95	109.71
3	C	104[B]	CYS	CB-CA-C	-7.74	98.95	109.71
1	A	346	ILE	CA-C-N	7.69	127.23	119.24
1	A	346	ILE	C-N-CA	7.69	127.23	119.24
1	D	108	LYS	N-CA-C	7.55	121.81	111.39
1	D	62	GLU	O-C-N	-7.40	114.38	123.33
1	A	42	ILE	O-C-N	-7.06	113.06	121.10
1	A	86	ASP	CA-C-N	7.04	130.41	122.59
1	A	86	ASP	C-N-CA	7.04	130.41	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	191	ASN	N-CA-C	-7.04	103.79	112.38
1	D	413	ILE	N-CA-C	6.81	118.62	108.54
1	D	155	GLU	O-C-N	-6.71	115.00	122.12
3	F	34	LYS	O-C-N	6.69	130.29	122.20
1	A	108	LYS	N-CA-C	6.65	120.72	111.74
2	B	31	PRO	N-CA-C	-6.58	103.53	110.58
1	A	177	CYS	N-CA-C	-6.53	102.10	110.53
1	D	139	ILE	N-CA-C	-6.51	100.30	108.89
1	A	62	GLU	O-C-N	-6.51	115.46	123.33
2	B	145	THR	O-C-N	-6.47	113.99	122.59
2	B	191	ASN	N-CA-C	-6.44	104.52	112.38
1	D	87	GLN	CA-C-N	6.39	125.89	119.24
1	D	87	GLN	C-N-CA	6.39	125.89	119.24
2	B	220	GLU	N-CA-C	6.39	119.23	111.82
2	E	222	CYS	N-CA-C	6.37	119.91	109.72
2	B	273	LEU	N-CA-C	6.37	123.62	114.39
2	E	144	HIS	N-CA-C	6.36	117.51	108.74
1	D	337	ASP	N-CA-C	6.33	120.68	113.15
3	C	104[A]	CYS	N-CA-C	-6.28	101.25	110.42
3	C	104[B]	CYS	N-CA-C	-6.28	101.25	110.42
1	A	117	ALA	O-C-N	-6.26	115.49	122.12
1	A	142	LEU	N-CA-C	6.23	118.94	108.23
2	E	47	LEU	CA-C-N	6.23	131.09	122.06
2	E	47	LEU	C-N-CA	6.23	131.09	122.06
1	A	413	ILE	N-CA-C	6.21	117.52	108.58
3	F	33	ALA	O-C-N	-6.19	114.66	122.27
1	D	276	ILE	O-C-N	6.11	128.04	121.87
1	D	336	LEU	CA-CB-CG	6.10	137.66	116.30
2	B	220	GLU	CG-CD-OE1	-6.08	104.41	118.40
1	A	226	VAL	N-CA-C	-6.04	106.43	112.17
2	B	30	PHE	CA-C-N	-5.99	115.34	119.66
2	B	30	PHE	C-N-CA	-5.99	115.34	119.66
2	B	213	ILE	O-C-N	-5.98	116.86	123.20
1	D	96	HIS	N-CA-C	-5.97	99.66	109.40
1	A	231	ARG	N-CA-C	5.94	119.75	111.56
3	C	105	VAL	CG1-CB-CG2	5.94	123.87	110.80
1	D	142	LEU	N-CA-C	5.94	119.15	108.17
2	B	144	HIS	N-CA-C	5.93	116.10	108.34
2	B	188[A]	CYS	CA-CB-SG	-5.92	100.80	114.40
2	B	188[B]	CYS	CA-CB-SG	-5.92	100.80	114.40
1	A	308	HIS	N-CA-C	5.91	118.20	111.11
1	D	334	PRO	N-CA-C	5.90	124.63	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	GLY	N-CA-C	-5.85	107.02	115.27
1	D	406	GLU	CA-C-N	-5.84	114.60	120.21
1	D	406	GLU	C-N-CA	-5.84	114.60	120.21
1	A	313	MET	CA-C-N	5.81	126.21	119.47
1	A	313	MET	C-N-CA	5.81	126.21	119.47
1	D	158	HIS	N-CA-C	5.80	117.68	111.36
2	B	346	TRP	N-CA-C	5.74	117.21	111.07
2	E	12	LYS	CA-C-N	5.73	126.12	119.47
2	E	12	LYS	C-N-CA	5.73	126.12	119.47
2	B	286	GLY	N-CA-C	5.72	123.22	115.32
1	D	207	ARG	CA-C-N	5.70	126.96	119.84
1	D	207	ARG	C-N-CA	5.70	126.96	119.84
3	C	103	GLY	CA-C-O	-5.67	116.51	122.01
1	D	329	VAL	N-CA-C	5.66	118.29	108.95
2	B	12	LYS	CA-C-N	5.64	126.02	119.47
2	B	12	LYS	C-N-CA	5.64	126.02	119.47
3	F	33	ALA	CA-C-N	5.62	130.12	121.19
3	F	33	ALA	C-N-CA	5.62	130.12	121.19
2	B	336	ARG	N-CA-C	-5.58	103.02	110.55
2	B	201	ILE	CA-C-N	5.54	125.88	121.61
2	B	201	ILE	C-N-CA	5.54	125.88	121.61
2	B	234	ALA	CA-C-N	5.53	129.96	120.72
2	B	234	ALA	C-N-CA	5.53	129.96	120.72
2	B	201	ILE	O-C-N	-5.49	117.14	123.07
2	E	142	ILE	O-C-N	-5.44	117.43	123.03
1	D	140	VAL	N-CA-C	5.39	115.62	107.80
1	A	13	GLU	N-CA-C	-5.36	106.91	113.50
2	E	260	TYR	N-CA-C	5.32	118.78	111.54
3	F	12	GLU	O-C-N	-5.32	116.38	122.93
1	D	349	ILE	O-C-N	-5.32	117.02	122.82
2	E	126	GLY	O-C-N	5.32	129.61	122.70
1	D	243	ASP	N-CA-C	5.31	118.39	110.52
1	A	380	GLY	CA-C-N	5.31	128.38	120.31
1	A	380	GLY	C-N-CA	5.31	128.38	120.31
3	C	63	ALA	N-CA-C	-5.29	102.52	110.24
1	D	13	GLU	N-CA-C	-5.27	106.89	113.38
2	B	212	MET	N-CA-C	-5.27	101.94	110.32
2	E	145	THR	N-CA-C	5.26	118.74	109.80
1	A	420	VAL	N-CA-C	5.25	113.06	107.76
1	A	334	PRO	CA-N-CD	-5.24	104.66	112.00
2	B	126	GLY	N-CA-C	5.24	120.72	114.48
2	E	286	GLY	N-CA-C	5.14	122.52	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ILE	N-CA-C	5.12	114.15	106.42
2	B	100	ASN	N-CA-C	-5.11	102.50	110.42
1	D	15	GLY	CA-C-N	5.10	124.41	118.85
1	D	15	GLY	C-N-CA	5.10	124.41	118.85
2	E	24	ARG	N-CA-C	-5.10	103.31	110.50
2	E	140	SER	N-CA-C	5.04	117.34	107.57
1	A	96	HIS	N-CA-C	-5.04	100.96	109.07
2	E	100	ASN	N-CA-C	-5.02	102.64	110.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	229	MET	Mainchain

