



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:09 PM UTC

PDB ID : 3MMC / pdb_00003mmc
Title : Structure of the dissimilatory sulfite reductase from *Archaeoglobus fulgidus*
Authors : Schiffer, A.; Parey, K.; Warkentin, E.; Diederichs, K.; Huber, H.; Stetter, K.O.;
Kroneck, P.M.H.; Ermler, U.
Deposited on : 2010-04-19
Resolution : 2.04 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

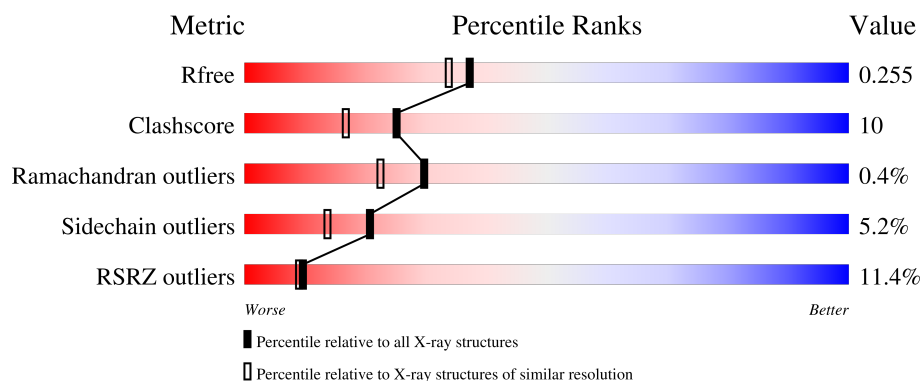
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	418	18% 82% 17% .
1	D	418	8% 83% 15% .
2	B	366	13% 83% 13% ..
2	E	366	5% 75% 21% ..

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
3	SRM	A	580	X	-	-	-
3	SRM	B	570	X	-	-	-
3	SRM	D	580	X	-	-	-
3	SRM	E	570	X	-	-	-
4	SF4	D	575	-	-	X	-
4	SF4	E	585	-	-	X	-
5	GOL	A	590	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13324 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.

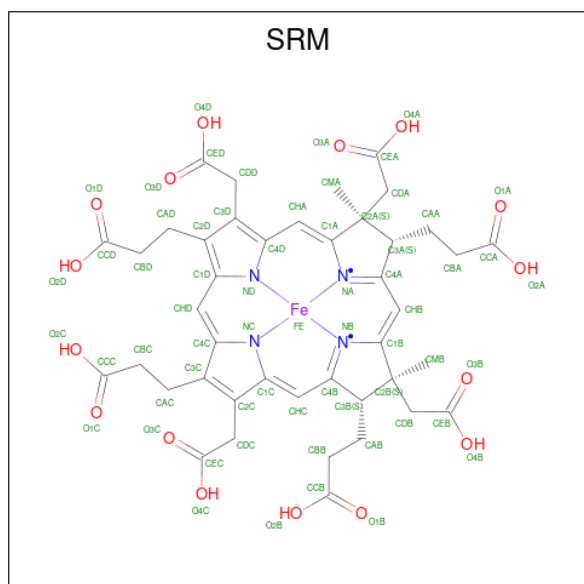
- Molecule 1 is a protein called Sulfite reductase, dissimilatory-type subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3329	2134	557	612	26			
1	D	417	Total	C	N	O	S	0	0	0
			3329	2134	557	612	26			

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

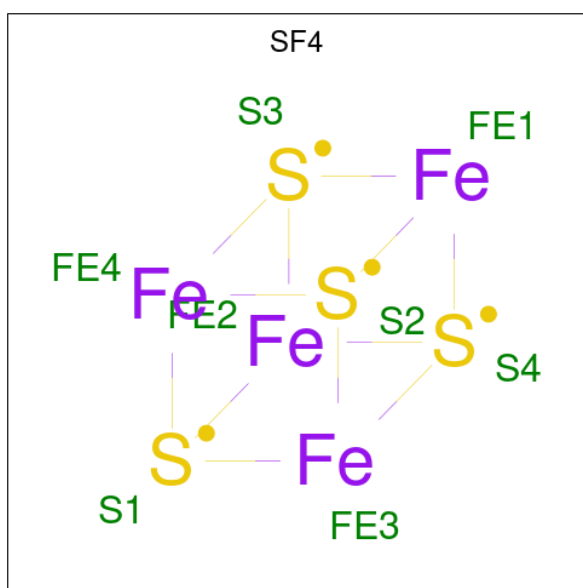
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			
2	E	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			

- Molecule 3 is SIROHEME (CCD ID: SRM) (formula: $C_{42}H_{44}FeN_4O_{16}$).



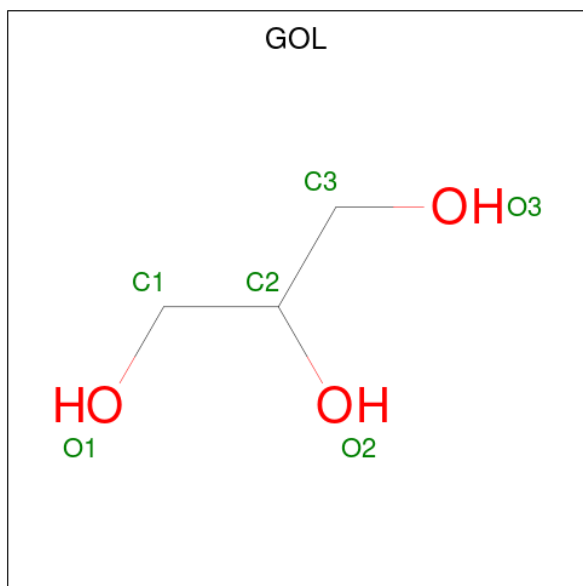
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	B	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	D	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	E	1	Total	C	Fe	N	O	
			63	42	1	4	16	

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

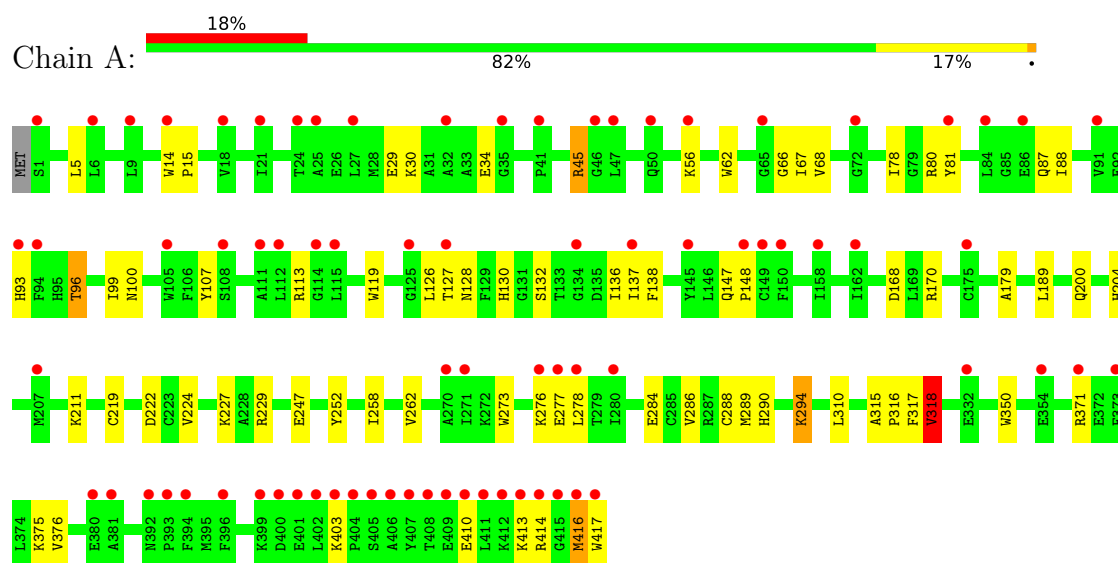
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	220	Total	O	0	0
			220	220		
6	B	265	Total	O	0	0
			265	265		
6	D	39	Total	O	0	0
			39	39		
6	E	18	Total	O	0	0
			18	18		

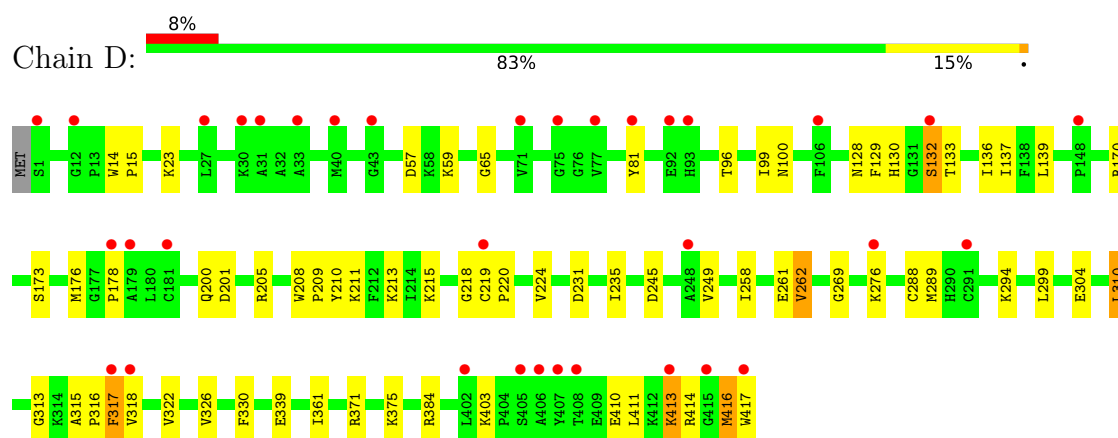
3 Residue-property plots

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

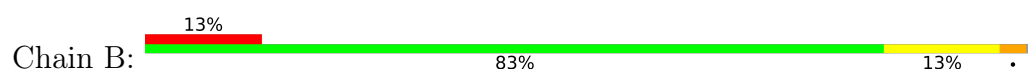
- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