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	3421	0	3275	126	0
1	D	3421	0	3275	134	0
2	B	3001	0	2969	93	0
2	E	2998	0	2964	89	0
3	C	793	0	776	32	0
3	F	790	0	771	32	0
4	A	16	0	0	1	0
4	B	15	0	0	2	0
4	D	16	0	0	1	0
4	E	15	0	0	0	0
5	A	8	0	0	2	0
5	D	8	0	0	0	0
6	A	63	0	34	9	0
6	B	62	0	34	6	0
6	D	63	0	34	15	0
6	E	62	0	34	4	0
7	A	157	0	0	2	0
7	B	139	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	8	0	0	0	0
7	D	212	0	0	2	0
7	E	149	0	0	2	0
7	F	16	0	0	1	0
All	All	15433	0	14166	427	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 (427) 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)
6:D:584:SRM:HHA	3:F:104:CYS:SG	1.48	1.54
2:B:188[B]:CYS:SG	4:B:803:SF4:S1	2.38	1.21
6:D:584:SRM:CHA	3:F:104:CYS:SG	2.28	1.19
1:D:170:ASN:HD22	1:D:208:PRO:HG3	1.21	1.04
1:D:167:SER:HB2	3:F:105:VAL:HG11	1.39	1.01
1:A:416:LYS:HB3	1:A:418:GLU:OE1	1.60	0.99
1:D:402:GLN:H	1:D:402:GLN:HE21	1.17	0.93
2:E:239:ILE:HD13	2:E:252:ALA:HB2	1.50	0.92
1:D:8:MET:HE2	2:E:311:PRO:HD3	1.53	0.90
1:D:131:ASN:HB2	1:D:140:VAL:HB	1.53	0.89
1:A:136:THR:H	6:A:582:SRM:HBB2	1.40	0.87
1:A:290:THR:HB	1:A:297:SER:OG	1.73	0.86
1:A:308:HIS:HD2	2:B:292:ARG:HE	1.21	0.86
1:A:230:ALA:HB2	2:B:289:ILE:HD13	1.55	0.86
1:A:131:ASN:HB2	1:A:140:VAL:HB	1.59	0.84
1:D:104:GLN:NE2	1:D:104:GLN:H	1.76	0.83
1:D:136:THR:H	6:D:584:SRM:HBB2	1.43	0.82
2:E:223:GLU:OE1	2:E:226:LEU:HD11	1.80	0.82
2:E:37:ASN:HD21	2:E:58:ASN:HD21	1.27	0.82
2:B:366:ARG:C	2:B:368:PRO:HD2	2.06	0.81
1:D:170:ASN:ND2	1:D:208:PRO:HG3	1.95	0.81
5:A:6573:SO3:O1	3:C:100:LYS:NZ	2.14	0.80
1:D:104:GLN:H	1:D:104:GLN:HE21	1.30	0.79
1:A:416:LYS:CB	1:A:418:GLU:OE1	2.31	0.79
1:D:170:ASN:HB3	1:D:208:PRO:HA	1.64	0.79
2:E:314:PRO:O	2:E:318:LYS:HG3	1.84	0.77
2:E:219:ALA:HB2	2:E:249:LYS:O	1.85	0.77
1:A:170:ASN:ND2	1:A:208:PRO:HG3	2.00	0.76
3:C:3:VAL:HG22	3:C:12:GLU:OE2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLN:H	1:A:104:GLN:NE2	1.84	0.75
2:E:117:ASP:O	2:E:120:THR:HG22	1.87	0.75
1:A:402:GLN:H	1:A:402:GLN:HE21	1.31	0.75
1:D:167:SER:CB	3:F:105:VAL:HG11	2.15	0.75
1:A:246:ILE:HG12	1:A:317:LEU:CD2	2.17	0.74
1:A:104:GLN:H	1:A:104:GLN:HE21	1.33	0.74
2:B:224:ILE:HB	2:B:225:PRO:HD3	1.70	0.74
1:A:229:MET:HG3	2:B:289:ILE:HD11	1.68	0.74
1:D:112:ALA:O	1:D:116:GLU:HG3	1.88	0.74
1:D:184:GLU:OE1	2:E:44:HIS:HD2	1.70	0.74
1:A:8:MET:HE3	1:A:59:HIS:CD2	2.23	0.73
1:A:135:SER:HB2	6:A:582:SRM:HHC	1.70	0.73
1:A:133:HIS:HA	1:A:138:ASP:O	1.88	0.73
1:A:263:ALA:HB1	2:B:45:GLU:HA	1.72	0.72
1:D:97:PHE:O	2:E:150:TYR:HE1	1.72	0.72
1:A:39:ASP:OD1	2:B:2:ALA:HA	1.88	0.71
1:A:285:PRO:HG3	2:B:293:ILE:HA	1.72	0.71
2:B:332:ARG:HG3	2:B:343:ARG:NH2	2.05	0.71
1:A:427:ASP:OD2	1:A:429:SER:HB3	1.90	0.71
2:B:37:ASN:HD21	2:B:58:ASN:HD21	1.39	0.71
1:D:89:GLU:CD	1:D:89:GLU:H	1.98	0.71
2:B:367:ASP:N	2:B:368:PRO:HD2	2.06	0.71
1:D:97:PHE:O	2:E:150:TYR:CE1	2.43	0.71
1:D:336:LEU:HD23	2:E:232:PRO:HG3	1.73	0.70
1:D:308:HIS:HD2	2:E:292:ARG:HE	1.39	0.70
1:A:196:GLN:HE22	1:A:354:PRO:HA	1.56	0.70
1:A:168:GLY:N	3:C:105:VAL:HG21	2.05	0.70
2:E:125:ALA:HB3	7:E:400:HOH:O	1.90	0.70
1:A:8:MET:HE3	1:A:59:HIS:HD2	1.57	0.70
1:A:431:TYR:CD2	2:E:212:MET:HE1	2.26	0.69
2:B:382:VAL:CG2	2:B:384:PHE:HD2	2.05	0.69
3:F:78:LYS:O	3:F:82:GLU:HG3	1.92	0.69
1:D:402:GLN:H	1:D:402:GLN:NE2	1.89	0.69
1:A:46:CYS:HB3	1:A:47:PRO:HD3	1.75	0.68
1:D:223:ASN:HD21	1:D:311:ASN:HD21	1.38	0.68
1:D:416:LYS:O	1:D:419:GLU:HG2	1.93	0.68
1:A:34:ASN:HD21	1:A:38:LEU:H	1.41	0.68
1:A:408:ARG:HH11	1:A:410:ASN:HD21	1.39	0.68
1:D:262:ASN:ND2	2:E:292:ARG:HH22	1.92	0.68
1:A:124:LEU:HD21	2:B:4:ILE:HD11	1.76	0.68
2:B:350:TYR:HB3	2:B:384:PHE:HZ	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:GLN:HE22	1:D:173:THR:HG21	1.58	0.67
1:D:408:ARG:HH11	1:D:410:ASN:HD21	1.41	0.67
1:A:136:THR:H	6:A:582:SRM:CBB	2.07	0.67
1:A:168:GLY:HA2	3:C:105:VAL:HB	1.76	0.67
3:C:12:GLU:HB3	3:C:20:ASN:HD22	1.60	0.67
3:C:49:ILE:HD12	3:C:84:PHE:HE1	1.60	0.67
6:D:584:SRM:HDA2	3:F:104:CYS:SG	2.35	0.67
1:A:170:ASN:HB2	1:A:204:GLU:O	1.95	0.66
1:A:262:ASN:ND2	2:B:292:ARG:HH22	1.94	0.66
1:A:290:THR:HB	1:A:297:SER:HG	1.57	0.66
1:A:219:ASP:OD1	1:A:226:VAL:HG12	1.95	0.66
1:A:418:GLU:CD	1:A:418:GLU:H	2.05	0.66
6:D:584:SRM:HMA2	3:F:104:CYS:HB3	1.78	0.65
1:D:336:LEU:CD2	2:E:232:PRO:HG3	2.26	0.65
1:D:136:THR:H	6:D:584:SRM:CBB	2.09	0.65
1:D:34:ASN:HD21	1:D:38:LEU:H	1.45	0.65
2:B:223:GLU:HB2	2:B:226:LEU:HD12	1.79	0.65
1:D:246:ILE:HG12	1:D:317:LEU:CD1	2.27	0.65
1:D:121:VAL:HG13	1:D:155:GLU:OE1	1.98	0.64
2:E:223:GLU:OE1	2:E:226:LEU:CD1	2.45	0.64
3:F:28:GLU:HA	3:F:31:LYS:HE2	1.78	0.64
1:A:410:ASN:HD22	1:A:412:TYR:H	1.44	0.64
1:D:33:LYS:HE3	1:D:35:PRO:HG3	1.79	0.64
1:A:170:ASN:HD22	1:A:208:PRO:HG3	1.62	0.64
1:D:434:ARG:NH1	1:D:434:ARG:HB2	2.13	0.64
2:B:37:ASN:HD21	2:B:58:ASN:ND2	1.96	0.64
1:A:402:GLN:H	1:A:402:GLN:NE2	1.95	0.64
2:E:281:ILE:O	2:E:306:VAL:HG22	1.98	0.64
2:B:281:ILE:O	2:B:306:VAL:HG22	1.98	0.63
6:D:584:SRM:O1A	2:E:150:TYR:HD2	1.80	0.63
1:D:155:GLU:HG3	2:E:6:SER:HB2	1.80	0.63
6:D:584:SRM:HMA2	3:F:104:CYS:CB	2.29	0.63
1:A:97:PHE:O	2:B:150:TYR:CE1	2.52	0.63
1:A:223:ASN:HD21	1:A:311:ASN:HD21	1.44	0.63
1:D:121:VAL:HG11	1:D:156:MET:HE2	1.81	0.62
1:D:196:GLN:HE22	1:D:354:PRO:HA	1.64	0.62
2:E:223:GLU:HB3	3:F:62:ILE:HG22	1.81	0.62
2:B:107:ASN:ND2	2:B:110:THR:H	1.97	0.62
3:C:4:VAL:O	3:C:10:ALA:HA	2.00	0.62
1:D:42:ILE:HD11	1:D:126:GLY:C	2.25	0.62
1:D:168:GLY:N	3:F:105:VAL:HG13	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:223:GLU:HB2	2:E:226:LEU:HD12	1.81	0.61
1:D:434:ARG:HB2	1:D:434:ARG:HH11	1.64	0.61
1:A:42:ILE:HD11	1:A:126:GLY:C	2.26	0.61
1:D:313:MET:HB2	1:D:317:LEU:HD23	1.81	0.61
2:E:243:VAL:HG12	2:E:244:ASN:ND2	2.15	0.61
1:A:83:ARG:H	1:A:98:HIS:HD2	1.49	0.61
1:D:83:ARG:H	1:D:98:HIS:HD2	1.49	0.61
1:A:418:GLU:OE2	1:A:418:GLU:N	2.30	0.61
1:D:410:ASN:HD22	1:D:412:TYR:H	1.49	0.61
1:A:436:MET:SD	1:D:89:GLU:OE1	2.59	0.60
1:D:98:HIS:HE1	1:D:146:THR:OG1	1.83	0.60
1:D:104:GLN:HE21	1:D:104:GLN:N	1.98	0.60
2:B:186:LEU:C	2:B:186:LEU:HD23	2.25	0.60
1:D:317:LEU:N	1:D:317:LEU:HD22	2.16	0.60
1:D:167:SER:OG	3:F:105:VAL:HG21	2.01	0.60
1:A:104:GLN:HE22	1:A:173:THR:HG21	1.66	0.60
2:E:146:GLN:HE21	2:E:150:TYR:HB3	1.65	0.60
1:A:184:GLU:OE1	2:B:44:HIS:HD2	1.85	0.60
2:B:350:TYR:HB3	2:B:384:PHE:CZ	2.37	0.60
2:E:356:GLU:HA	2:E:356:GLU:OE2	2.01	0.60
2:E:315:THR:O	2:E:319:ILE:HG13	2.02	0.59
1:A:308:HIS:CD2	2:B:292:ARG:HE	2.11	0.59
2:B:382:VAL:HG22	1:D:402:GLN:OE1	2.03	0.59
2:B:153:THR:N	2:B:154:PRO:CD	2.66	0.59
1:D:248:GLN:HE22	1:D:296:LEU:H	1.49	0.59
1:A:402:GLN:OE1	2:E:382:VAL:HG22	2.02	0.59
3:C:26:CYS:SG	3:C:28:GLU:HG2	2.42	0.59
1:D:168:GLY:H	3:F:105:VAL:HG13	1.68	0.59
3:F:21:ALA:HB3	3:F:24:ASP:OD2	2.02	0.59
1:D:402:GLN:HE21	1:D:402:GLN:N	1.97	0.58
1:A:427:ASP:CG	1:A:429:SER:HB3	2.27	0.58
1:D:229:MET:HG3	2:E:289:ILE:HD11	1.86	0.58
1:D:418:GLU:CD	1:D:418:GLU:H	2.11	0.58
1:A:97:PHE:O	2:B:150:TYR:HE1	1.86	0.58
1:D:220:GLY:HA3	4:D:806:SF4:S4	2.43	0.58
2:B:223:GLU:HG2	3:C:62:ILE:HA	1.84	0.57
1:D:170:ASN:HB2	1:D:204:GLU:O	2.05	0.57
2:B:188[B]:CYS:SG	4:B:803:SF4:S2	3.03	0.57
1:D:416:LYS:HB3	1:D:418:GLU:OE2	2.05	0.57
1:A:70:ILE:HG13	3:C:100:LYS:HG3	1.85	0.57
1:A:168:GLY:H	3:C:105:VAL:HG21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:LYS:HE3	2:B:42:ASP:O	2.04	0.57
1:A:406:GLU:HG3	2:E:346:TRP:HE1	1.70	0.56
2:B:207:HIS:HD2	2:B:279:ASP:OD1	1.88	0.56
2:B:236:VAL:HG22	2:B:253:ILE:HG12	1.88	0.56
1:D:306:CYS:O	1:D:307:MET:HB2	2.04	0.56
3:C:104[B]:CYS:HB3	3:C:105:VAL:HG23	1.88	0.56
6:A:582:SRM:O1A	2:B:150:TYR:HD2	1.89	0.56
1:A:416:LYS:HE3	1:A:418:GLU:OE1	2.06	0.56
2:B:242:GLU:HA	2:B:246:GLN:O	2.06	0.55
3:C:52:PHE:CE1	3:C:72:VAL:HG11	2.42	0.55
2:E:280:GLY:HA3	2:E:305:PHE:CE1	2.41	0.55
2:E:152:HIS:C	2:E:154:PRO:HD2	2.31	0.55
2:B:382:VAL:HG21	2:B:384:PHE:HD2	1.70	0.55
1:D:308:HIS:CD2	2:E:292:ARG:HE	2.22	0.55
2:E:211:PRO:HG2	2:E:253:ILE:CD1	2.37	0.55
6:D:584:SRM:CED	3:F:104:CYS:SG	2.95	0.54
1:A:246:ILE:HD11	1:A:298:ILE:HD12	1.87	0.54
1:A:335:VAL:HG12	7:B:405:HOH:O	2.07	0.54
1:D:34:ASN:N	1:D:35:PRO:HD3	2.22	0.54
2:E:306:VAL:HG11	2:E:319:ILE:HD12	1.89	0.54
1:D:230:ALA:HB2	2:E:289:ILE:HD13	1.90	0.54
1:A:229:MET:CG	2:B:289:ILE:HD11	2.37	0.54
2:B:31:PRO:HG2	2:B:34:ILE:CG1	2.38	0.54
1:D:202:GLN:OE1	1:D:206:HIS:HE1	1.90	0.54
1:D:246:ILE:HG12	1:D:317:LEU:HD13	1.88	0.54
2:B:9:ASN:ND2	2:B:11:ALA:H	2.05	0.54
2:B:224:ILE:HD13	7:B:451:HOH:O	2.07	0.54
1:A:50:LEU:C	1:A:50:LEU:HD13	2.33	0.54
1:A:69:GLY:O	1:A:70:ILE:HD13	2.07	0.54
1:A:245:LYS:HB2	1:A:318:LYS:HB2	1.89	0.54
2:B:367:ASP:N	2:B:368:PRO:CD	2.70	0.54
1:D:316:ALA:C	1:D:317:LEU:HD22	2.33	0.54
1:A:104:GLN:HE21	1:A:104:GLN:N	2.05	0.54
2:B:300:LYS:CB	1:D:407:PRO:HG2	2.39	0.54
1:D:17:TRP:CD2	1:D:18:PRO:HD2	2.43	0.54
1:D:55:GLU:OE2	1:D:59:HIS:HE1	1.91	0.54
1:D:133:HIS:HA	1:D:138:ASP:O	2.07	0.53
2:B:289:ILE:HG22	6:B:581:SRM:CCC	2.37	0.53
1:A:306:CYS:O	1:A:307:MET:HB2	2.09	0.53
1:A:383:MET:HE3	1:A:391:LEU:HD12	1.90	0.53
1:D:131:ASN:HB2	1:D:140:VAL:CB	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:211:PRO:HG2	2:E:253:ILE:HD13	1.90	0.53
1:A:435:HIS:HE1	1:D:62:GLU:OE2	1.92	0.53
2:E:254:ASN:ND2	2:E:256:ASP:H	2.07	0.53
2:B:300:LYS:HB3	1:D:407:PRO:HG2	1.90	0.53
1:D:4:HIS:N	1:D:5:PRO:HD2	2.24	0.53
1:A:99:THR:N	2:B:150:TYR:OH	2.42	0.53
1:D:42:ILE:HD11	1:D:126:GLY:O	2.09	0.53
2:E:153:THR:N	2:E:154:PRO:CD	2.72	0.52
2:E:186:LEU:C	2:E:186:LEU:HD23	2.34	0.52
1:A:98:HIS:HE1	1:A:146:THR:OG1	1.92	0.52
2:B:9:ASN:HD21	2:B:11:ALA:HB3	1.75	0.52
1:D:136:THR:OG1	6:D:584:SRM:HBB1	2.10	0.52
3:C:21:ALA:HB3	3:C:24:ASP:OD2	2.09	0.52
2:E:211:PRO:HA	2:E:273:LEU:HB3	1.91	0.52
3:F:105:VAL:CG2	3:F:105:VAL:OXT	2.58	0.52
1:A:70:ILE:HG12	3:C:100:LYS:HD2	1.91	0.52
1:D:56:LEU:HD13	1:D:64:HIS:CE1	2.45	0.51
2:B:142:ILE:O	2:B:144:HIS:HD2	1.94	0.51
2:B:212:MET:HE1	1:D:431:TYR:CD2	2.46	0.51
1:D:76:TYR:CD1	1:D:206:HIS:HB3	2.46	0.51
2:E:254:ASN:C	2:E:254:ASN:HD22	2.19	0.51
3:F:77:LEU:HD22	3:F:81:TYR:CE1	2.46	0.51
2:E:246:GLN:HA	2:E:246:GLN:OE1	2.11	0.51
1:A:124:LEU:HD21	2:B:4:ILE:CD1	2.40	0.51
1:A:146:THR:HB	1:A:147:PRO:HD3	1.92	0.50
1:D:170:ASN:HD22	1:D:208:PRO:CG	2.10	0.50
2:E:153:THR:N	2:E:154:PRO:HD2	2.26	0.50
1:A:220:GLY:HA3	4:A:802:SF4:S1	2.51	0.50
1:D:209:ALA:HB2	3:F:77:LEU:HD12	1.94	0.50
1:A:103:ALA:HB1	2:B:23:PRO:HB3	1.93	0.50
1:A:363:GLU:O	1:A:367:GLU:HG3	2.11	0.50
1:D:50:LEU:C	1:D:50:LEU:HD13	2.36	0.50
1:D:375:ASN:HA	3:F:65:MET:HE3	1.93	0.50
1:A:196:GLN:HE22	1:A:354:PRO:CA	2.25	0.50
1:D:46:CYS:HB3	1:D:47:PRO:HD3	1.93	0.50
3:C:11:PHE:CE2	3:C:29:TRP:HB2	2.47	0.50
1:D:221:CYS:SG	1:D:307:MET:HE2	2.52	0.50
2:E:37:ASN:HD21	2:E:58:ASN:ND2	2.02	0.50
1:A:136:THR:OG1	6:A:582:SRM:HBB1	2.12	0.49
1:A:36:LYS:HB2	7:A:506:HOH:O	2.10	0.49
1:A:205:LEU:HD23	1:A:205:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:370:TYR:CE1	1:D:340:GLN:HG2	2.47	0.49
2:E:207:HIS:HD2	2:E:279:ASP:OD1	1.94	0.49
2:B:9:ASN:C	2:B:9:ASN:HD22	2.20	0.49
2:E:382:VAL:CG2	2:E:384:PHE:HD1	2.26	0.49
2:B:223:GLU:OE1	2:B:226:LEU:HD11	2.12	0.49
1:D:83:ARG:H	1:D:98:HIS:CD2	2.31	0.49
1:A:131:ASN:HB2	1:A:140:VAL:CB	2.37	0.49
2:B:52:LEU:HD21	6:B:581:SRM:CCA	2.43	0.49
1:A:102:LEU:HB3	1:A:139:ILE:HB	1.93	0.49
1:A:17:TRP:CD2	1:A:18:PRO:HD2	2.47	0.48
2:B:217:ASN:ND2	1:D:437:ARG:NH1	2.60	0.48
1:A:205:LEU:HD23	1:A:205:LEU:C	2.38	0.48
2:B:289:ILE:HG22	6:B:581:SRM:O2C	2.12	0.48
3:C:78:LYS:O	3:C:82:GLU:HG3	2.12	0.48
1:D:3:LYS:HD3	1:D:3:LYS:N	2.28	0.48
2:B:382:VAL:HG21	2:B:384:PHE:CD2	2.47	0.48
1:D:104:GLN:NE2	1:D:104:GLN:N	2.55	0.48
6:A:582:SRM:HMA2	3:C:104[B]:CYS:HA	1.96	0.48
2:B:192:MET:HE3	2:B:196:VAL:HG12	1.95	0.48
3:F:50:ILE:O	3:F:54:GLN:HG3	2.14	0.48
1:D:135:SER:HB2	6:D:584:SRM:HHC	1.96	0.48
1:A:170:ASN:HD22	1:A:208:PRO:CG	2.27	0.48
1:A:410:ASN:C	1:A:410:ASN:ND2	2.72	0.48
2:B:31:PRO:HG2	2:B:34:ILE:HG12	1.95	0.47
2:B:179:PRO:HG2	2:B:331:ALA:HB3	1.95	0.47
1:D:225:CYS:SG	6:E:583:SRM:NC	2.87	0.47
1:A:167:SER:C	3:C:105:VAL:HG11	2.39	0.47
2:E:293:ILE:HG22	2:E:294:LYS:CD	2.44	0.47
1:A:312:THR:C	1:A:314:PRO:HD3	2.39	0.47
2:E:293:ILE:HG22	2:E:294:LYS:HD3	1.96	0.47
1:D:60:GLU:OE1	1:D:64:HIS:CE1	2.68	0.47
3:C:37:GLU:OE1	3:C:91:GLY:HA2	2.15	0.47
1:D:20:PHE:O	1:D:24:ILE:HG13	2.15	0.47
2:E:138:SER:HB2	2:E:172:GLU:O	2.15	0.47
2:B:220:GLU:H	2:B:220:GLU:HG2	1.57	0.47
1:D:89:GLU:CD	1:D:89:GLU:N	2.71	0.47
1:D:102:LEU:HB3	1:D:139:ILE:HB	1.95	0.47
6:D:584:SRM:HHB	6:D:584:SRM:HBA1	1.96	0.47
3:F:46:HIS:O	3:F:50:ILE:HG12	2.14	0.47
1:D:111:THR:HG23	2:E:29:PHE:HD2	1.80	0.47
3:F:39:ILE:HD12	3:F:95:MET:HE1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ILE:CD1	2:E:214:ASP:HB2	2.45	0.47
3:C:13:VAL:HG12	3:C:14:ASP:N	2.30	0.46
1:D:237:ILE:HD12	1:D:328:LEU:HD13	1.96	0.46
2:B:223:GLU:O	2:B:224:ILE:C	2.57	0.46
1:D:8:MET:HE2	2:E:311:PRO:CD	2.34	0.46
1:D:245:LYS:NZ	1:D:321:ASP:OD1	2.48	0.46
2:E:200:ASP:O	2:E:285:VAL:HA	2.15	0.46
2:E:52:LEU:HD21	6:E:583:SRM:O2A	2.15	0.46
1:A:42:ILE:HD11	1:A:126:GLY:O	2.15	0.46
1:D:262:ASN:HD21	2:E:292:ARG:HH12	1.64	0.46
1:A:28:CYS:SG	1:A:47:PRO:HB2	2.56	0.46
2:B:107:ASN:HD21	2:B:110:THR:H	1.61	0.46
1:D:317:LEU:N	1:D:317:LEU:CD2	2.77	0.46
1:A:70:ILE:H	3:C:16:ASP:CG	2.24	0.46
1:D:217:LYS:HB2	1:D:232:SER:HB3	1.98	0.46
2:E:270:ALA:O	2:E:271:LEU:HD12	2.15	0.46
1:A:410:ASN:HD22	1:A:410:ASN:C	2.24	0.45
1:D:67:HIS:CG	2:E:269:PRO:HB3	2.51	0.45
2:E:216:GLU:HA	2:E:243:VAL:HG21	1.99	0.45
1:A:202:GLN:OE1	1:A:206:HIS:HE1	2.00	0.45
2:B:300:LYS:HE2	1:D:406:GLU:OE1	2.16	0.45
1:D:335:VAL:HA	1:D:336:LEU:HA	1.69	0.45
1:A:86:ASP:OD2	1:D:435:HIS:HD2	1.99	0.45
2:B:108:GLU:O	2:B:112:LYS:HG3	2.17	0.45
2:B:148:TRP:CE3	2:B:157:ASP:HB2	2.51	0.45
3:C:49:ILE:HG23	3:C:69:LEU:HD11	1.98	0.45
1:D:434:ARG:HH11	1:D:434:ARG:CB	2.29	0.45
1:A:225:CYS:SG	6:B:581:SRM:NC	2.90	0.45
1:A:406:GLU:HG2	2:E:300:LYS:HE2	1.99	0.45
1:A:121:VAL:HG13	1:A:155:GLU:OE1	2.17	0.44
2:B:153:THR:N	2:B:154:PRO:HD2	2.31	0.44
2:B:382:VAL:CG2	2:B:384:PHE:CD2	2.95	0.44
1:D:279:GLU:O	1:D:308:HIS:HE1	1.99	0.44
6:D:584:SRM:HMA2	3:F:104:CYS:SG	2.57	0.44
1:A:246:ILE:HG12	1:A:317:LEU:HD23	1.97	0.44
2:B:138:SER:HB2	2:B:172:GLU:O	2.17	0.44
6:B:581:SRM:HBA1	6:B:581:SRM:HMA3	1.99	0.44
1:A:430:ASP:O	1:A:433:LYS:HB3	2.17	0.44
6:D:584:SRM:C1A	3:F:104:CYS:SG	3.00	0.44
2:E:200:ASP:HB3	2:E:337:ILE:HD12	1.99	0.44
1:D:13:GLU:HB3	2:E:125:ALA:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLU:OE1	1:D:435:HIS:HE1	2.00	0.44
1:A:427:ASP:OD1	1:A:429:SER:HB3	2.18	0.44
2:B:259:MET:SD	2:B:261:CYS:HB3	2.57	0.44
2:E:332:ARG:O	2:E:335:GLU:HB2	2.17	0.44
1:A:340:GLN:OE1	1:A:384:LYS:HD2	2.18	0.44
1:D:219:ASP:CG	1:D:224:GLY:HA2	2.43	0.44
3:F:77:LEU:HD22	3:F:81:TYR:HE1	1.82	0.44
1:A:122:TRP:O	1:A:126:GLY:N	2.49	0.44
2:B:152:HIS:C	2:B:154:PRO:HD2	2.43	0.44
6:D:584:SRM:O1A	2:E:150:TYR:CD2	2.65	0.44
2:E:29:PHE:O	2:E:92:HIS:HD2	2.00	0.44
3:F:49:ILE:HD12	3:F:84:PHE:HE1	1.80	0.44
1:D:88:PRO:HG3	7:D:504:HOH:O	2.18	0.44
1:A:284:CYS:HA	1:A:285:PRO:HD3	1.89	0.43
1:A:406:GLU:O	2:E:372:THR:HB	2.18	0.43
2:B:125:ALA:HB3	7:B:407:HOH:O	2.18	0.43
3:C:13:VAL:HG11	3:C:17:GLY:HA2	1.99	0.43
1:D:31:ARG:HD3	1:D:47:PRO:HG2	2.01	0.43
1:D:219:ASP:OD1	1:D:226:VAL:HG12	2.17	0.43
1:A:219:ASP:CG	1:A:226:VAL:HG12	2.42	0.43
1:D:87:GLN:N	1:D:88:PRO:HD3	2.33	0.43
2:E:190:ILE:C	2:E:192:MET:N	2.73	0.43
1:A:209:ALA:HB2	3:C:77:LEU:CD1	2.49	0.43
3:C:50:ILE:HG23	3:C:96:ALA:HA	2.00	0.43
3:F:6:PHE:CD2	3:F:32:TYR:HB2	2.53	0.43
1:A:113:GLU:HG3	7:A:484:HOH:O	2.18	0.43
1:A:225:CYS:HA	6:B:581:SRM:C1C	2.49	0.43
2:B:218:LEU:C	2:B:218:LEU:HD23	2.42	0.43
2:B:259:MET:C	2:B:260:TYR:CG	2.94	0.43
2:B:366:ARG:CB	2:B:368:PRO:HD2	2.49	0.43
1:D:130:THR:HB	1:D:140:VAL:O	2.18	0.43
1:D:181:SER:O	2:E:34:ILE:HG23	2.19	0.43
1:A:106:ALA:O	1:A:107:ALA:HB3	2.19	0.43
1:A:209:ALA:HB2	3:C:77:LEU:HD12	2.00	0.43
6:A:582:SRM:O1A	2:B:150:TYR:CD2	2.71	0.43
1:D:34:ASN:HD21	1:D:38:LEU:N	2.15	0.43
2:E:379:PHE:CD1	2:E:379:PHE:C	2.97	0.43
5:A:6573:SO3:S	3:C:100:LYS:NZ	2.91	0.43
1:D:125:ARG:HE	1:D:155:GLU:CD	2.26	0.43
2:E:259:MET:C	2:E:260:TYR:CG	2.96	0.43
2:B:192:MET:HE2	2:B:197:HIS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:LYS:HB2	1:D:4:HIS:H	1.58	0.42
1:D:252:LYS:HE2	7:D:632:HOH:O	2.19	0.42
1:A:202:GLN:OE1	1:A:206:HIS:CE1	2.73	0.42
6:A:582:SRM:HBA1	6:A:582:SRM:HHB	2.01	0.42
2:B:171:GLU:HA	2:B:171:GLU:OE1	2.19	0.42
1:D:70:ILE:HG13	3:F:100:LYS:HG3	2.01	0.42
2:B:288:LYS:NZ	7:B:402:HOH:O	2.51	0.42
2:E:12:LYS:HD3	2:E:15:GLU:OE2	2.20	0.42
6:E:583:SRM:HBA1	6:E:583:SRM:HMA3	2.02	0.42
1:A:9:LEU:HD21	1:A:54:LEU:HD13	2.02	0.42
2:B:52:LEU:CD1	2:B:135:THR:HG21	2.48	0.42
2:B:259:MET:C	2:B:260:TYR:CD1	2.97	0.42
2:E:350:TYR:HB3	2:E:384:PHE:CZ	2.54	0.42
2:E:37:ASN:ND2	2:E:58:ASN:HD21	2.06	0.42
6:A:582:SRM:C4C	2:B:193:CYS:HA	2.49	0.42
2:E:264:CYS:SG	2:E:271:LEU:HD23	2.60	0.42
1:D:161:ASN:HD22	2:E:21:ILE:HD12	1.84	0.42
2:E:75:THR:O	2:E:79:ARG:HG3	2.19	0.42
2:B:115:VAL:CG1	2:B:119:LYS:HE3	2.50	0.42
1:A:188:TYR:OH	1:A:218:PHE:HB3	2.20	0.41
1:A:308:HIS:HD2	2:B:292:ARG:NE	2.02	0.41
1:A:419:GLU:OE2	2:E:360:HIS:HE1	2.04	0.41
1:D:168:GLY:CA	3:F:105:VAL:HG22	2.50	0.41
1:A:400:VAL:HG22	1:A:403:HIS:CE1	2.54	0.41
2:B:254:ASN:C	2:B:254:ASN:HD22	2.27	0.41
3:F:52:PHE:CD2	3:F:69:LEU:HD12	2.54	0.41
3:F:90:LYS:HE2	7:F:642:HOH:O	2.19	0.41
1:A:99:THR:HG23	1:A:140:VAL:HG13	2.01	0.41
1:A:428:ILE:HD13	2:E:214:ASP:HB2	2.02	0.41
2:B:9:ASN:ND2	2:B:9:ASN:C	2.78	0.41
2:B:117:ASP:O	2:B:120:THR:OG1	2.30	0.41
2:E:142:ILE:O	2:E:144:HIS:HD2	2.03	0.41
2:E:147:GLY:N	2:E:188:CYS:SG	2.91	0.41
1:A:42:ILE:HG22	1:A:145:GLN:HG3	2.01	0.41
1:A:148:GLN:O	1:A:152:ILE:HG13	2.21	0.41
1:D:17:TRP:O	2:E:163:LYS:NZ	2.51	0.41
1:D:18:PRO:HD3	2:E:131:PRO:HG3	2.01	0.41
2:E:155:ALA:O	2:E:279:ASP:HB3	2.21	0.41
2:E:382:VAL:HG21	2:E:384:PHE:HD1	1.86	0.41
2:E:218:LEU:HD23	2:E:218:LEU:C	2.46	0.41
2:B:144:HIS:CG	2:B:162:VAL:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:347:GLU:HG2	7:E:392:HOH:O	2.21	0.41
2:B:346:TRP:CZ2	1:D:407:PRO:HD2	2.55	0.41
1:A:83:ARG:H	1:A:98:HIS:CD2	2.33	0.41
1:A:346:ILE:HG21	1:A:349:ILE:HB	2.02	0.41
3:C:19:LEU:HD21	3:C:29:TRP:CE3	2.56	0.41
1:D:33:LYS:HE3	1:D:33:LYS:HB3	1.87	0.41
1:D:42:ILE:CD1	1:D:126:GLY:C	2.93	0.41
1:D:225:CYS:HA	6:E:583:SRM:C1C	2.51	0.41
1:D:253:ALA:HB3	1:D:259:PHE:CD2	2.56	0.41
3:F:103:GLY:O	3:F:105:VAL:N	2.54	0.41
1:A:168:GLY:CA	3:C:105:VAL:HB	2.45	0.41
1:A:193:MET:HA	1:A:355:PHE:CE1	2.56	0.41
2:B:217:ASN:O	2:B:221:LEU:HD22	2.20	0.41
2:E:62:VAL:O	2:E:62:VAL:HG13	2.20	0.41
2:B:190:ILE:C	2:B:192:MET:N	2.78	0.40
1:D:333:ALA:HB1	1:D:334:PRO:HD2	2.03	0.40
1:A:45:GLU:HA	1:A:48:ASP:OD2	2.21	0.40
1:A:171:LEU:O	1:A:205:LEU:HG	2.21	0.40
1:D:13:GLU:HB3	2:E:125:ALA:HB1	2.03	0.40
1:D:81:ILE:O	2:E:150:TYR:OH	2.33	0.40
1:D:226:VAL:HG22	1:D:226:VAL:O	2.22	0.40
1:A:248:GLN:HA	1:A:248:GLN:NE2	2.36	0.40
2:B:377:THR:HG21	1:D:237:ILE:HG21	2.03	0.40
2:B:314:PRO:O	2:B:318:LYS:HG3	2.21	0.40
1:D:331:ALA:HA	1:D:340:GLN:O	2.22	0.40
1:D:340:GLN:CD	1:D:384:LYS:HE3	2.47	0.40
2:E:333:LYS:O	2:E:334:TYR:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/435 (100%)	412 (95%)	21 (5%)	0	100	100
1	D	433/435 (100%)	417 (96%)	15 (4%)	1 (0%)	43	37
2	B	384/385 (100%)	370 (96%)	11 (3%)	3 (1%)	16	9
2	E	383/385 (100%)	364 (95%)	17 (4%)	2 (0%)	24	16
3	C	103/104 (99%)	100 (97%)	3 (3%)	0	100	100
3	F	102/104 (98%)	98 (96%)	3 (3%)	1 (1%)	12	6
All	All	1838/1848 (100%)	1761 (96%)	70 (4%)	7 (0%)	30	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	141	ASN
3	F	104	CYS
2	B	293	ILE
1	D	133	HIS
2	E	153	THR
2	E	293	ILE
2	B	153	THR