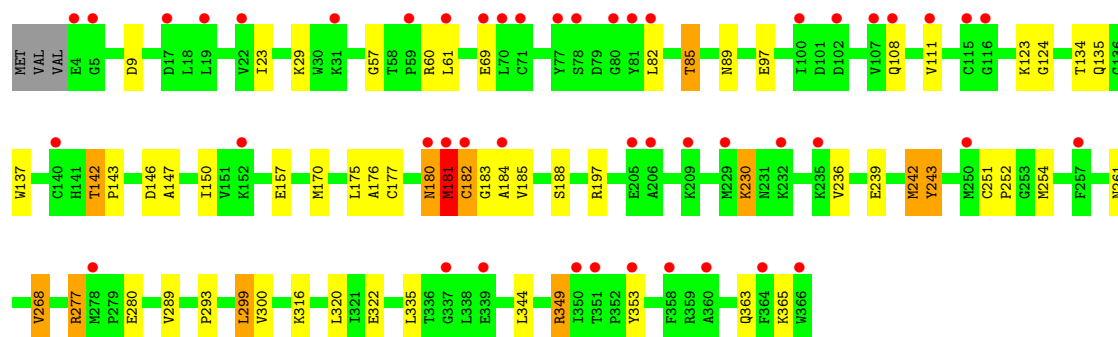


- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

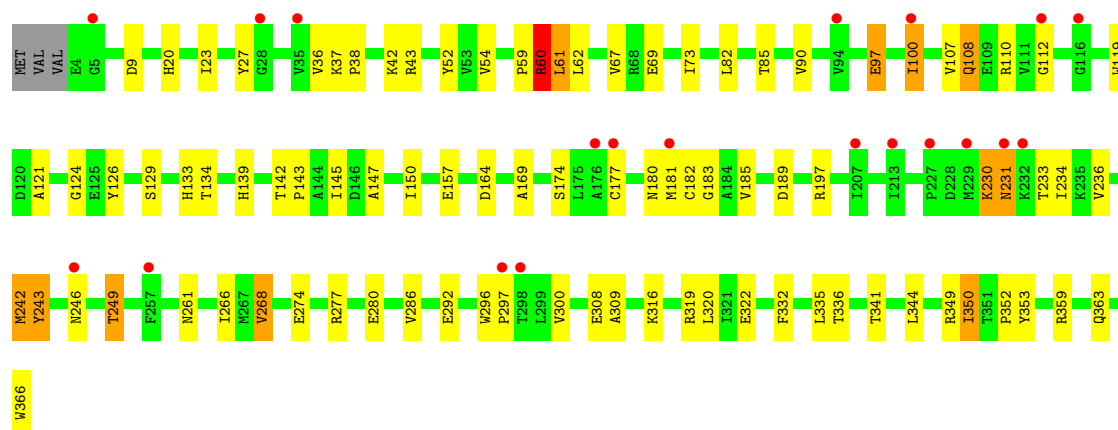
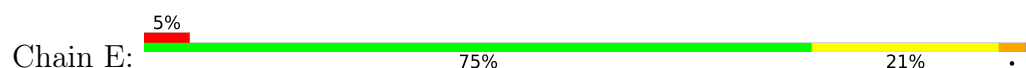


- Molecule 2: Sulfite reductase, dissimilatory-type subunit beta





• Molecule 2: Sulfite reductase, dissimilatory-type subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.91Å 69.26Å 147.21Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	20.11 – 2.04 20.11 – 2.04	Depositor EDS
% Data completeness (in resolution range)	97.9 (20.11-2.04) 97.8 (20.11-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.186 , 0.223 0.227 , 0.255	Depositor DCC
R_{free} test set	5740 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	13324	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, GOL, 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	0.96	1/3416 (0.0%)	0.99	2/4610 (0.0%)
1	D	0.60	1/3416 (0.0%)	0.88	1/4610 (0.0%)
2	B	1.04	5/2984 (0.2%)	1.06	3/4058 (0.1%)
2	E	0.66	0/2984	0.93	6/4058 (0.1%)
All	All	0.84	7/12800 (0.1%)	0.97	12/17336 (0.1%)

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

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	289	VAL	CA-CB	6.39	1.62	1.54
1	D	23	LYS	CD-CE	6.21	1.71	1.52
2	B	182	CYS	C-O	5.75	1.30	1.23
2	B	181	MET	CA-C	-5.62	1.45	1.53
1	A	88	ILE	CA-CB	5.51	1.61	1.54
2	B	293	PRO	CA-C	5.18	1.54	1.51
2	B	85	THR	N-CA	5.17	1.52	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	VAL	N-CA-C	8.41	126.83	109.34
1	D	317	PHE	N-CA-C	7.83	121.77	110.10
2	E	308	GLU	O-C-N	7.09	129.75	122.09
2	E	350	ILE	N-CA-C	6.92	117.71	110.72
2	E	230	LYS	CA-C-N	6.75	133.85	121.70
2	E	230	LYS	C-N-CA	6.75	133.85	121.70
2	B	254	MET	CA-C-N	-6.36	113.43	119.85
2	B	254	MET	C-N-CA	-6.36	113.43	119.85
2	B	182	CYS	N-CA-C	-6.27	101.40	110.24
1	A	66	GLY	N-CA-C	-6.12	104.70	112.54
2	E	309	ALA	CA-C-N	5.16	129.32	120.71
2	E	309	ALA	C-N-CA	5.16	129.32	120.71

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	PHE	Peptide
2	B	180	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3329	0	3276	58	0
1	D	3329	0	3276	58	0
2	B	2901	0	2838	65	0
2	E	2901	0	2838	81	0
3	A	63	0	34	9	0
3	B	63	0	34	2	0
3	D	63	0	34	18	0
3	E	63	0	34	13	0
4	A	16	0	0	0	0
4	B	16	0	0	1	0
4	D	16	0	0	2	0
4	E	16	0	0	3	0
5	A	6	0	8	8	0
6	A	220	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	265	0	0	16	0
6	D	39	0	0	5	0
6	E	18	0	0	2	0
All	All	13324	0	12372	245	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 10.

All (245) 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)
2:E:134:THR:HG21	2:E:182:CYS:HB2	1.39	1.00
2:E:177:CYS:HB2	4:E:585:SF4:S3	2.09	0.92
2:B:134:THR:CG2	6:B:4370:HOH:O	2.17	0.92
2:B:69:GLU:HG2	6:B:4358:HOH:O	1.70	0.92
2:E:90:VAL:HG23	6:E:4492:HOH:O	1.70	0.90
3:E:570:SRM:HDD1	3:E:570:SRM:HBD1	1.51	0.89
1:A:403:LYS:H	2:E:261:ASN:HD21	1.20	0.89
1:D:176:MET:HE1	3:E:570:SRM:HBA2	1.53	0.89
4:D:575:SF4:S4	6:E:4464:HOH:O	2.32	0.86
1:D:128:ASN:HB2	1:D:137:ILE:HB	1.58	0.85
2:E:134:THR:CG2	2:E:182:CYS:HB2	2.05	0.85
1:A:316:PRO:HG2	2:B:181:MET:HE3	1.59	0.84
2:B:124:GLY:HA3	2:B:316:LYS:HD2	1.60	0.83
1:A:170:ARG:HH22	5:A:590:GOL:H11	1.42	0.83
1:D:316:PRO:HG2	2:E:181:MET:HE3	1.62	0.81
2:B:182:CYS:C	6:B:4408:HOH:O	2.24	0.81
2:B:183:GLY:N	6:B:4408:HOH:O	2.14	0.81
2:B:60:ARG:HB2	6:B:4420:HOH:O	1.81	0.80
2:E:134:THR:HB	4:E:585:SF4:S4	2.22	0.79
2:E:124:GLY:HA3	2:E:316:LYS:HD2	1.65	0.79
2:B:185:VAL:CG2	6:B:4392:HOH:O	2.30	0.79
2:B:134:THR:HG21	6:B:4370:HOH:O	1.82	0.79
3:D:580:SRM:HAB2	2:E:183:GLY:H	1.46	0.76
2:E:52:TYR:CE1	2:E:97:GLU:HB3	2.20	0.76
1:A:211:LYS:HZ3	5:A:590:GOL:H32	1.51	0.75
2:B:261:ASN:HD21	1:D:403:LYS:H	1.32	0.75
1:A:211:LYS:NZ	5:A:590:GOL:H32	2.02	0.73
1:D:316:PRO:HG2	2:E:181:MET:CE	2.19	0.72
3:A:580:SRM:CBB	3:A:580:SRM:HMB1	2.19	0.72
2:E:230:LYS:CB	2:E:231:ASN:HB2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ARG:O	1:A:375:LYS:HD3	1.90	0.72
2:B:146:ASP:C	6:B:4376:HOH:O	2.32	0.72
3:A:580:SRM:HBA1	3:A:580:SRM:HHB	1.71	0.71
1:A:128:ASN:HD21	2:B:135:GLN:HE22	1.36	0.70
1:A:128:ASN:ND2	2:B:135:GLN:HE22	1.89	0.70
1:A:286:VAL:HG23	2:B:363:GLN:HG2	1.74	0.69
1:D:211:LYS:HZ3	3:D:580:SRM:HDA2	1.58	0.69
2:E:42:LYS:HG3	2:E:52:TYR:CE2	2.28	0.69
1:D:176:MET:CE	3:E:570:SRM:HBA2	2.24	0.67
1:D:132:SER:HB2	3:D:580:SRM:HBB2	1.76	0.66
1:A:211:LYS:HZ3	5:A:590:GOL:C3	2.08	0.66
2:E:85:THR:HB	3:E:570:SRM:HAB2	1.77	0.66
1:D:14:TRP:CD2	1:D:15:PRO:HD2	2.31	0.65
2:E:230:LYS:HB2	2:E:231:ASN:ND2	2.12	0.64
2:E:119:TRP:HE1	3:E:570:SRM:HDD2	1.63	0.64
2:B:185:VAL:HG21	6:B:4392:HOH:O	1.95	0.64
1:D:211:LYS:NZ	3:D:580:SRM:HDA2	2.12	0.63
2:E:197:ARG:HH21	2:E:261:ASN:HD22	1.43	0.63
1:A:14:TRP:CD2	1:A:15:PRO:HD2	2.35	0.62
1:D:288:CYS:O	1:D:289:MET:HB2	1.97	0.62
1:A:316:PRO:HG2	2:B:181:MET:CE	2.27	0.62
3:D:580:SRM:HMB2	2:E:182:CYS:HA	1.82	0.62
2:E:157:GLU:HG3	2:E:300:VAL:HG11	1.82	0.62
2:E:230:LYS:CA	2:E:231:ASN:HB2	2.29	0.62
1:A:107:TYR:OH	1:A:130:HIS:HE1	1.83	0.61
1:A:262:VAL:HG22	1:A:294:LYS:HG2	1.82	0.61
1:D:261:GLU:HB3	1:D:294:LYS:HE2	1.81	0.61
2:E:266:ILE:HB	2:E:286:VAL:HB	1.84	0.60
1:A:375:LYS:HD2	1:A:375:LYS:N	2.17	0.59
1:A:229:ARG:CD	2:B:184:ALA:HB2	2.32	0.59
2:B:175:LEU:HD23	2:B:175:LEU:C	2.28	0.59
1:A:170:ARG:HH12	5:A:590:GOL:H31	1.68	0.58
2:E:292:GLU:HB2	2:E:296:TRP:HA	1.85	0.58
1:A:170:ARG:HH12	5:A:590:GOL:C3	2.16	0.58
3:A:580:SRM:HMB1	3:A:580:SRM:HBB1	1.86	0.58
2:E:230:LYS:HB2	2:E:231:ASN:HB2	1.86	0.57
1:A:315:ALA:HB1	1:A:316:PRO:HD2	1.87	0.57
2:B:85:THR:HB	3:B:570:SRM:HAB1	1.87	0.56
2:B:147:ALA:HB2	2:B:177:CYS:SG	2.45	0.56
2:B:177:CYS:HB2	4:B:585:SF4:S3	2.46	0.56
2:B:261:ASN:HD21	1:D:403:LYS:N	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:GLN:HE21	2:E:9:ASP:HA	1.70	0.56
3:A:580:SRM:CBB	3:A:580:SRM:CMB	2.84	0.56
2:E:43:ARG:NH2	3:E:570:SRM:O4A	2.32	0.55
3:E:570:SRM:CBA	3:E:570:SRM:HHB	2.36	0.55
1:A:119:TRP:CH2	1:A:138:PHE:HB3	2.42	0.55
1:A:276:LYS:HG2	1:A:277:GLU:HG2	1.89	0.55
1:A:252:TYR:OH	6:A:4162:HOH:O	2.17	0.55
1:D:258:ILE:HA	1:D:262:VAL:HG23	1.89	0.55
1:D:57:ASP:HB3	1:D:59:LYS:HG2	1.89	0.54
1:D:261:GLU:CD	2:E:316:LYS:HE3	2.32	0.54
1:A:286:VAL:CG2	2:B:363:GLN:HG2	2.37	0.54
1:D:132:SER:HB2	3:D:580:SRM:CBB	2.38	0.53
1:D:213:LYS:NZ	3:D:580:SRM:HDB2	2.23	0.53
3:D:580:SRM:HMA1	2:E:180:ASN:ND2	2.23	0.53
3:E:570:SRM:O4D	3:E:570:SRM:HHA	2.08	0.53
2:E:20:HIS:HB3	2:E:23:ILE:HD12	1.90	0.53
1:D:14:TRP:CG	1:D:15:PRO:HD2	2.44	0.53
1:A:29:GLU:OE2	1:A:45:ARG:HD2	2.09	0.53
1:A:127:THR:O	2:B:61:LEU:HD12	2.08	0.53
1:D:213:LYS:HZ1	3:D:580:SRM:HDB2	1.73	0.53
2:E:230:LYS:HB2	2:E:231:ASN:CB	2.39	0.53
2:B:57:GLY:HA2	2:B:89:ASN:ND2	2.23	0.53
1:D:262:VAL:HG22	1:D:294:LYS:HG2	1.90	0.53
1:A:30:LYS:O	1:A:34:GLU:HG3	2.09	0.52
2:B:134:THR:HG21	2:B:182:CYS:HB2	1.92	0.52
2:B:146:ASP:O	2:B:150:ILE:HD12	2.10	0.52
1:A:229:ARG:HD3	2:B:184:ALA:HB2	1.92	0.51
2:B:268:VAL:HG13	2:B:320:LEU:CD2	2.40	0.51
1:D:416:MET:O	1:D:417:TRP:HB3	2.09	0.51
1:D:178:PRO:HG2	2:E:27:TYR:CZ	2.46	0.51
2:B:277:ARG:NH2	2:B:280:GLU:OE1	2.40	0.51
1:D:245:ASP:O	1:D:249:VAL:HG23	2.11	0.51
1:A:219:CYS:SG	1:A:289:MET:HE2	2.51	0.51
2:B:184:ALA:HB3	6:B:4380:HOH:O	2.10	0.50
2:B:349:ARG:NH2	2:E:350:ILE:O	2.44	0.50
1:D:170:ARG:HG3	1:D:213:LYS:HE2	1.94	0.50
1:D:235:ILE:HD12	1:D:310:LEU:HD22	1.93	0.50
2:B:137:TRP:CE3	2:B:146:ASP:HB2	2.46	0.50
1:A:416:MET:O	1:A:417:TRP:HB3	2.12	0.50
1:D:99:ILE:HB	1:D:136:ILE:HB	1.92	0.50
1:D:261:GLU:HB3	1:D:294:LYS:CE	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:PHE:CD2	2:E:180:ASN:ND2	2.80	0.49
1:A:403:LYS:N	2:E:261:ASN:HD21	1.98	0.49
2:E:134:THR:CG2	2:E:182:CYS:CB	2.84	0.49
1:A:262:VAL:HG22	1:A:294:LYS:CG	2.42	0.49
2:E:69:GLU:HG2	2:E:110:ARG:HH21	1.78	0.49
2:E:121:ALA:CB	3:E:570:SRM:O3D	2.61	0.49
2:E:268:VAL:HG22	2:E:320:LEU:HD22	1.95	0.49
3:A:580:SRM:C2D	2:B:180:ASN:HB2	2.43	0.49
1:A:62:TRP:HB3	1:A:80:ARG:HD2	1.95	0.49
1:A:410:GLU:O	1:A:414:ARG:HG2	2.13	0.48
2:E:230:LYS:HB2	2:E:231:ASN:HD22	1.79	0.48
2:E:37:LYS:HB2	2:E:38:PRO:CD	2.43	0.48
1:A:416:MET:O	1:A:417:TRP:CB	2.61	0.48
3:D:580:SRM:CAB	2:E:183:GLY:H	2.22	0.48
2:E:277:ARG:HG2	2:E:322:GLU:HG2	1.95	0.48
1:A:99:ILE:HB	1:A:136:ILE:HB	1.94	0.48
2:B:157:GLU:HG3	2:B:300:VAL:HG11	1.95	0.48
3:D:580:SRM:CMB	2:E:182:CYS:HA	2.43	0.48
3:A:580:SRM:HMB1	3:A:580:SRM:HBB2	1.92	0.47
2:B:175:LEU:HD23	2:B:176:ALA:N	2.30	0.47
1:D:213:LYS:HZ2	3:D:580:SRM:HDB1	1.79	0.47
3:E:570:SRM:HDD1	3:E:570:SRM:CBD	2.26	0.47
2:B:134:THR:HG23	6:B:4370:HOH:O	1.97	0.47
2:B:197:ARG:HH21	2:B:261:ASN:HD22	1.63	0.47
1:D:315:ALA:HB1	1:D:316:PRO:CD	2.45	0.47
2:E:145:ILE:HD12	2:E:150:ILE:HD12	1.96	0.47
3:E:570:SRM:HHB	3:E:570:SRM:HBA1	1.95	0.47
2:E:142:THR:N	2:E:143:PRO:HD3	2.29	0.47
2:B:242:MET:C	2:B:243:TYR:CG	2.93	0.46
1:D:173:SER:OG	1:D:215:LYS:HG2	2.15	0.46
1:D:218:GLY:HA3	4:D:575:SF4:S2	2.54	0.46
1:D:416:MET:O	1:D:417:TRP:CB	2.63	0.46
1:D:213:LYS:NZ	3:D:580:SRM:CDB	2.78	0.46
2:E:296:TRP:N	2:E:297:PRO:HD3	2.30	0.46
2:B:60:ARG:HD3	6:B:4420:HOH:O	2.15	0.46
1:D:129:PHE:HA	1:D:130:HIS:HA	1.73	0.46
3:D:580:SRM:CCD	3:D:580:SRM:HDD1	2.46	0.46
2:E:189:ASP:O	2:E:268:VAL:HA	2.16	0.46
2:E:197:ARG:NH2	2:E:261:ASN:HD22	2.12	0.46
1:A:222:ASP:OD1	1:A:227:LYS:NZ	2.48	0.46
2:E:230:LYS:HB2	2:E:231:ASN:CG	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:LEU:HD13	1:D:417:TRP:HA	1.98	0.45
2:E:108:GLN:H	2:E:108:GLN:HE21	1.64	0.45
2:E:147:ALA:HB2	2:E:177:CYS:SG	2.56	0.45
1:A:130:HIS:HD2	6:B:4031:HOH:O	1.99	0.45
1:A:290:HIS:O	1:A:294:LYS:HB2	2.15	0.45
1:D:317:PHE:HD2	2:E:180:ASN:HD22	1.65	0.45
2:E:73:ILE:HD13	2:E:107:VAL:HG22	1.99	0.45
1:A:119:TRP:CZ3	1:A:138:PHE:HB3	2.52	0.45
2:B:251:CYS:HA	2:B:252:PRO:HD2	1.84	0.45
2:B:349:ARG:HH22	2:E:352:PRO:HD3	1.82	0.45
2:E:142:THR:N	2:E:143:PRO:CD	2.79	0.45
3:E:570:SRM:HCD1	3:E:570:SRM:HAC2	1.78	0.45
1:A:284:GLU:HA	2:B:365:LYS:HD3	1.99	0.45
2:B:29:LYS:HE3	6:B:4374:HOH:O	2.17	0.45
3:D:580:SRM:HAA1	3:D:580:SRM:HDA1	1.71	0.45
1:A:288:CYS:O	1:A:289:MET:HB2	2.16	0.45
2:B:182:CYS:CB	6:B:4408:HOH:O	2.64	0.45
1:A:211:LYS:NZ	5:A:590:GOL:C3	2.71	0.44
1:A:81:TYR:CE2	1:A:93:HIS:CD2	3.05	0.44
1:D:201:ASP:OD1	1:D:205:ARG:HD2	2.18	0.44
2:E:126:TYR:CE1	2:E:169:ALA:HA	2.52	0.44
2:B:268:VAL:HG13	2:B:320:LEU:HD22	1.99	0.44
2:E:177:CYS:CB	4:E:585:SF4:S3	2.95	0.44
2:B:142:THR:N	2:B:143:PRO:CD	2.81	0.44
6:D:4535:HOH:O	2:E:182:CYS:SG	2.62	0.44
1:A:128:ASN:HB2	1:A:137:ILE:HB	2.00	0.43
2:B:277:ARG:HG2	2:B:322:GLU:HG2	1.99	0.43
1:D:208:TRP:HB3	1:D:209:PRO:CD	2.48	0.43
1:D:219:CYS:HB2	1:D:220:PRO:CD	2.48	0.43
1:D:330:PHE:HB2	2:E:366:TRP:CH2	2.53	0.43
1:A:316:PRO:CG	2:B:181:MET:HE3	2.41	0.43
1:D:139:LEU:HD11	2:E:139:HIS:CG	2.54	0.43
1:D:65:GLY:HA3	1:D:81:TYR:CD1	2.53	0.43
2:B:349:ARG:NH2	2:E:352:PRO:HD3	2.34	0.43
1:D:129:PHE:HB2	2:E:62:LEU:HD22	1.99	0.43
2:E:119:TRP:HB2	2:E:126:TYR:CD2	2.53	0.43
1:A:168:ASP:OD1	1:A:170:ARG:HD3	2.19	0.43
2:B:176:ALA:HB1	2:B:181:MET:HA	2.00	0.43
2:B:268:VAL:HG13	2:B:320:LEU:HD21	2.01	0.43
2:B:320:LEU:C	2:B:320:LEU:HD23	2.44	0.43
1:A:273:TRP:HB2	1:A:278:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:GLU:O	1:D:414:ARG:HG2	2.18	0.43
2:E:62:LEU:HD23	2:E:67:VAL:HG22	2.01	0.43
2:B:82:LEU:N	2:B:82:LEU:HD23	2.34	0.42
1:A:96:THR:HG21	6:A:4356:HOH:O	2.19	0.42
1:A:229:ARG:HD2	2:B:184:ALA:N	2.33	0.42
1:D:310:LEU:HD12	1:D:326:VAL:HA	2.00	0.42
1:A:179:ALA:O	2:B:23:ILE:HG23	2.19	0.42
2:E:174:SER:HB3	2:E:185:VAL:HG22	2.02	0.42
2:E:332:PHE:CE1	2:E:336:THR:HG21	2.55	0.42
1:D:384:ARG:O	2:E:359:ARG:HD2	2.19	0.42
3:A:580:SRM:CMB	3:A:580:SRM:HBB2	2.49	0.42
2:E:277:ARG:NH2	2:E:280:GLU:OE1	2.52	0.42
1:D:213:LYS:HZ2	3:D:580:SRM:CDB	2.33	0.42
2:E:60:ARG:HD3	2:E:133:HIS:CE1	2.55	0.42
3:A:580:SRM:O3B	2:B:135:GLN:HG2	2.18	0.42
1:D:128:ASN:OD1	2:E:60:ARG:NH2	2.52	0.42
1:D:315:ALA:HB3	3:D:580:SRM:HBA1	2.02	0.42
1:D:403:LYS:NZ	6:D:4208:HOH:O	2.52	0.42
2:E:42:LYS:HE2	2:E:42:LYS:HB3	1.86	0.42
2:E:59:PRO:O	2:E:61:LEU:N	2.53	0.42
1:D:269:GLY:HA2	6:D:4331:HOH:O	2.19	0.42
1:A:81:TYR:HE2	1:A:93:HIS:CD2	2.38	0.42
1:D:231:ASP:HB3	1:D:361:ILE:CG2	2.50	0.42
2:E:108:GLN:HE21	2:E:108:GLN:N	2.18	0.42
2:E:242:MET:C	2:E:243:TYR:CG	2.98	0.42
1:A:147:GLN:HB3	1:A:148:PRO:CD	2.50	0.41
1:A:170:ARG:NH1	5:A:590:GOL:H31	2.34	0.41
2:B:299:LEU:HD23	2:B:299:LEU:C	2.45	0.41
2:B:353:TYR:HA	2:E:353:TYR:HA	2.02	0.41
2:E:246:ASN:O	2:E:249:THR:HB	2.20	0.41
1:D:176:MET:HE1	3:E:570:SRM:CBA	2.37	0.41
3:A:580:SRM:HHB	3:A:580:SRM:CBA	2.47	0.41
1:A:375:LYS:N	1:A:375:LYS:CD	2.81	0.41
2:B:182:CYS:HB3	6:B:4408:HOH:O	2.21	0.41
2:E:230:LYS:N	2:E:231:ASN:HB2	2.36	0.41
2:B:170:MET:SD	3:B:570:SRM:HBD1	2.60	0.41
1:A:200:GLN:HE21	2:B:9:ASP:HA	1.85	0.41
3:D:580:SRM:CHD	6:D:4535:HOH:O	2.69	0.41
1:A:200:GLN:NE2	1:A:204:HIS:NE2	2.69	0.41
2:B:69:GLU:OE2	2:B:111:VAL:HG12	2.20	0.41
1:D:413:LYS:HE2	6:D:4364:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:TRP:CG	1:A:376:VAL:HG21	2.55	0.41
2:E:100:ILE:H	2:E:100:ILE:HG13	1.61	0.41
1:A:113:ARG:HH11	1:A:113:ARG:HD2	1.77	0.40
2:B:185:VAL:H	2:B:185:VAL:HG23	1.50	0.40
2:B:230:LYS:H	2:B:230:LYS:HG2	1.59	0.40
2:E:108:GLN:HA	2:E:112:GLY:HA2	2.02	0.40
2:E:319:ARG:O	2:E:320:LEU:C	2.63	0.40
1:D:313:GLY:HA2	1:D:322:VAL:O	2.21	0.40
2:E:233:THR:OG1	2:E:234:ILE:N	2.54	0.40
2:E:274:GLU:OE1	2:E:363:GLN:HG3	2.21	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	415/418 (99%)	402 (97%)	12 (3%)	1 (0%)	43	37
1	D	415/418 (99%)	395 (95%)	19 (5%)	1 (0%)	43	37
2	B	361/366 (99%)	346 (96%)	14 (4%)	1 (0%)	36	30
2	E	361/366 (99%)	324 (90%)	34 (9%)	3 (1%)	16	9
All	All	1552/1568 (99%)	1467 (94%)	79 (5%)	6 (0%)	30	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	VAL
2	E	231	ASN
2	E	60	ARG
1	D	318	VAL
2	E	36	VAL