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	364/364 (100%)	353 (97%)	11 (3%)	36	32
1	D	364/364 (100%)	350 (96%)	14 (4%)	29	24
2	B	325/324 (100%)	320 (98%)	5 (2%)	57	58
2	E	324/324 (100%)	317 (98%)	7 (2%)	45	44
3	C	81/80 (101%)	79 (98%)	2 (2%)	42	39
3	F	80/80 (100%)	77 (96%)	3 (4%)	29	24
All	All	1538/1536 (100%)	1496 (97%)	42 (3%)	39	36

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	54	LEU
1	A	56	LEU
1	A	104	GLN
1	A	192	LEU
1	A	335	VAL
1	A	341	MET
1	A	391	LEU
1	A	402	GLN
1	A	406	GLU
1	A	410	ASN
2	B	220	GLU
2	B	221	LEU
2	B	259	MET
2	B	260	TYR
2	B	329	GLU
3	C	12	GLU
3	C	77	LEU
1	D	3	LYS
1	D	4	HIS
1	D	33	LYS
1	D	45	GLU
1	D	54	LEU
1	D	56	LEU
1	D	89	GLU
1	D	104	GLN
1	D	317	LEU
1	D	336	LEU
1	D	345	LEU
1	D	402	GLN
1	D	418	GLU
1	D	432	ARG
2	E	188	CYS
2	E	189	CYS
2	E	203	LEU
2	E	246	GLN
2	E	259	MET
2	E	260	TYR
2	E	273	LEU
3	F	12	GLU
3	F	77	LEU
3	F	105	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62)