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Mol	Chain	Res	Type
2	B	142	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	353/354 (100%)	333 (94%)	20 (6%)	18	11
1	D	353/354 (100%)	337 (96%)	16 (4%)	24	18
2	B	314/317 (99%)	298 (95%)	16 (5%)	21	14
2	E	314/317 (99%)	296 (94%)	18 (6%)	18	11
All	All	1334/1342 (99%)	1264 (95%)	70 (5%)	21	14

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	45	ARG
1	A	56	LYS
1	A	67	ILE
1	A	68	VAL
1	A	78	ILE
1	A	87	GLN
1	A	96	THR
1	A	100	ASN
1	A	126	LEU
1	A	132	SER
1	A	189	LEU
1	A	224	VAL
1	A	247	GLU
1	A	258	ILE
1	A	294	LYS
1	A	310	LEU
1	A	318	VAL
1	A	413	LYS
1	A	416	MET

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Mol	Chain	Res	Type
2	B	97	GLU
2	B	108	GLN
2	B	123	LYS
2	B	181	MET
2	B	188	SER
2	B	230	LYS
2	B	236	VAL
2	B	239	GLU
2	B	242	MET
2	B	243	TYR
2	B	268	VAL
2	B	277	ARG
2	B	299	LEU
2	B	335	LEU
2	B	344	LEU
2	B	349	ARG
1	D	96	THR
1	D	100	ASN
1	D	132	SER
1	D	133	THR
1	D	210	TYR
1	D	224	VAL
1	D	262	VAL
1	D	276	LYS
1	D	299	LEU
1	D	304	GLU
1	D	310	LEU
1	D	339	GLU
1	D	371	ARG
1	D	375	LYS
1	D	413	LYS
1	D	416	MET
2	E	54	VAL
2	E	60	ARG
2	E	61	LEU
2	E	82	LEU
2	E	97	GLU
2	E	100	ILE
2	E	108	GLN
2	E	129	SER
2	E	164	ASP
2	E	236	VAL

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Mol	Chain	Res	Type
2	E	242	MET
2	E	243	TYR
2	E	249	THR
2	E	268	VAL
2	E	335	LEU
2	E	341	THR
2	E	344	LEU
2	E	349	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	130	HIS
1	A	200	GLN
2	B	89	ASN
2	B	186	HIS
2	B	231	ASN
2	B	261	ASN
2	B	363	GLN
1	D	100	ASN
1	D	200	GLN
2	E	89	ASN
2	E	180	ASN
2	E	196	HIS
2	E	203	ASN
2	E	231	ASN
2	E	261	ASN
2	E	313	ASN
2	E	363	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
3	SRM	B	570	1	68,70,70	2.12	14 (20%)	86,112,112	2.99	39 (45%)
4	SF4	A	576	1	0,12,12	-	-	-		
4	SF4	B	586	2	0,12,12	-	-	-		
4	SF4	E	586	2	0,12,12	-	-	-		
4	SF4	D	575	1	0,12,12	-	-	-		
4	SF4	B	585	2	0,12,12	-	-	-		
4	SF4	A	575	1	0,12,12	-	-	-		
4	SF4	E	585	6,2	0,12,12	-	-	-		
3	SRM	D	580	-	68,70,70	2.13	17 (25%)	86,112,112	2.90	26 (30%)
4	SF4	D	576	1	0,12,12	-	-	-		
3	SRM	A	580	2	68,70,70	2.14	21 (30%)	86,112,112	2.71	29 (33%)
5	GOL	A	590	-	5,5,5	0.45	0	5,5,5	1.05	0
3	SRM	E	570	1	68,70,70	2.10	14 (20%)	86,112,112	2.75	34 (39%)

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
3	SRM	B	570	1	1/1/19/23	16/38/126/126	-
4	SF4	A	576	1	-	-	0/6/5/5
4	SF4	B	586	2	-	-	0/6/5/5
4	SF4	E	586	2	-	-	0/6/5/5
4	SF4	D	575	1	-	-	0/6/5/5
4	SF4	B	585	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	A	575	1	-	-	0/6/5/5
4	SF4	E	585	6,2	-	-	0/6/5/5
3	SRM	D	580	-	2/2/19/23	20/38/126/126	-
5	GOL	A	590	-	-	4/4/4/4	-
3	SRM	A	580	2	1/1/19/23	12/38/126/126	-
4	SF4	D	576	1	-	-	0/6/5/5
3	SRM	E	570	1	2/2/19/23	20/38/126/126	-

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	570	SRM	C4A-NA	-8.22	1.29	1.35
3	E	570	SRM	C3C-C2C	7.44	1.52	1.36
3	D	580	SRM	C3C-C2C	6.44	1.50	1.36
3	B	570	SRM	C3C-C2C	6.11	1.49	1.36
3	A	580	SRM	C3C-C2C	6.06	1.49	1.36
3	E	570	SRM	C4A-NA	-5.99	1.31	1.35
3	E	570	SRM	C1C-NC	-5.51	1.29	1.39
3	E	570	SRM	C4C-NC	-5.24	1.29	1.39
3	A	580	SRM	C3A-C4A	-5.24	1.40	1.51
3	A	580	SRM	FE-NA	5.22	2.11	1.94
3	D	580	SRM	C3B-C4B	-5.13	1.40	1.51
3	D	580	SRM	C3A-C4A	-5.02	1.40	1.51
3	D	580	SRM	FE-NA	4.62	2.09	1.94
3	B	570	SRM	C1D-C2D	4.47	1.53	1.44
3	A	580	SRM	FE-NB	4.32	2.08	1.94
3	B	570	SRM	C4D-C3D	4.20	1.53	1.44
3	D	580	SRM	FE-NB	4.13	2.07	1.94
3	A	580	SRM	C1D-C2D	4.10	1.52	1.44
3	A	580	SRM	C4A-NA	-4.03	1.32	1.35
3	B	570	SRM	C2B-C3B	-3.97	1.44	1.55
3	B	570	SRM	C4C-NC	-3.93	1.32	1.39
3	E	570	SRM	C1D-C2D	3.90	1.52	1.44
3	D	580	SRM	FE-NC	3.79	2.07	1.95
3	D	580	SRM	C1D-C2D	3.79	1.52	1.44
3	D	580	SRM	C4D-ND	-3.63	1.32	1.39
3	A	580	SRM	C3B-C4B	-3.59	1.43	1.51
3	E	570	SRM	C4D-C3D	3.59	1.51	1.44
3	A	580	SRM	C4D-C3D	3.57	1.51	1.44
3	E	570	SRM	C1C-C2C	3.52	1.51	1.45
3	A	580	SRM	C1C-C2C	3.50	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	580	SRM	CDD-C3D	3.49	1.56	1.51
3	E	570	SRM	C4C-C3C	3.48	1.51	1.45
3	D	580	SRM	C1C-NC	-3.33	1.33	1.39
3	D	580	SRM	C4C-NC	-3.27	1.33	1.39
3	D	580	SRM	C3D-C2D	3.23	1.54	1.40
3	A	580	SRM	C4C-NC	-3.20	1.33	1.39
3	B	570	SRM	CDC-CEC	3.16	1.56	1.51
3	D	580	SRM	C1C-C2C	3.14	1.50	1.45
3	A	580	SRM	FE-NC	3.14	2.05	1.95
3	D	580	SRM	C4D-C3D	3.09	1.50	1.44
3	E	570	SRM	C3D-C2D	3.09	1.54	1.40
3	A	580	SRM	C4D-ND	-3.09	1.33	1.39
3	A	580	SRM	C3D-C2D	3.05	1.53	1.40
3	B	570	SRM	C1C-NC	-3.04	1.33	1.39
3	B	570	SRM	C1C-C2C	2.95	1.50	1.45
3	B	570	SRM	C4C-C3C	2.88	1.50	1.45
3	B	570	SRM	C4D-ND	-2.85	1.34	1.39
3	B	570	SRM	C3D-C2D	2.81	1.52	1.40
3	E	570	SRM	C4D-ND	-2.64	1.34	1.39
3	A	580	SRM	O3B-CEB	2.60	1.30	1.22
3	B	570	SRM	C1D-ND	-2.54	1.34	1.39
3	D	580	SRM	C1D-ND	-2.52	1.34	1.39
3	E	570	SRM	CDC-C2C	2.51	1.54	1.51
3	A	580	SRM	C4C-C3C	2.40	1.49	1.45
3	D	580	SRM	CAB-C3B	-2.38	1.49	1.54
3	D	580	SRM	FE-ND	-2.34	1.87	1.95
3	A	580	SRM	C4B-NB	2.29	1.36	1.35
3	B	570	SRM	O4C-CEC	-2.27	1.23	1.30
3	A	580	SRM	C1C-NC	-2.11	1.35	1.39
3	A	580	SRM	CDA-CEA	2.10	1.57	1.50
3	A	580	SRM	CAA-C3A	-2.08	1.49	1.54
3	E	570	SRM	C1D-ND	-2.07	1.35	1.39
3	A	580	SRM	O4C-CEC	-2.05	1.24	1.30
3	E	570	SRM	C2B-C3B	-2.04	1.49	1.55
3	E	570	SRM	CDD-C3D	2.03	1.54	1.51
3	D	580	SRM	C4C-C3C	2.01	1.48	1.45