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	170	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	90	ASN
2	B	99	ASN
2	B	107	ASN
2	B	144	HIS
2	B	191	ASN
2	B	207	HIS
2	B	215	HIS
2	B	217	ASN
2	B	254	ASN
2	B	263	ASN
3	C	20	ASN
3	C	60	ASN
1	D	30	ASN
1	D	34	ASN
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

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Mol	Chain	Res	Type
1	D	262	ASN
1	D	308	HIS
1	D	311	ASN
1	D	402	GLN
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	217	ASN
2	E	244	ASN
2	E	254	ASN
2	E	263	ASN
2	E	360	HIS
3	F	47	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](#)

16 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	SF4	D	806	1	0,12,12	-	-	-		
4	SF4	E	807	2	0,9,12	-	-	-		
4	SF4	D	805	1	0,12,12	-	-	-		
4	SF4	E	808	2	0,12,12	-	-	-		
5	SO3	D	6576	6	1,3,3	1.17	0	0,3,3	-	-
6	SRM	A	582	5,2	68,70,70	2.04	11 (16%)	86,112,112	1.73	19 (22%)
4	SF4	A	801	1	0,12,12	-	-	-		
6	SRM	E	583	-	54,66,70	1.93	9 (16%)	56,98,112	1.82	12 (21%)
6	SRM	B	581	-	54,66,70	1.98	9 (16%)	56,98,112	1.80	13 (23%)
4	SF4	A	802	1	0,12,12	-	-	-		
4	SF4	B	803	2	0,9,12	-	-	-		
5	SO3	A	6573	-	1,3,3	0.48	0	0,3,3	-	-
5	SO3	A	6574	6	1,3,3	1.10	0	0,3,3	-	-
4	SF4	B	804	2	0,12,12	-	-	-		
6	SRM	D	584	5,2	68,70,70	2.10	11 (16%)	86,112,112	1.79	18 (20%)
5	SO3	D	6575	-	1,3,3	0.46	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
4	SF4	D	806	1	-	-	0/6/5/5
4	SF4	E	807	2	-	-	0/3/3/5
4	SF4	D	805	1	-	-	0/6/5/5
6	SRM	E	583	-	-	9/38/94/126	0/4/4/8
6	SRM	A	582	5,2	1/1/19/23	13/38/126/126	-
4	SF4	E	808	2	-	-	0/6/5/5
4	SF4	A	801	1	-	-	0/6/5/5
6	SRM	B	581	-	-	11/38/94/126	0/4/4/8
4	SF4	A	802	1	-	-	0/6/5/5
4	SF4	B	803	2	-	-	0/3/2/5
4	SF4	B	804	2	-	-	0/6/5/5
6	SRM	D	584	5,2	1/1/19/23	11/38/126/126	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	584	SRM	C4B-NB	8.22	1.41	1.35
6	A	582	SRM	C4B-NB	7.73	1.40	1.35
6	B	581	SRM	C1D-C2D	6.83	1.47	1.39
6	E	583	SRM	C1D-C2D	6.66	1.46	1.39
6	A	582	SRM	FE-NA	5.52	2.11	1.94
6	D	584	SRM	FE-NB	5.50	2.11	1.94
6	B	581	SRM	C1C-C2C	5.23	1.45	1.39
6	D	584	SRM	FE-NA	5.23	2.11	1.94
6	A	582	SRM	FE-NB	5.05	2.10	1.94
6	E	583	SRM	C1C-C2C	4.97	1.45	1.39
6	D	584	SRM	FE-NC	4.95	2.11	1.95
6	A	582	SRM	FE-NC	4.90	2.11	1.95
6	B	581	SRM	CMB-C2B	4.79	1.62	1.54
6	A	582	SRM	CMB-C2B	4.78	1.62	1.54
6	D	584	SRM	CMB-C2B	4.68	1.62	1.54
6	D	584	SRM	C3B-C4B	4.65	1.61	1.51
6	E	583	SRM	C4C-C3C	4.61	1.44	1.39
6	A	582	SRM	FE-ND	4.44	2.09	1.95
6	A	582	SRM	C3B-C4B	4.43	1.60	1.51
6	E	583	SRM	CMB-C2B	4.42	1.61	1.54
6	D	584	SRM	FE-ND	4.38	2.09	1.95
6	B	581	SRM	C4C-C3C	4.05	1.44	1.39
6	B	581	SRM	C4D-C3D	3.28	1.43	1.39
6	E	583	SRM	C4D-C3D	2.94	1.42	1.39
6	B	581	SRM	C4B-C3B	2.83	1.57	1.51
6	E	583	SRM	C2A-C1A	2.74	1.56	1.52
6	E	583	SRM	CAB-C3B	2.64	1.58	1.54
6	E	583	SRM	C4B-C3B	2.53	1.56	1.51
6	B	581	SRM	CAB-C3B	2.45	1.57	1.54
6	D	584	SRM	C4A-NA	2.43	1.37	1.35
6	D	584	SRM	CDD-C3D	2.40	1.54	1.51
6	B	581	SRM	C2A-C1A	2.35	1.56	1.52
6	B	581	SRM	CMA-C2A	2.26	1.58	1.54
6	E	583	SRM	CMA-C2A	2.22	1.58	1.54
6	A	582	SRM	CAA-C3A	-2.10	1.49	1.54
6	D	584	SRM	CMA-C2A	2.06	1.58	1.54
6	A	582	SRM	CMA-C2A	2.04	1.57	1.54
6	A	582	SRM	CDD-C3D	2.02	1.54	1.51
6	A	582	SRM	CBB-CCB	2.01	1.55	1.50
6	D	584	SRM	C4C-NC	-2.01	1.35	1.39

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	584	SRM	C2A-C1A-CHA	6.41	129.30	123.54
6	D	584	SRM	CAB-C3B-C4B	5.72	121.17	111.19
6	A	582	SRM	C2A-C1A-CHA	5.35	128.35	123.54
6	A	582	SRM	CAB-C3B-C4B	5.35	120.53	111.19
6	E	583	SRM	CBD-CAD-C2D	-5.32	103.59	112.54
6	B	581	SRM	CBD-CAD-C2D	-5.14	103.90	112.54
6	D	584	SRM	C2C-C1C-NC	-4.37	106.11	110.32
6	B	581	SRM	C2C-C1C-NC	-4.28	106.34	109.43
6	E	583	SRM	CMA-C2A-C3A	4.23	119.73	112.07
6	E	583	SRM	C2C-C1C-NC	-4.20	106.40	109.43
6	A	582	SRM	C2C-C1C-NC	-4.20	106.27	110.32
6	B	581	SRM	C2C-CDC-CEC	4.19	119.05	114.20
6	B	581	SRM	CMA-C2A-C3A	4.12	119.52	112.07
6	B	581	SRM	CMB-C2B-C3B	3.56	118.52	112.07
6	E	583	SRM	CDA-C2A-C1A	3.48	116.07	110.16
6	D	584	SRM	C1A-NA-C4A	3.41	109.56	105.34
6	E	583	SRM	CMB-C2B-C3B	3.35	118.14	112.07
6	E	583	SRM	CDB-C2B-C1B	-3.34	104.49	110.16
6	D	584	SRM	CMB-C2B-C3B	3.31	118.16	112.05
6	A	582	SRM	C1A-NA-C4A	3.31	109.42	105.34
6	E	583	SRM	C2C-CDC-CEC	3.27	117.98	114.20
6	A	582	SRM	CMB-C2B-C3B	3.26	118.07	112.05
6	B	581	SRM	CAB-C3B-C2B	-3.16	105.49	114.19
6	E	583	SRM	CAB-C3B-C2B	-3.13	105.57	114.19
6	A	582	SRM	C4B-NB-C1B	3.07	109.13	105.34
6	D	584	SRM	CAB-C3B-C2B	-3.06	105.77	114.19
6	D	584	SRM	C4D-CHA-C1A	3.06	131.50	125.87
6	A	582	SRM	CAB-C3B-C2B	-2.91	106.18	114.19
6	D	584	SRM	C4B-NB-C1B	2.90	108.93	105.34
6	D	584	SRM	C4A-CHB-C1B	2.87	130.05	125.84
6	A	582	SRM	C4A-CHB-C1B	2.83	130.00	125.84
6	A	582	SRM	C4D-CHA-C1A	2.74	130.93	125.87
6	B	581	SRM	CDA-C2A-C1A	2.71	114.77	110.16
6	B	581	SRM	CDB-C2B-C1B	-2.69	105.59	110.16
6	A	582	SRM	CMA-C2A-C3A	2.48	116.63	112.05
6	D	584	SRM	C3D-C4D-ND	-2.43	107.45	110.15
6	D	584	SRM	CMA-C2A-C3A	2.38	116.44	112.05
6	E	583	SRM	CBC-CAC-C3C	2.36	116.51	112.54
6	B	581	SRM	CMA-C2A-C1A	-2.29	104.39	109.77
6	A	582	SRM	CMA-C2A-CDA	2.28	114.61	110.74
6	A	582	SRM	C3D-C4D-ND	-2.28	107.63	110.15
6	D	584	SRM	CDA-C2A-C1A	2.25	114.07	107.11
6	A	582	SRM	C4D-C3D-C2D	2.24	109.17	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	584	SRM	CAA-C3A-C4A	2.18	114.99	111.19
6	B	581	SRM	CAA-CBA-CCA	2.18	118.31	112.49
6	A	582	SRM	C4C-NC-C1C	2.18	109.37	105.82
6	B	581	SRM	O2D-CCD-CBD	2.17	120.84	114.00
6	A	582	SRM	C1C-C2C-C3C	2.16	109.25	106.84
6	B	581	SRM	CBC-CAC-C3C	2.15	116.15	112.54
6	D	584	SRM	C1C-C2C-C3C	2.14	109.23	106.84
6	D	584	SRM	C4D-ND-C1D	2.14	109.31	105.82
6	E	583	SRM	O2D-CCD-CBD	2.13	120.74	114.00
6	D	584	SRM	C4C-NC-C1C	2.13	109.29	105.82
6	D	584	SRM	C1D-C2D-C3D	-2.13	104.58	106.81
6	A	582	SRM	O2B-CCB-CBB	2.10	120.64	114.00
6	E	583	SRM	CMA-C2A-C1A	-2.10	104.82	109.77
6	E	583	SRM	O3B-CEB-CDB	-2.10	117.00	122.95
6	B	581	SRM	O3B-CEB-CDB	-2.08	117.05	122.95
6	D	584	SRM	C4D-C3D-C2D	2.05	108.96	106.81
6	A	582	SRM	C1D-C2D-C3D	-2.03	104.69	106.81
6	A	582	SRM	C4D-ND-C1D	2.01	109.09	105.82
6	A	582	SRM	CAA-C3A-C4A	2.00	114.68	111.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	582	SRM	NC
6	D	584	SRM	NC

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	582	SRM	C1A-C2A-CDA-CEA
6	A	582	SRM	CMA-C2A-CDA-CEA
6	A	582	SRM	C3A-C2A-CDA-CEA
6	D	584	SRM	C1A-C2A-CDA-CEA
6	D	584	SRM	C3A-C2A-CDA-CEA
6	E	583	SRM	C3C-CAC-CBC-CCC
6	A	582	SRM	C4A-C3A-CAA-CBA
6	D	584	SRM	C4A-C3A-CAA-CBA
6	B	581	SRM	C3C-CAC-CBC-CCC
6	A	582	SRM	C2A-C3A-CAA-CBA
6	A	582	SRM	C2A-CDA-CEA-O4A
6	D	584	SRM	C3D-CDD-CED-O4D
6	A	582	SRM	C2A-CDA-CEA-O3A