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	SRM	C2B-C3B-C4B	11.51	115.47	100.89
3	A	580	SRM	C2A-C3A-C4A	11.25	115.14	100.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	580	SRM	CAA-C3A-C4A	10.11	128.81	111.19
3	D	580	SRM	C2A-C3A-C4A	9.41	112.82	100.89
3	E	570	SRM	C2B-C1B-CHB	-9.38	115.12	123.54
3	D	580	SRM	C2B-C3B-C4B	8.86	112.11	100.89
3	E	570	SRM	CAB-C3B-C4B	8.04	125.21	111.19
3	B	570	SRM	C2B-C1B-CHB	-7.54	116.77	123.54
3	A	580	SRM	CMB-C2B-C3B	7.40	125.70	112.05
3	E	570	SRM	C1D-C2D-C3D	-6.97	99.50	106.81
3	B	570	SRM	C3B-C2B-C1B	-6.90	89.21	100.92
3	A	580	SRM	C2B-C3B-C4B	6.80	109.51	100.89
3	D	580	SRM	C4D-C3D-C2D	-6.56	99.93	106.81
3	E	570	SRM	C4C-C3C-C2C	-6.35	99.74	106.84
3	B	570	SRM	C1D-C2D-C3D	-6.21	100.30	106.81
3	D	580	SRM	CAB-C3B-C4B	6.05	121.73	111.19
3	B	570	SRM	CMB-C2B-C3B	6.01	123.14	112.05
3	D	580	SRM	C1D-C2D-C3D	-5.99	100.53	106.81
3	A	580	SRM	CAA-C3A-C4A	5.98	121.62	111.19
3	E	570	SRM	C2B-C3B-C4B	5.80	108.24	100.89
3	B	570	SRM	CBC-CAC-C3C	-5.65	96.90	112.53
3	D	580	SRM	C1A-NA-C4A	5.56	112.21	105.34
3	A	580	SRM	C3A-C2A-C1A	-5.49	91.60	100.92
3	E	570	SRM	C2D-C1D-ND	5.21	115.94	110.15
3	D	580	SRM	CAD-C2D-C1D	-5.17	114.84	124.94
3	B	570	SRM	C2A-C1A-CHA	-5.16	118.90	123.54
3	E	570	SRM	CAC-C3C-C2C	-5.07	117.33	129.24
3	B	570	SRM	C2D-C1D-ND	5.00	115.70	110.15
3	E	570	SRM	C3A-C4A-NA	4.88	120.36	110.83
3	A	580	SRM	CDA-C2A-C1A	4.87	122.18	107.11
3	D	580	SRM	C3C-C4C-NC	4.87	115.02	110.32
3	D	580	SRM	C4C-C3C-C2C	-4.75	101.53	106.84
3	B	570	SRM	CBD-CAD-C2D	4.70	125.53	112.53
3	E	570	SRM	CAD-C2D-C1D	-4.68	115.80	124.94
3	B	570	SRM	C3C-C4C-NC	4.60	114.76	110.32
3	A	580	SRM	C3C-C4C-NC	4.47	114.64	110.32
3	A	580	SRM	CBD-CAD-C2D	4.44	124.81	112.53
3	B	570	SRM	C4C-C3C-C2C	-4.42	101.90	106.84
3	A	580	SRM	C4C-C3C-C2C	-4.41	101.91	106.84
3	E	570	SRM	C1C-C2C-C3C	-4.38	101.94	106.84
3	B	570	SRM	CHD-C4C-C3C	-4.35	118.00	124.86
3	D	580	SRM	CHD-C4C-NC	-4.33	119.73	124.45
3	A	580	SRM	CMB-C2B-CDB	-4.28	103.46	110.74
3	D	580	SRM	C3D-C4D-ND	-4.24	105.45	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	580	SRM	CHC-C1C-NC	-4.14	119.94	124.45
3	D	580	SRM	C4D-ND-C1D	4.06	112.43	105.82
3	B	570	SRM	CAB-C3B-C4B	3.93	118.05	111.19
3	B	570	SRM	CHC-C1C-C2C	-3.91	118.68	124.86
3	E	570	SRM	CAB-C3B-C2B	3.89	124.88	114.19
3	A	580	SRM	C1D-C2D-C3D	-3.87	102.75	106.81
3	B	570	SRM	C3B-C4B-NB	-3.87	103.28	110.83
3	B	570	SRM	C3D-C4D-ND	3.74	114.31	110.15
3	D	580	SRM	CBA-CAA-C3A	3.73	125.22	114.65
3	A	580	SRM	CBB-CAB-C3B	3.73	125.21	114.65
3	B	570	SRM	C4D-C3D-C2D	-3.64	102.99	106.81
3	E	570	SRM	C3B-C2B-C1B	-3.64	94.73	100.92
3	B	570	SRM	C1C-C2C-C3C	-3.62	102.79	106.84
3	B	570	SRM	CDA-C2A-C1A	3.57	118.17	107.11
3	A	580	SRM	C2B-C1B-CHB	-3.56	120.34	123.54
3	A	580	SRM	CAB-C3B-C2B	-3.52	104.51	114.19
3	A	580	SRM	C4D-ND-C1D	3.42	111.40	105.82
3	E	570	SRM	CAC-C3C-C4C	-3.41	117.92	124.85
3	E	570	SRM	CAD-C2D-C3D	-3.33	114.94	125.30
3	B	570	SRM	C2C-C1C-NC	3.33	113.53	110.32
3	E	570	SRM	C3C-C4C-NC	3.30	113.50	110.32
3	E	570	SRM	CAA-CBA-CCA	3.29	121.27	112.49
3	A	580	SRM	CAC-CBC-CCC	-3.22	105.13	113.67
3	E	570	SRM	C2A-C3A-C4A	-3.17	96.88	100.89
3	A	580	SRM	C3B-C2B-C1B	-3.15	95.58	100.92
3	D	580	SRM	C1C-C2C-C3C	-3.09	103.39	106.84
3	B	570	SRM	CHC-C1C-NC	3.06	127.78	124.45
3	B	570	SRM	CBB-CAB-C3B	3.05	123.29	114.65
3	D	580	SRM	C3B-C2B-C1B	-3.04	95.77	100.92
3	D	580	SRM	C3A-C4A-CHB	3.01	129.74	123.33
3	E	570	SRM	C3A-C4A-CHB	-2.99	116.96	123.33
3	A	580	SRM	CAB-C3B-C4B	-2.97	106.01	111.19
3	B	570	SRM	CAA-CBA-CCA	2.94	120.33	112.49
3	B	570	SRM	C3A-C4A-NA	2.94	116.56	110.83
3	B	570	SRM	CAA-C3A-C2A	-2.91	106.17	114.19
3	B	570	SRM	CAD-CBD-CCD	-2.89	106.00	113.67
3	E	570	SRM	C4D-CHA-C1A	-2.86	120.60	125.87
3	B	570	SRM	CMA-C2A-CDA	-2.85	105.90	110.74
3	A	580	SRM	CAC-C3C-C4C	2.82	130.59	124.85
3	D	580	SRM	CAD-C2D-C3D	-2.81	116.56	125.30
3	B	570	SRM	CHA-C4D-C3D	-2.81	119.15	125.30
3	E	570	SRM	C2A-C1A-CHA	-2.80	121.03	123.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	580	SRM	C3A-C2A-C1A	-2.73	96.28	100.92
3	E	570	SRM	C3D-C4D-ND	2.68	113.13	110.15
3	D	580	SRM	C4B-NB-C1B	2.67	108.63	105.34
3	A	580	SRM	C4D-C3D-C2D	-2.67	104.01	106.81
3	B	570	SRM	CED-CDD-C3D	2.64	120.41	113.76
3	E	570	SRM	C4D-C3D-C2D	-2.63	104.05	106.81
3	E	570	SRM	C2C-C1C-NC	2.61	112.84	110.32
3	A	580	SRM	O2B-CCB-CBB	2.60	122.21	114.00
3	B	570	SRM	CAC-C3C-C4C	2.58	130.10	124.85
3	B	570	SRM	CHD-C1D-C2D	-2.58	119.65	125.30
3	E	570	SRM	CHC-C1C-C2C	-2.56	120.82	124.86
3	A	580	SRM	C1C-C2C-C3C	-2.53	104.01	106.84
3	B	570	SRM	CAA-C3A-C4A	-2.48	106.85	111.19
3	B	570	SRM	C2A-C3A-C4A	2.48	104.03	100.89
3	D	580	SRM	C2C-C1C-NC	2.48	112.71	110.32
3	B	570	SRM	C1C-CHC-C4B	-2.44	120.73	126.62
3	E	570	SRM	CBC-CAC-C3C	-2.42	105.84	112.53
3	A	580	SRM	CHD-C4C-C3C	-2.41	121.05	124.86
3	D	580	SRM	C3A-C4A-NA	-2.38	106.18	110.83
3	A	580	SRM	CAD-CBD-CCD	-2.36	107.40	113.67
3	B	570	SRM	C3A-C2A-C1A	-2.35	96.93	100.92
3	B	570	SRM	C1A-NA-C4A	-2.33	102.45	105.34
3	E	570	SRM	O4D-CED-CDD	2.33	121.72	114.51
3	A	580	SRM	CMA-C2A-C3A	-2.32	107.77	112.05
3	E	570	SRM	O4A-CEA-CDA	2.30	121.63	114.35
3	A	580	SRM	C4D-CHA-C1A	2.29	130.08	125.87
3	B	570	SRM	CEC-CDC-C2C	-2.28	108.03	113.76
3	E	570	SRM	CDA-C2A-C3A	2.26	114.34	108.37
3	A	580	SRM	O4A-CEA-O3A	-2.26	117.52	123.33
3	E	570	SRM	C1C-CHC-C4B	-2.26	121.18	126.62
3	D	580	SRM	CBB-CAB-C3B	2.22	120.93	114.65
3	B	570	SRM	O2A-CCA-CBA	2.20	120.94	114.00
3	D	580	SRM	C2D-C1D-ND	-2.17	107.75	110.15
3	D	580	SRM	C3B-C4B-CHC	2.16	127.92	123.33
3	A	580	SRM	C1A-NA-C4A	2.15	108.00	105.34
3	B	570	SRM	CAC-C3C-C2C	-2.13	124.24	129.24
3	E	570	SRM	O1C-CCC-CBC	-2.13	116.35	123.09
3	E	570	SRM	CDB-C2B-C3B	2.12	113.97	108.37
3	E	570	SRM	C1A-NA-C4A	-2.11	102.73	105.34
3	E	570	SRM	CMA-C2A-C3A	-2.04	108.28	112.05
3	E	570	SRM	CHD-C1D-ND	-2.03	120.18	123.86
3	A	580	SRM	O1B-CCB-CBB	-2.00	116.75	123.09

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	580	SRM	NC
3	B	570	SRM	NC
3	D	580	SRM	NC
3	D	580	SRM	C3A
3	E	570	SRM	C3B
3	E	570	SRM	NC

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	570	SRM	C4A-C3A-CAA-CBA
3	B	570	SRM	C4D-C3D-CDD-CED
3	D	580	SRM	C1A-C2A-CDA-CEA
3	D	580	SRM	C4A-C3A-CAA-CBA
3	D	580	SRM	C1B-C2B-CDB-CEB
3	D	580	SRM	C4D-C3D-CDD-CED
3	E	570	SRM	C1B-C2B-CDB-CEB
3	E	570	SRM	C4C-C3C-CAC-CBC
3	E	570	SRM	C2D-C3D-CDD-CED
5	A	590	GOL	O1-C1-C2-O2
5	A	590	GOL	O1-C1-C2-C3
5	A	590	GOL	C1-C2-C3-O3
3	E	570	SRM	C1D-C2D-CAD-CBD
3	B	570	SRM	C4B-C3B-CAB-CBB
3	D	580	SRM	C1D-C2D-CAD-CBD
3	D	580	SRM	C3C-CAC-CBC-CCC
3	E	570	SRM	C3B-CAB-CBB-CCB
3	E	570	SRM	CMB-C2B-CDB-CEB
3	E	570	SRM	C3B-C2B-CDB-CEB
3	A	580	SRM	C4D-C3D-CDD-CED
3	E	570	SRM	C2B-C3B-CAB-CBB
5	A	590	GOL	O2-C2-C3-O3
3	E	570	SRM	C2B-CDB-CEB-O4B
3	A	580	SRM	C2A-C3A-CAA-CBA
3	A	580	SRM	C3B-CAB-CBB-CCB
3	D	580	SRM	C2D-CAD-CBD-CCD
3	A	580	SRM	C1D-C2D-CAD-CBD
3	D	580	SRM	CMA-C2A-CDA-CEA
3	D	580	SRM	CMB-C2B-CDB-CEB
3	B	570	SRM	C3D-CDD-CED-O3D
3	B	570	SRM	C3D-CDD-CED-O4D
3	B	570	SRM	C2B-CDB-CEB-O3B

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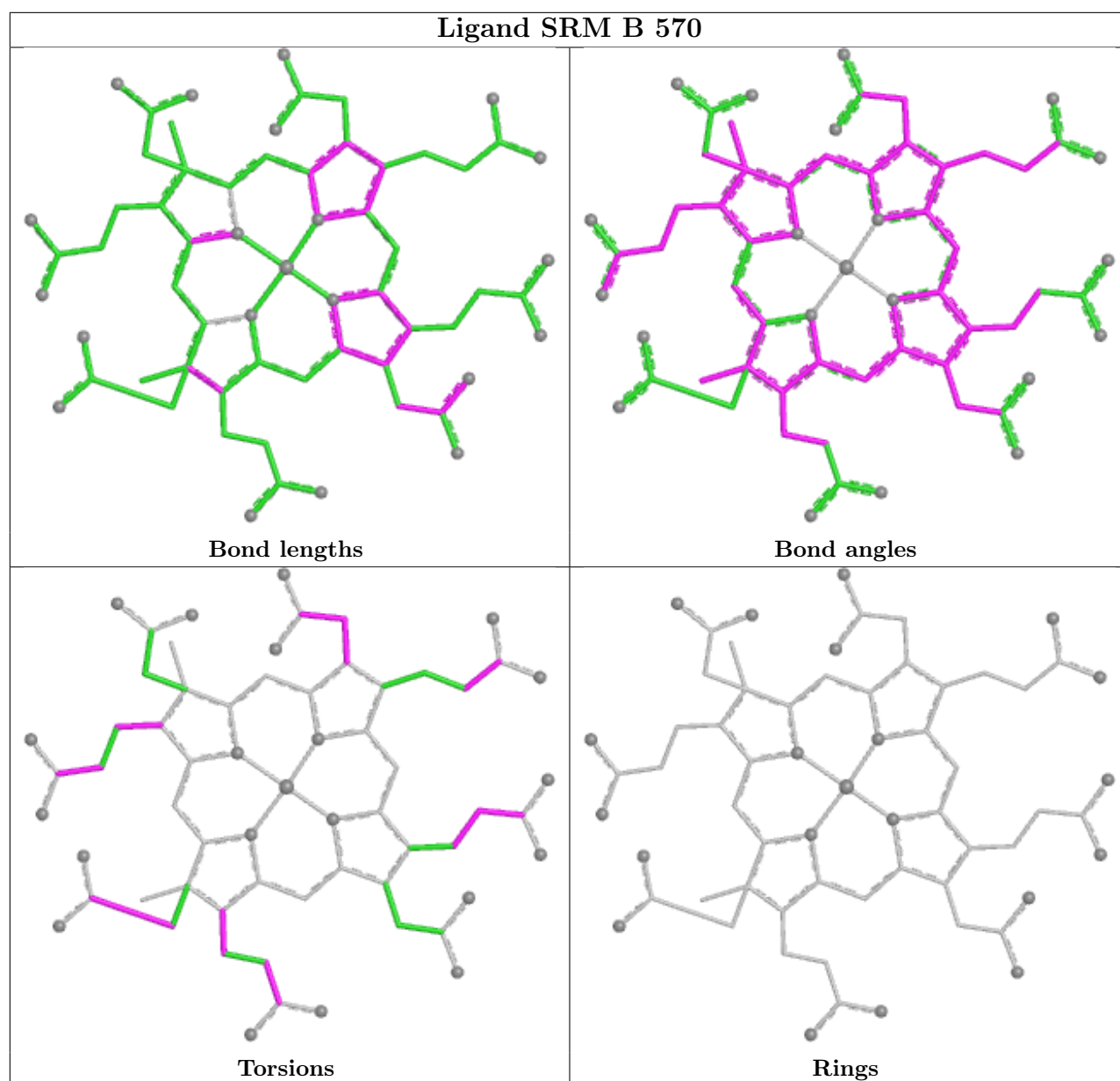
Mol	Chain	Res	Type	Atoms
3	E	570	SRM	C2B-CDB-CEB-O3B
3	B	570	SRM	C2B-CDB-CEB-O4B
3	A	580	SRM	C3D-CDD-CED-O3D
3	A	580	SRM	C3D-CDD-CED-O4D
3	D	580	SRM	C2C-CDC-CEC-O3C
3	E	570	SRM	C3D-CDD-CED-O3D
3	B	570	SRM	C3C-CAC-CBC-CCC
3	A	580	SRM	CAB-CBB-CCB-O1B
3	A	580	SRM	CAB-CBB-CCB-O2B
3	D	580	SRM	CAC-CBC-CCC-O1C
3	E	570	SRM	CAD-CBD-CCD-O1D
3	B	570	SRM	CAD-CBD-CCD-O1D
3	B	570	SRM	CAA-CBA-CCA-O1A
3	B	570	SRM	CAC-CBC-CCC-O1C
3	D	580	SRM	CAD-CBD-CCD-O1D
3	E	570	SRM	CAD-CBD-CCD-O2D
3	A	580	SRM	C2B-C3B-CAB-CBB
3	E	570	SRM	C2A-CDA-CEA-O3A
3	D	580	SRM	C2C-CDC-CEC-O4C
3	E	570	SRM	C3D-CDD-CED-O4D
3	B	570	SRM	CAC-CBC-CCC-O2C
3	D	580	SRM	CAC-CBC-CCC-O2C
3	B	570	SRM	CAA-CBA-CCA-O2A
3	D	580	SRM	CAD-CBD-CCD-O2D
3	B	570	SRM	CAD-CBD-CCD-O2D
3	E	570	SRM	C4A-C3A-CAA-CBA
3	A	580	SRM	CAC-CBC-CCC-O1C
3	D	580	SRM	CAA-CBA-CCA-O1A
3	D	580	SRM	CAB-CBB-CCB-O2B
3	E	570	SRM	C3A-CAA-CBA-CCA
3	D	580	SRM	CAA-CBA-CCA-O2A
3	B	570	SRM	CAB-CBB-CCB-O2B
3	B	570	SRM	CAB-CBB-CCB-O1B
3	D	580	SRM	CAB-CBB-CCB-O1B
3	A	580	SRM	CAC-CBC-CCC-O2C
3	E	570	SRM	C2A-CDA-CEA-O4A
3	E	570	SRM	CAC-CBC-CCC-O1C
3	E	570	SRM	CAC-CBC-CCC-O2C
3	A	580	SRM	CAA-CBA-CCA-O1A
3	D	580	SRM	C2B-C3B-CAB-CBB

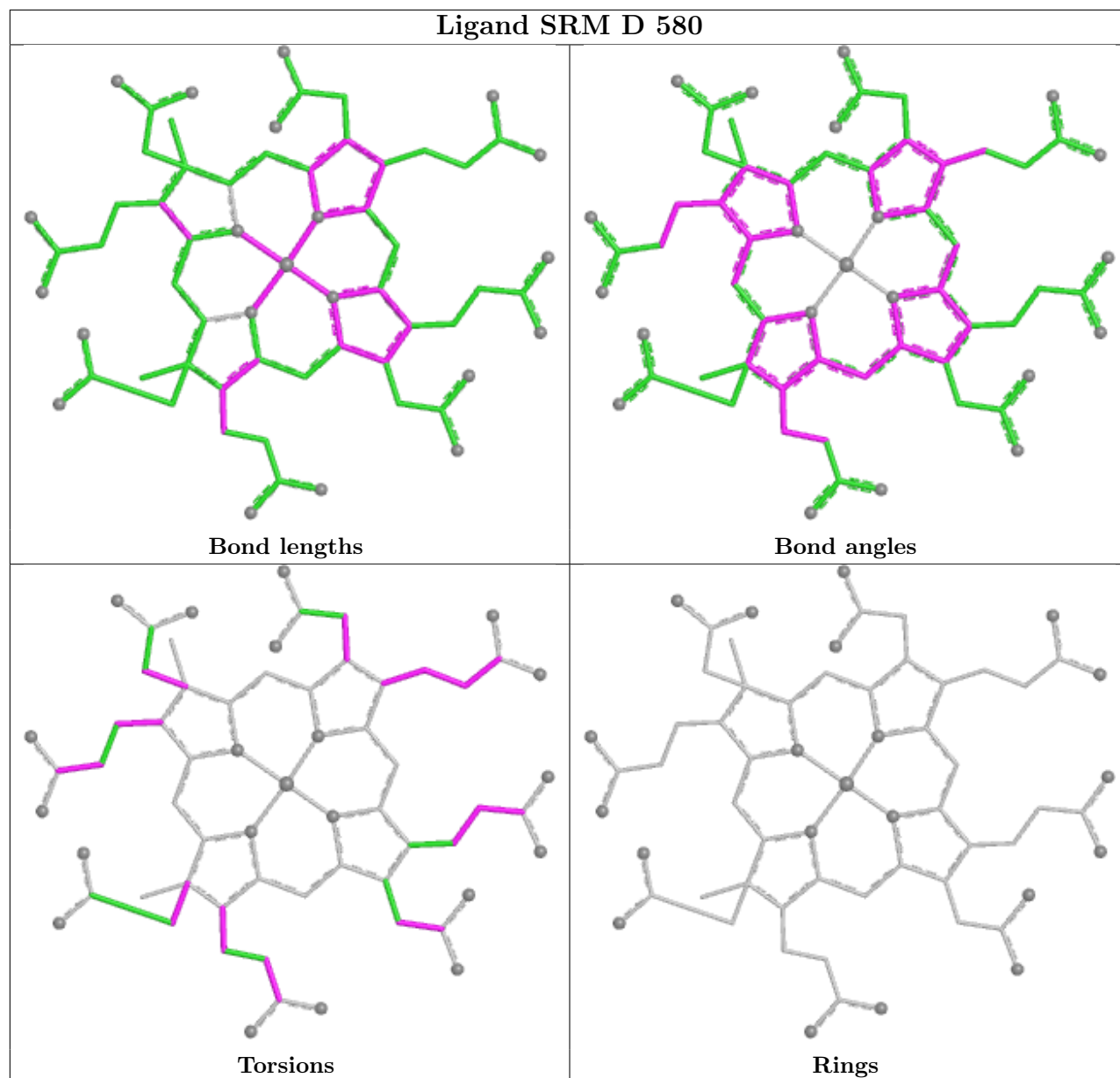
There are no ring outliers.