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Mol	Chain	Res	Type	Atoms
6	B	581	SRM	C2B-CDB-CEB-O3B
6	B	581	SRM	C2B-CDB-CEB-O4B
6	E	583	SRM	CAC-CBC-CCC-O2C
6	A	582	SRM	CAC-CBC-CCC-O1C
6	D	584	SRM	CAA-CBA-CCA-O1A
6	D	584	SRM	CAC-CBC-CCC-O1C
6	D	584	SRM	CMA-C2A-CDA-CEA
6	D	584	SRM	CAC-CBC-CCC-O2C
6	A	582	SRM	CAA-CBA-CCA-O2A
6	B	581	SRM	CAA-CBA-CCA-O1A
6	D	584	SRM	CAA-CBA-CCA-O2A
6	E	583	SRM	CAC-CBC-CCC-O1C
6	A	582	SRM	CAB-CBB-CCB-O1B
6	A	582	SRM	CAC-CBC-CCC-O2C
6	E	583	SRM	CAA-CBA-CCA-O1A
6	E	583	SRM	C2B-CDB-CEB-O4B
6	A	582	SRM	CAA-CBA-CCA-O1A
6	B	581	SRM	CAC-CBC-CCC-O2C
6	E	583	SRM	CAA-CBA-CCA-O2A
6	A	582	SRM	CAB-CBB-CCB-O2B
6	E	583	SRM	CAB-CBB-CCB-O2B
6	B	581	SRM	CAA-CBA-CCA-O2A
6	B	581	SRM	CAB-CBB-CCB-O1B
6	E	583	SRM	CAB-CBB-CCB-O1B
6	B	581	SRM	CAC-CBC-CCC-O1C
6	D	584	SRM	C2A-C3A-CAA-CBA
6	B	581	SRM	CAB-CBB-CCB-O2B
6	E	583	SRM	C2B-CDB-CEB-O3B
6	D	584	SRM	C3D-CDD-CED-O3D
6	B	581	SRM	CAD-CBD-CCD-O1D
6	B	581	SRM	CAD-CBD-CCD-O2D

There are no ring outliers.

8 monomers are involved in 40 short contacts:

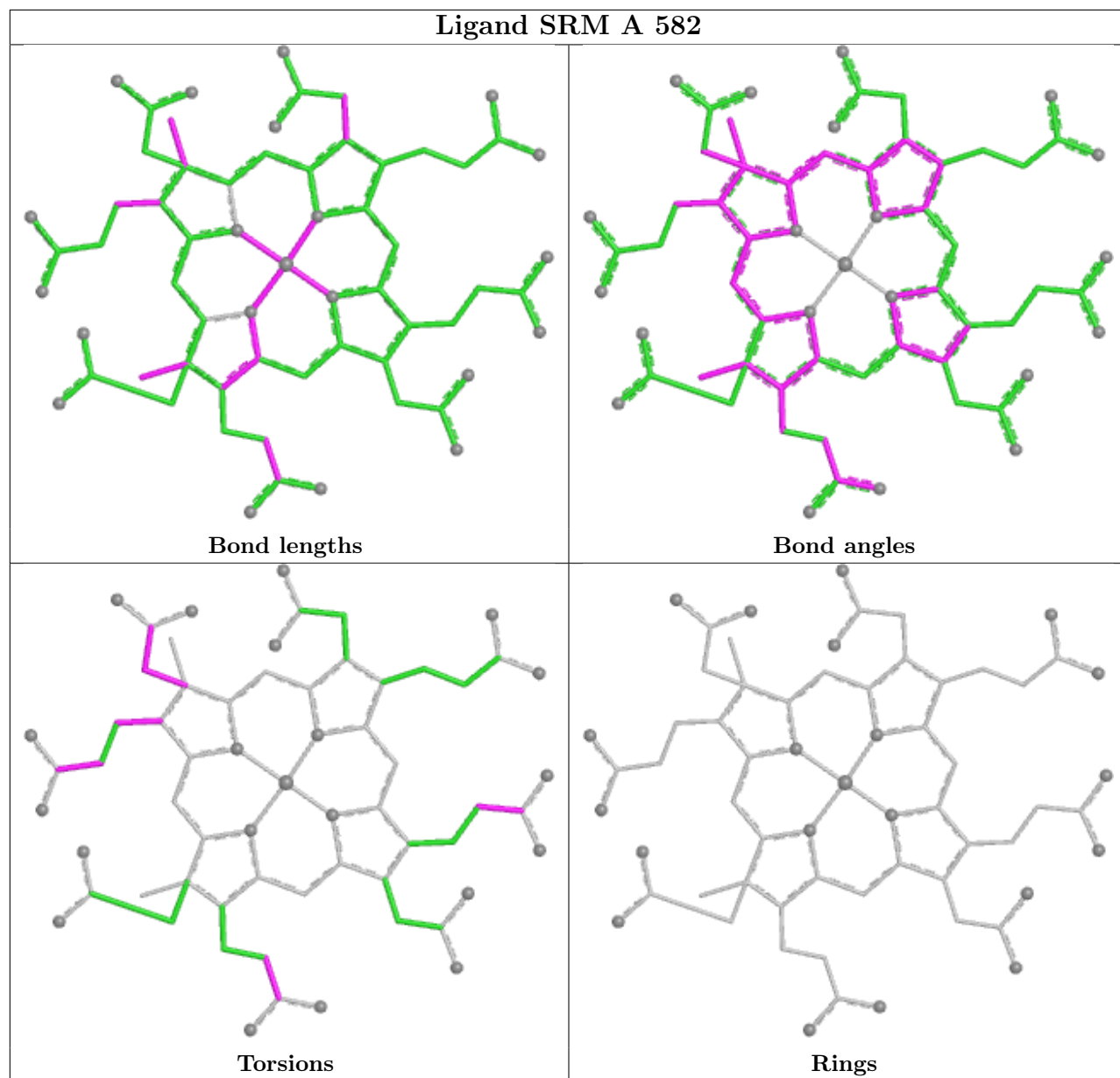
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	806	SF4	1	0
6	A	582	SRM	9	0
6	E	583	SRM	4	0
6	B	581	SRM	6	0
4	A	802	SF4	1	0
4	B	803	SF4	2	0

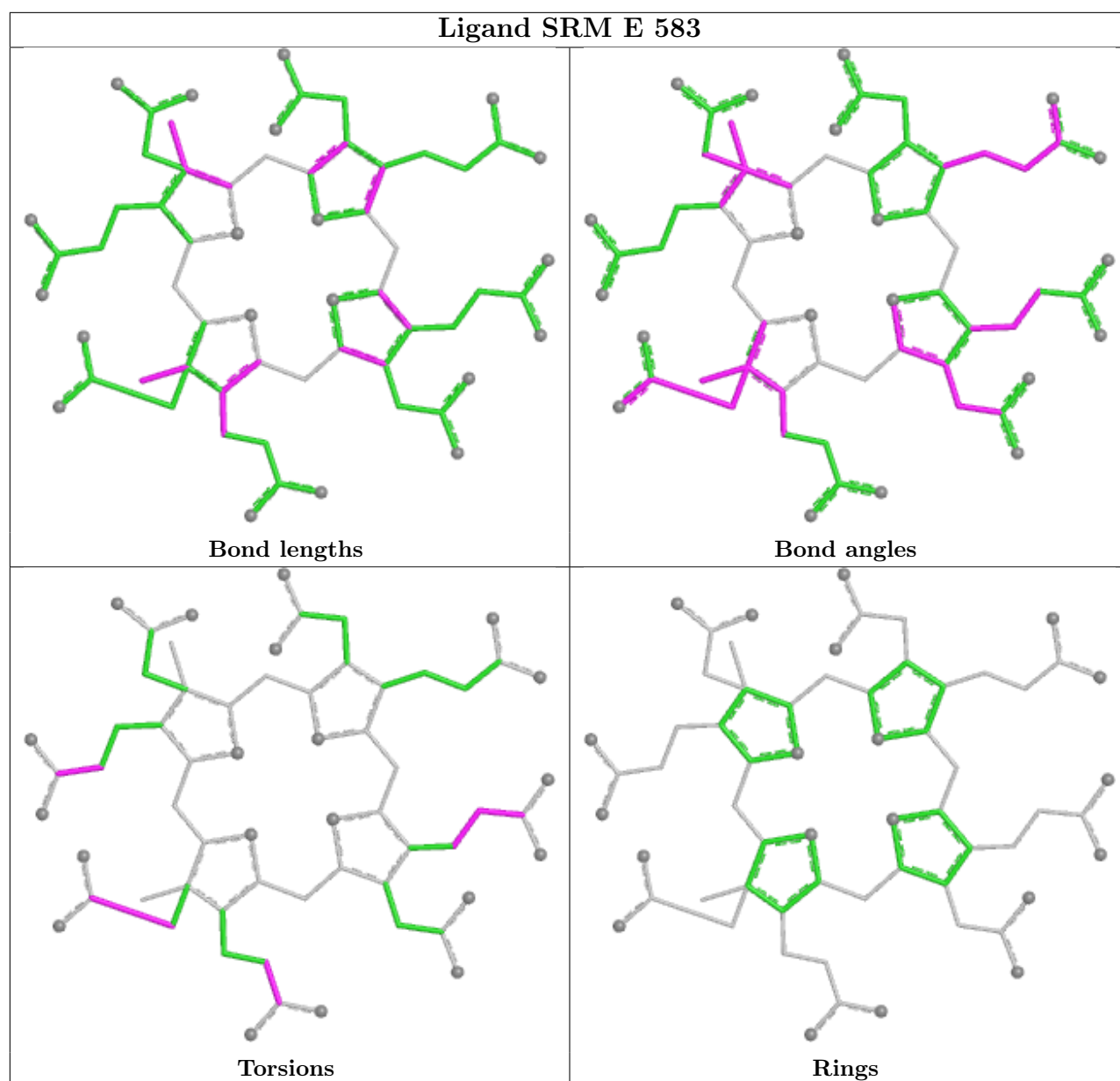
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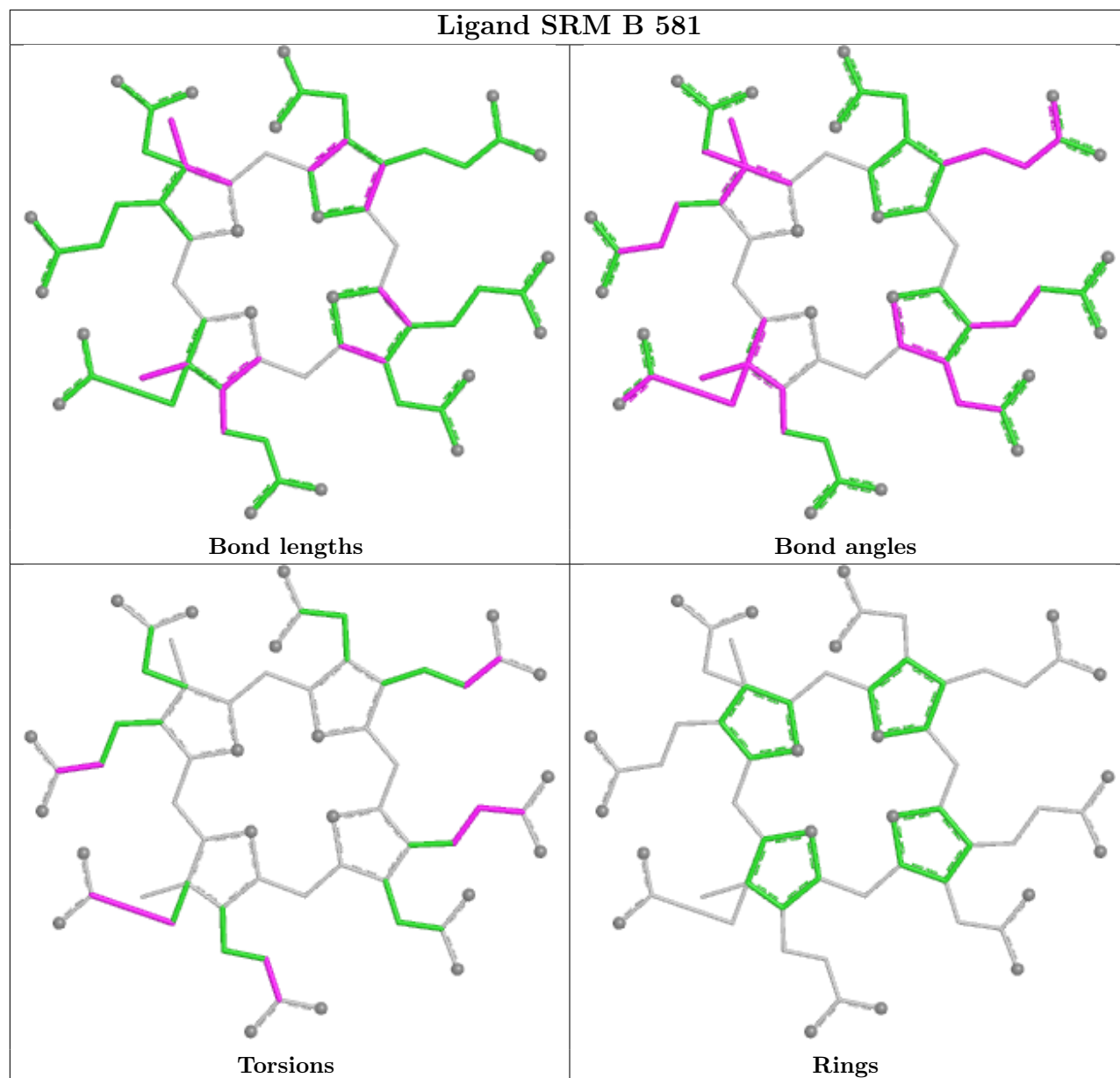
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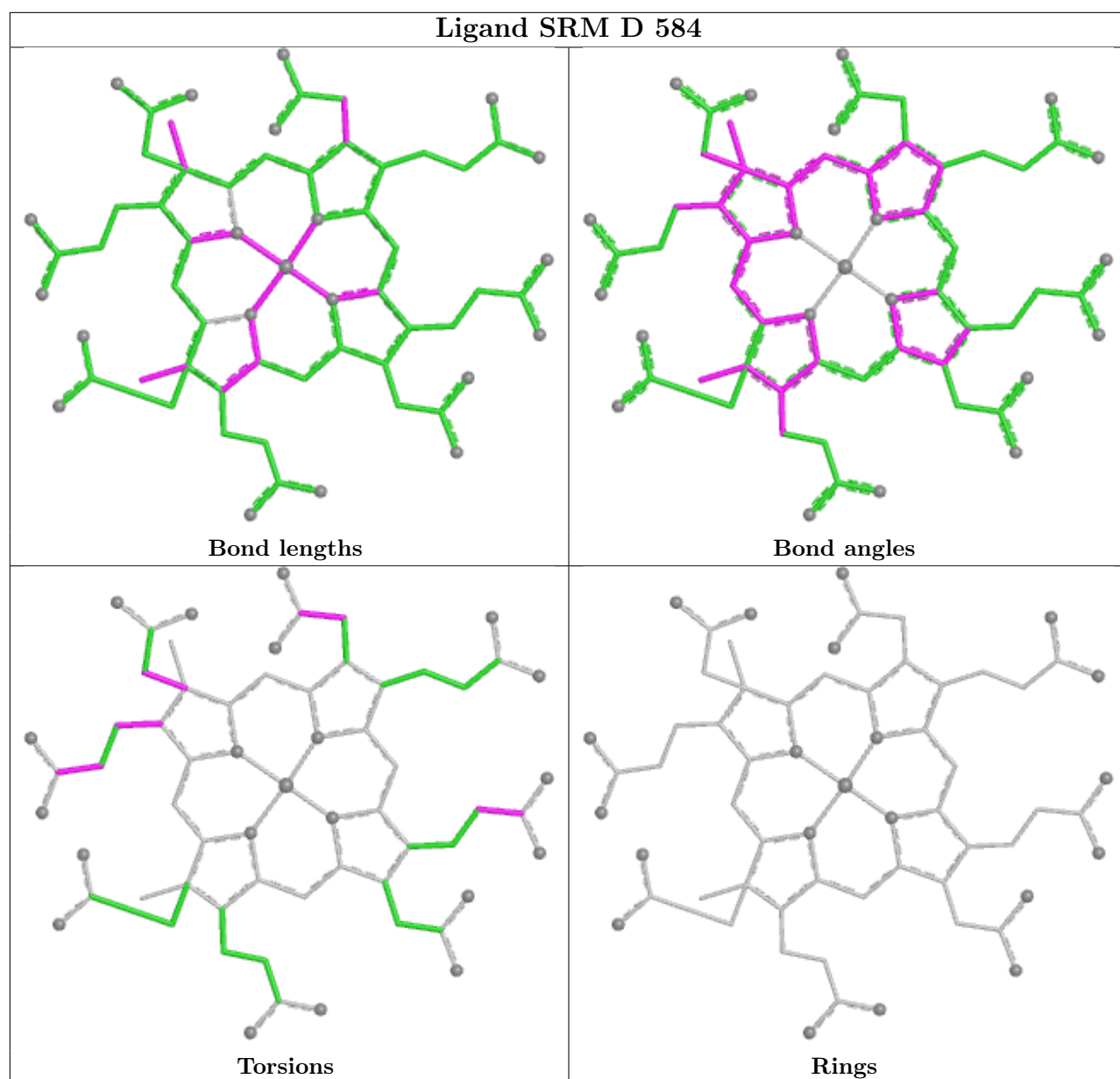
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	6573	SO3	2	0
6	D	584	SRM	15	0

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	435/435 (100%)	0.02	10 (2%) 61 63	8, 15, 32, 60	0
1	D	435/435 (100%)	-0.21	9 (2%) 63 65	6, 12, 26, 60	0
2	B	385/385 (100%)	0.02	10 (2%) 57 59	6, 15, 28, 46	1 (0%)
2	E	385/385 (100%)	-0.05	12 (3%) 51 52	6, 13, 29, 54	0
3	C	104/104 (100%)	1.45	23 (22%) 2 1	23, 35, 59, 74	1 (0%)
3	F	104/104 (100%)	0.69	4 (3%) 44 44	15, 25, 34, 50	0
All	All	1848/1848 (100%)	0.07	68 (3%) 45 45	6, 15, 35, 74	2 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	10	ALA	5.0
3	F	105	VAL	4.9
3	C	105	VAL	4.8
2	B	120	THR	4.5
2	E	386	SER	4.5
3	F	26	CYS	4.1
3	C	2	ALA	4.1
3	C	6	PHE	4.0
3	C	104[A]	CYS	4.0
2	E	244	ASN	3.9
3	C	33	ALA	3.8
1	D	3	LYS	3.7
1	D	4	HIS	3.7
2	B	2	ALA	3.7
3	C	3	VAL	3.6
3	C	4	VAL	3.6
3	F	23	ASP	3.5
1	A	418	GLU	3.3
3	C	34	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	3	PHE	3.1
3	C	7	ALA	3.0
3	C	5	GLU	3.0
2	E	246	GLN	3.0
3	C	8	GLY	3.0
2	B	4	ILE	2.9
1	D	430	ASP	2.9
1	A	4	HIS	2.9
1	D	5	PRO	2.8
1	A	433	LYS	2.8
2	B	245	GLY	2.8
2	E	124	ALA	2.8
2	E	384	PHE	2.7
2	E	220	GLU	2.7
3	C	35	GLY	2.7
1	D	89	GLU	2.6
3	C	11	PHE	2.6
1	D	431	TYR	2.6
3	C	49	ILE	2.6
2	E	245	GLY	2.6
3	C	32	TYR	2.6
2	E	216	GLU	2.6
3	F	21	ALA	2.5
1	D	432	ARG	2.5
2	B	169	LEU	2.3
3	C	23	ASP	2.3
3	C	20	ASN	2.3
1	A	337	ASP	2.3
1	A	429	SER	2.3
3	C	44	ALA	2.3
2	B	243	VAL	2.2
2	B	246	GLN	2.2
1	A	5	PRO	2.2
1	A	427	ASP	2.2
3	C	79	GLN	2.2
2	E	277	THR	2.1
2	E	219	ALA	2.1
3	C	9	SER	2.1
1	D	436	MET	2.1
1	A	371	GLU	2.1
2	E	120	THR	2.1
1	D	437	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	223	GLU	2.1
1	A	171	LEU	2.0
1	A	422	GLY	2.0
2	B	171	GLU	2.0
2	B	384	PHE	2.0
3	C	36	SER	2.0
3	C	26	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