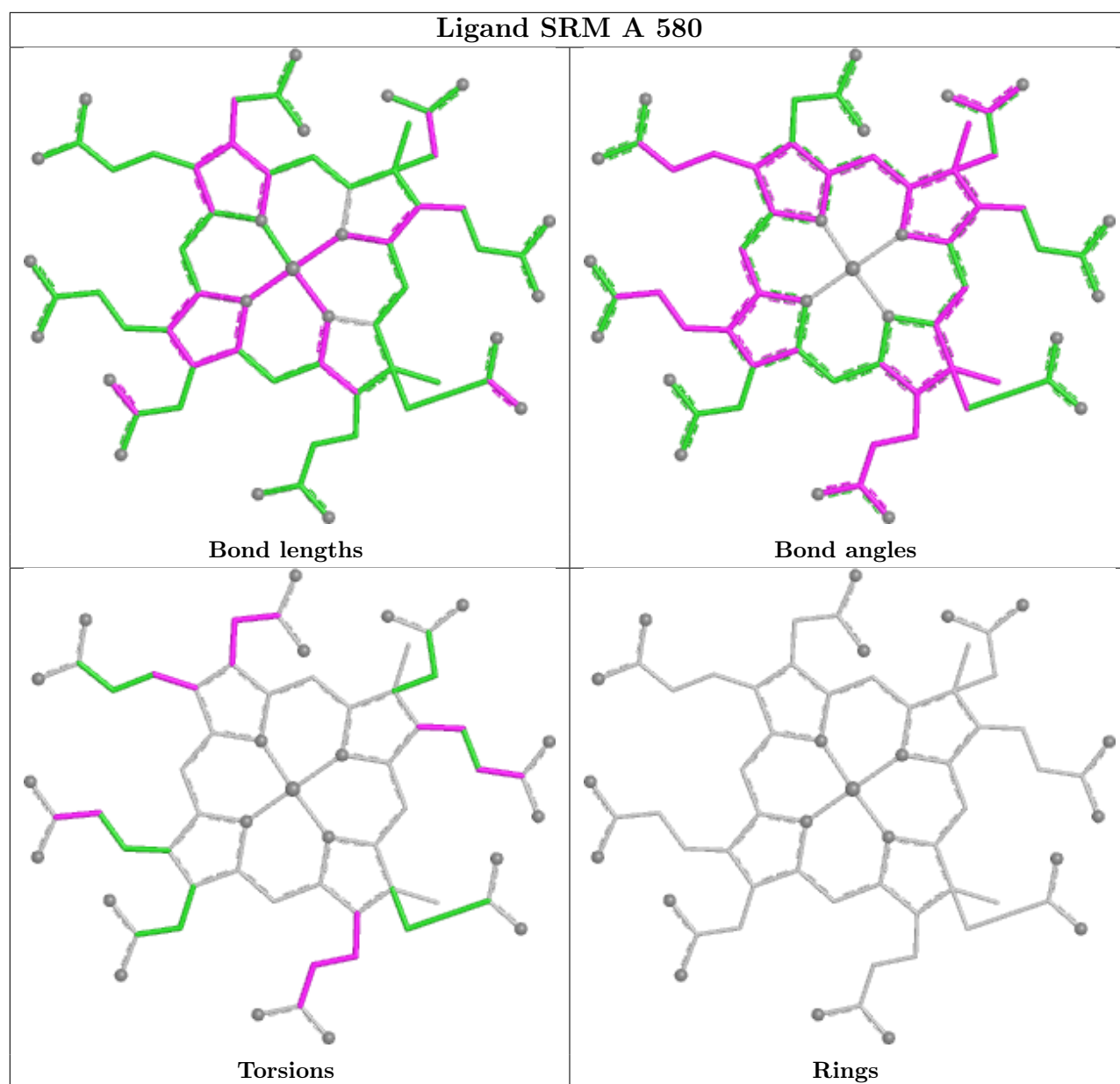
8 monomers are involved in 56 short contacts:

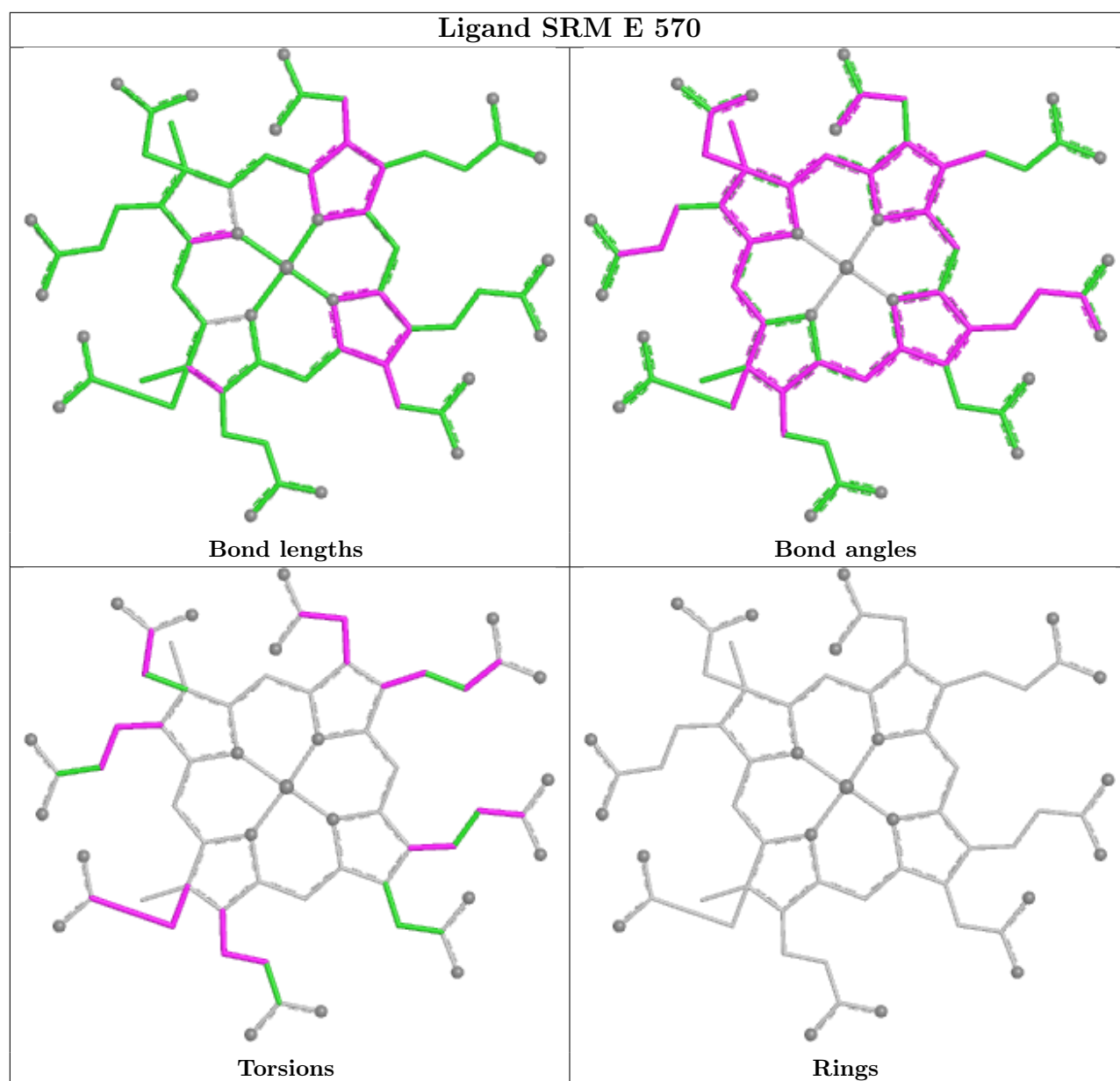
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	570	SRM	2	0
4	D	575	SF4	2	0
4	B	585	SF4	1	0
4	E	585	SF4	3	0
3	D	580	SRM	18	0
3	A	580	SRM	9	0
5	A	590	GOL	8	0
3	E	570	SRM	13	0