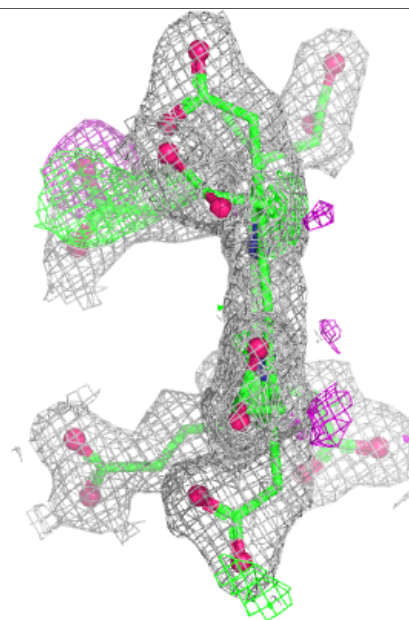
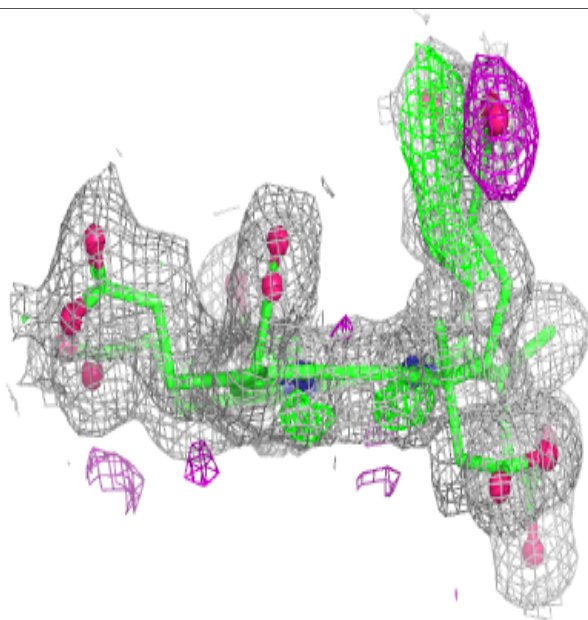
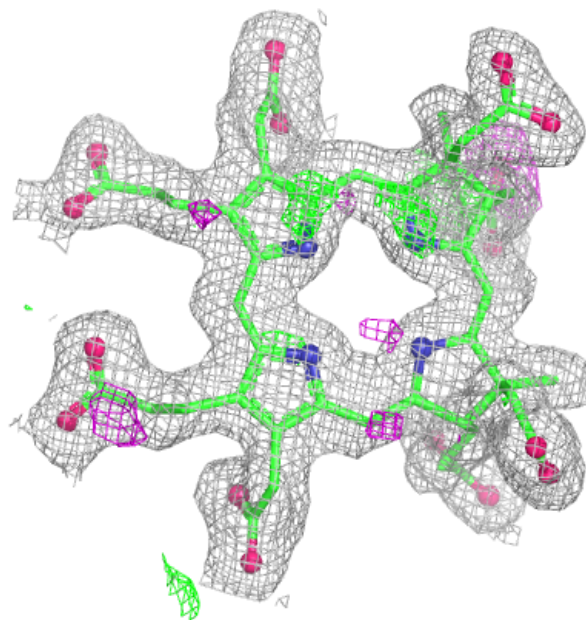
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO3	A	6573	4/4	0.59	0.26	68,68,68,70	0
5	SO3	D	6575	4/4	0.71	0.25	67,67,67,68	0
6	SRM	B	581	62/63	0.86	0.11	11,18,22,33	0
6	SRM	E	583	62/63	0.88	0.10	8,12,16,30	0
6	SRM	A	582	63/63	0.91	0.12	11,16,24,30	0
6	SRM	D	584	63/63	0.93	0.10	7,14,22,30	0
4	SF4	A	801	8/8	0.94	0.07	16,18,19,19	0
4	SF4	E	808	8/8	0.94	0.07	18,19,20,21	0
4	SF4	E	807	7/8	0.95	0.06	14,14,17,18	0
5	SO3	D	6576	4/4	0.95	0.10	21,22,25,25	0
4	SF4	D	806	8/8	0.96	0.06	9,11,12,13	0
4	SF4	B	804	8/8	0.96	0.06	14,15,16,17	0
5	SO3	A	6574	4/4	0.96	0.07	24,25,26,28	0
4	SF4	D	805	8/8	0.97	0.05	12,12,13,14	0
4	SF4	B	803	7/8	0.97	0.05	14,14,16,17	0
4	SF4	A	802	8/8	0.97	0.05	13,14,15,15	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.

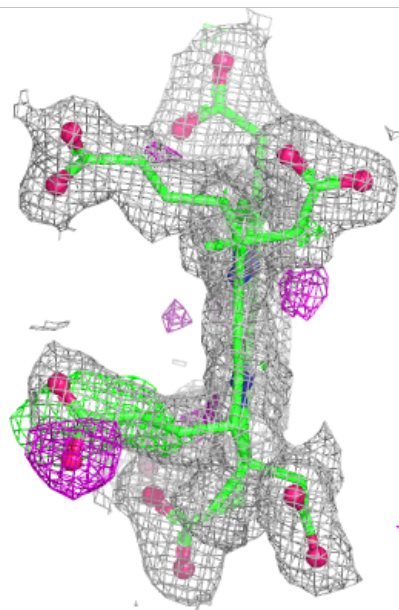
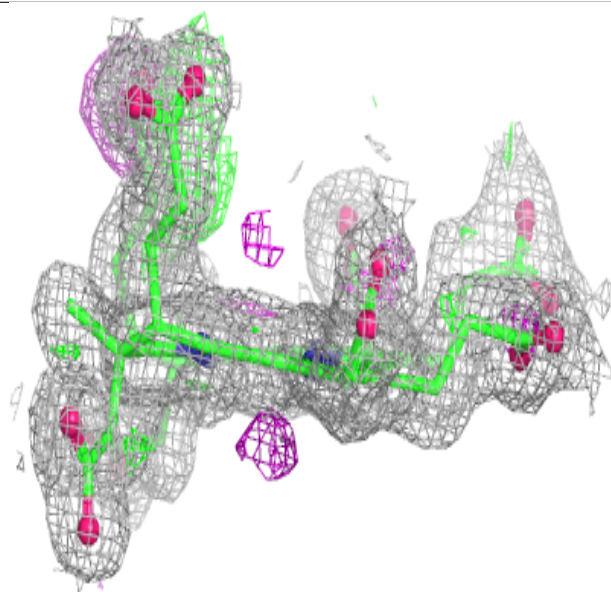
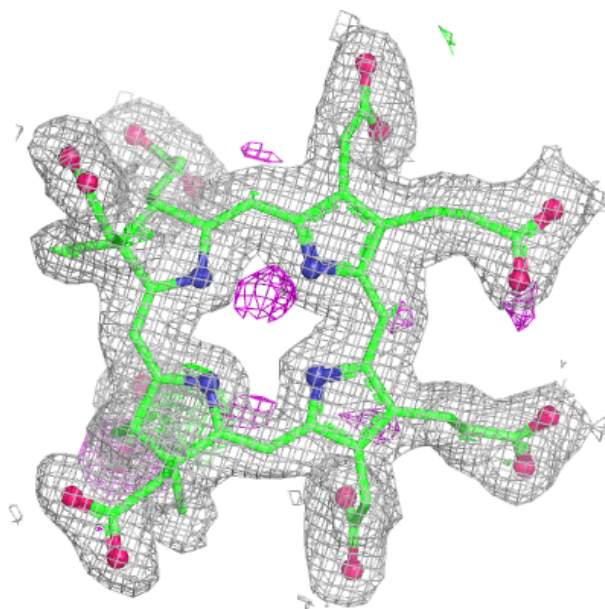
Electron density around SRM B 581:

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



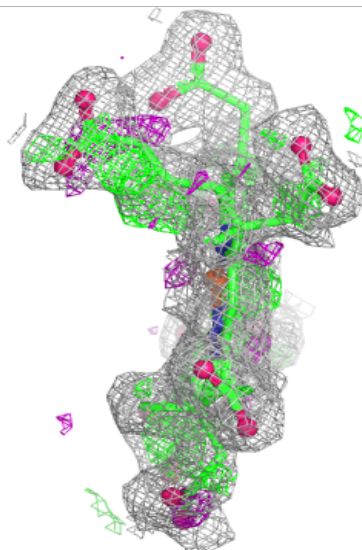
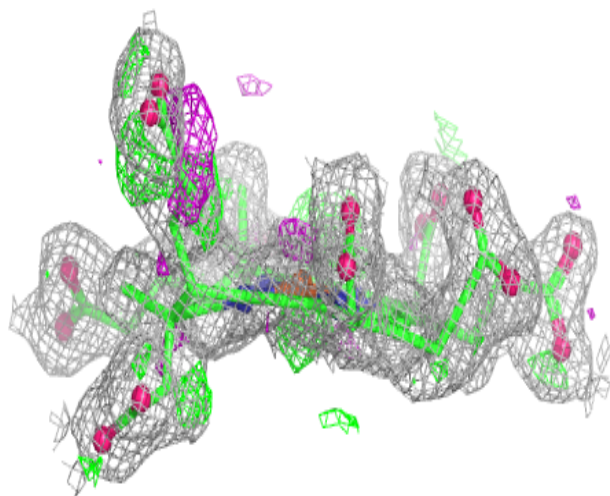
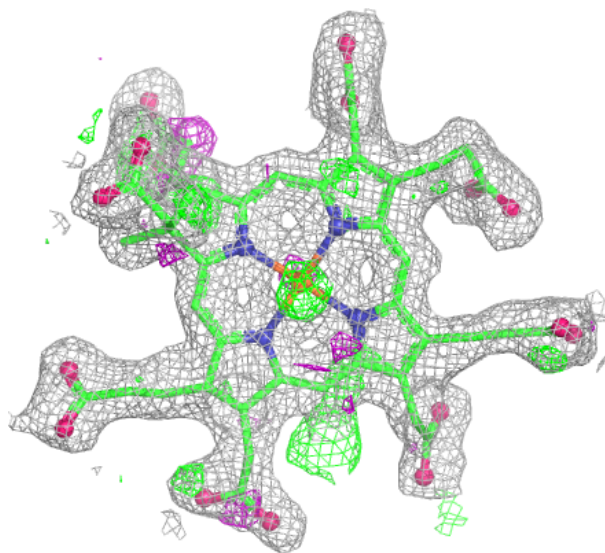
Electron density around SRM E 583:

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



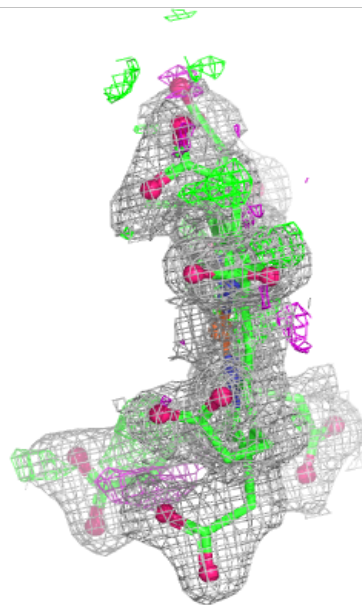
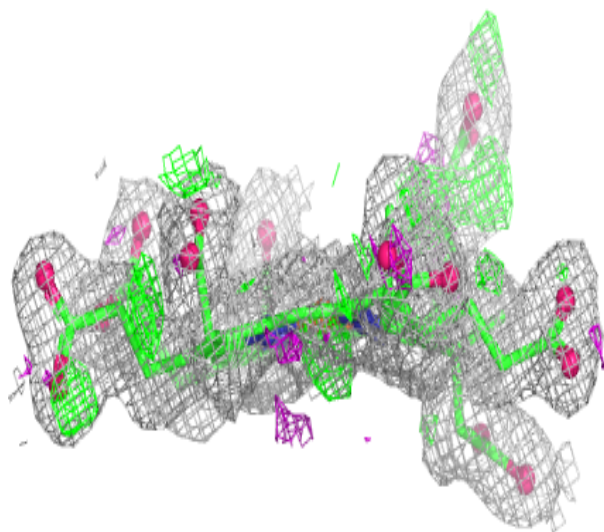
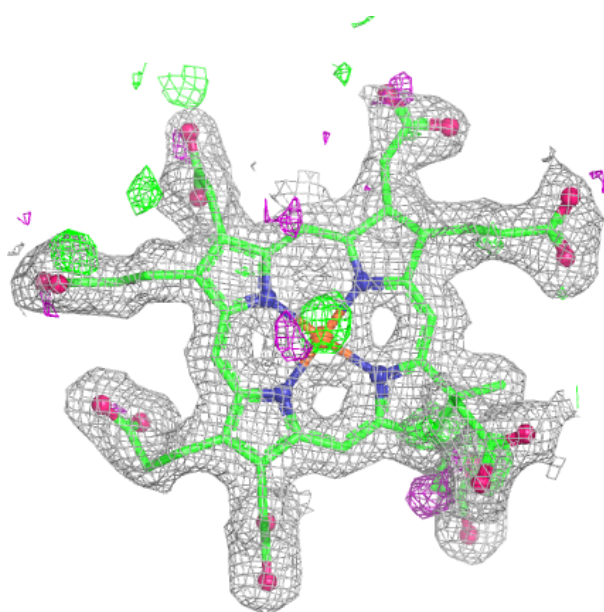
Electron density around SRM A 582:

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



Electron density around SRM D 584:

$2mF_o-DF_c$ (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.