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	417/418 (99%)	1.20	77 (18%) 3 2	5, 12, 25, 58	0
1	D	417/418 (99%)	0.90	34 (8%) 17 18	4, 13, 25, 41	0
2	B	363/366 (99%)	1.12	47 (12%) 7 7	5, 11, 19, 57	0
2	E	363/366 (99%)	0.77	20 (5%) 30 30	2, 12, 33, 54	0
All	All	1560/1568 (99%)	1.00	178 (11%) 10 9	2, 12, 26, 58	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	415	GLY	9.1
1	A	417	TRP	8.3
2	B	5	GLY	7.3
1	A	406	ALA	6.7
2	B	4	GLU	5.4
1	A	407	TYR	4.9
1	A	404	PRO	4.8
1	D	417	TRP	4.7
1	A	409	GLU	4.4
2	B	366	TRP	4.3
1	A	413	LYS	4.3
1	A	402	LEU	4.3
2	B	257	PHE	3.8
1	A	414	ARG	3.8
1	A	410	GLU	3.7
1	D	148	PRO	3.7
1	A	396	PHE	3.7
1	A	9	LEU	3.6
2	B	181	MET	3.6
1	A	18	VAL	3.6
1	A	412	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	180	ASN	3.5
1	A	72	GLY	3.5
1	D	132	SER	3.5
2	E	207	ILE	3.4
1	A	393	PRO	3.3
2	E	232	LYS	3.2
2	B	232	LYS	3.2
1	A	371	ARG	3.2
1	A	32	ALA	3.2
1	A	405	SER	3.1
2	E	100	ILE	3.1
1	A	394	PHE	3.1
1	D	407	TYR	3.0
2	B	69	GLU	3.0
1	D	31	ALA	3.0
1	A	145	TYR	3.0
1	D	81	TYR	3.0
1	D	219	CYS	3.0
2	B	205	GLU	3.0
1	D	408	THR	3.0
1	A	93	HIS	3.0
1	D	415	GLY	3.0
1	D	33	ALA	2.9
2	B	184	ALA	2.9
1	A	380	GLU	2.9
2	B	182	CYS	2.9
1	A	278	LEU	2.8
1	A	162	ILE	2.8
1	A	111	ALA	2.8
1	A	115	LEU	2.8
2	B	351	THR	2.8
1	D	402	LEU	2.8
1	A	14	TRP	2.8
2	B	107	VAL	2.8
1	A	408	THR	2.8
2	B	229	MET	2.7
2	B	116	GLY	2.7
1	D	178	PRO	2.7
2	B	70	LEU	2.7
1	A	41	PRO	2.7
1	A	416	MET	2.7
1	D	181	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	413	LYS	2.7
1	D	93	HIS	2.6
1	D	77	VAL	2.6
1	D	106	PHE	2.6
1	A	158	ILE	2.6
2	E	229	MET	2.6
1	D	406	ALA	2.6
1	D	71	VAL	2.6
2	B	350	ILE	2.6
2	E	5	GLY	2.6
1	A	81	TYR	2.5
2	E	177	CYS	2.5
1	A	148	PRO	2.5
2	B	78	SER	2.5
1	A	411	LEU	2.5
1	A	277	GLU	2.5
1	A	137	ILE	2.5
1	A	399	LYS	2.5
1	A	276	LYS	2.5
1	D	75	GLY	2.5
2	B	17	ASP	2.5
1	A	27	LEU	2.5
1	A	86	GLU	2.4
1	A	25	ALA	2.4
1	A	108	SER	2.4
1	A	114	GLY	2.4
2	E	28	GLY	2.4
1	A	94	PHE	2.4
1	D	318	VAL	2.4
1	D	1	SER	2.4
2	B	209	LYS	2.4
2	B	77	TYR	2.4
1	D	317	PHE	2.4
1	A	91	VAL	2.4
1	D	30	LYS	2.4
1	A	125	GLY	2.3
1	A	150	PHE	2.3
2	B	278	MET	2.3
1	A	373	PHE	2.3
2	B	358	PHE	2.3
2	E	257	PHE	2.3
1	A	1	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	22	VAL	2.3
2	B	339	GLU	2.3
2	B	115	CYS	2.3
1	A	47	LEU	2.3
2	B	81	TYR	2.3
1	A	332	GLU	2.3
2	B	100	ILE	2.3
2	B	140	CYS	2.3
1	D	179	ALA	2.3
1	A	84	LEU	2.3
1	A	21	ILE	2.2
2	E	94	VAL	2.2
1	A	400	ASP	2.2
1	A	134	GLY	2.2
1	A	149	CYS	2.2
1	D	43	GLY	2.2
1	D	248	ALA	2.2
2	B	80	GLY	2.2
2	B	206	ALA	2.2
1	D	27	LEU	2.2
2	B	353	TYR	2.2
1	A	105	TRP	2.2
2	B	111	VAL	2.2
1	A	270	ALA	2.2
1	D	291	CYS	2.2
2	B	31	LYS	2.2
2	B	102	ASP	2.2
1	A	35	GLY	2.2
2	E	116	GLY	2.2
1	A	50	GLN	2.2
2	E	176	ALA	2.2
2	B	19	LEU	2.2
2	B	61	LEU	2.2
2	B	82	LEU	2.2
1	D	40	MET	2.2
2	E	297	PRO	2.1
1	A	271	ILE	2.1
2	B	108	GLN	2.1
1	A	381	ALA	2.1
2	B	360	ALA	2.1
1	A	56	LYS	2.1
2	B	250	MET	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	181	MET	2.1
2	B	364	PHE	2.1
2	E	35	VAL	2.1
2	E	112	GLY	2.1
1	A	6	LEU	2.1
1	A	112	LEU	2.1
1	D	405	SER	2.1
2	E	231	ASN	2.1
2	B	59	PRO	2.1
2	B	337	GLY	2.1
1	D	276	LYS	2.1
1	A	354	GLU	2.1
1	A	24	THR	2.1
1	A	127	THR	2.1
1	A	403	LYS	2.1
1	A	207	MET	2.0
1	D	92	GLU	2.0
1	A	392	ASN	2.0
2	E	246	ASN	2.0
1	A	175	CYS	2.0
2	E	298	THR	2.0
2	B	152	LYS	2.0
1	D	12	GLY	2.0
1	A	280	ILE	2.0
2	E	213	ILE	2.0
1	A	401	GLU	2.0
2	B	71	CYS	2.0
2	B	235	LYS	2.0
2	E	227	PRO	2.0
1	A	46	GLY	2.0
1	A	65	GLY	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

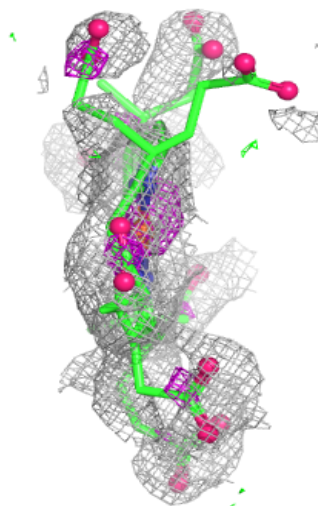
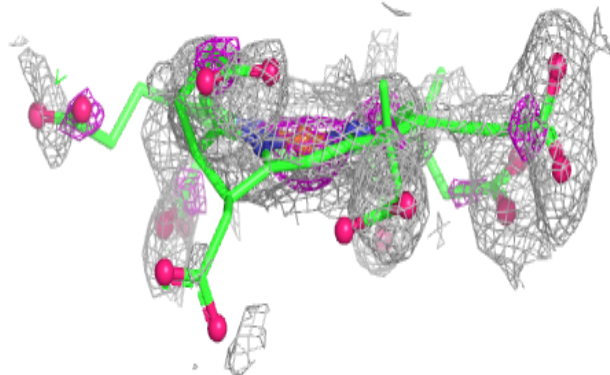
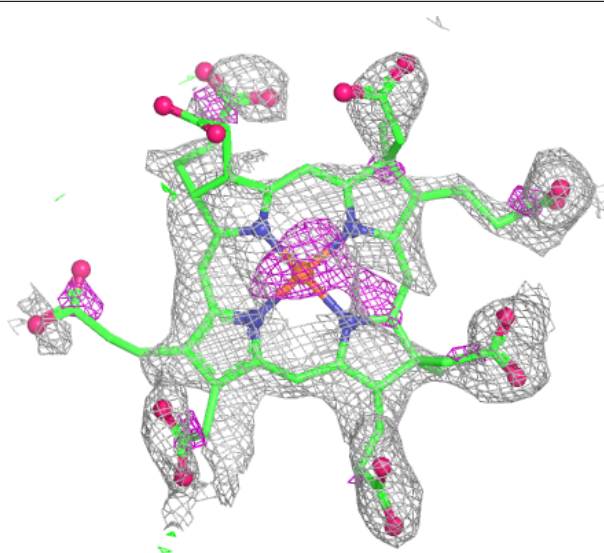
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SRM	D	580	63/63	0.73	0.17	40,56,68,71	0
3	SRM	E	570	63/63	0.84	0.12	11,15,19,22	0
4	SF4	E	585	8/8	0.92	0.22	32,34,36,40	0
5	GOL	A	590	6/6	0.93	0.11	25,30,37,42	0
4	SF4	D	576	8/8	0.94	0.17	7,10,10,10	0
3	SRM	A	580	63/63	0.94	0.09	16,23,33,41	0
3	SRM	B	570	63/63	0.94	0.08	6,8,13,16	0
4	SF4	D	575	8/8	0.95	0.19	6,7,7,8	0
4	SF4	E	586	8/8	0.95	0.14	20,22,24,24	0
4	SF4	A	576	8/8	0.95	0.10	4,5,6,6	0
4	SF4	B	585	8/8	0.97	0.05	16,19,20,36	0
4	SF4	A	575	8/8	0.97	0.06	7,8,10,11	0
4	SF4	B	586	8/8	0.99	0.04	19,22,24,25	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.

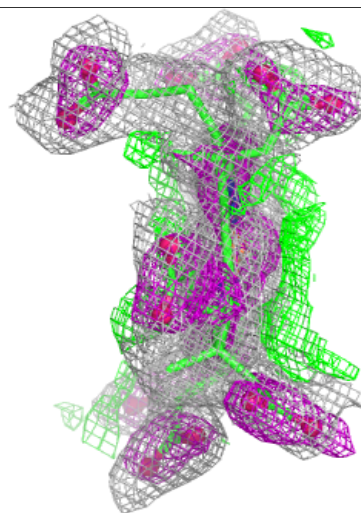
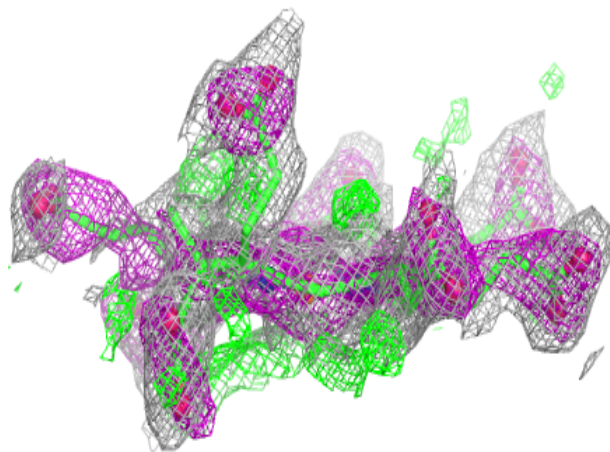
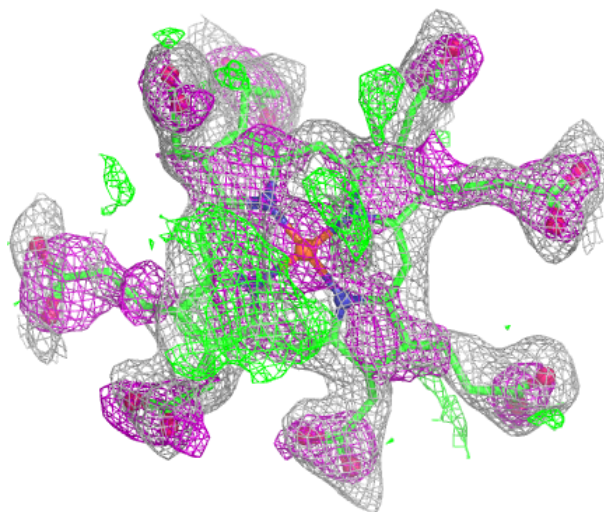
Electron density around SRM D 580:

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



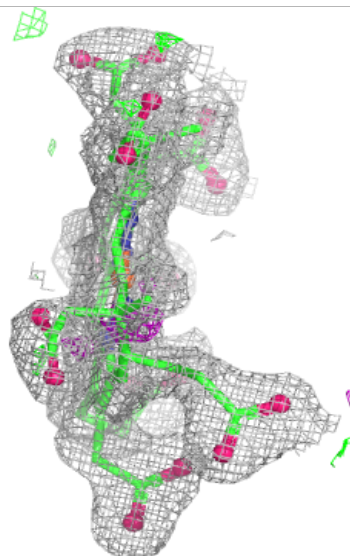
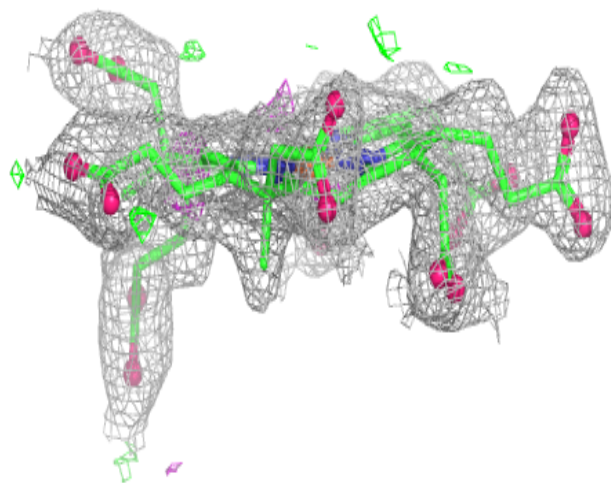
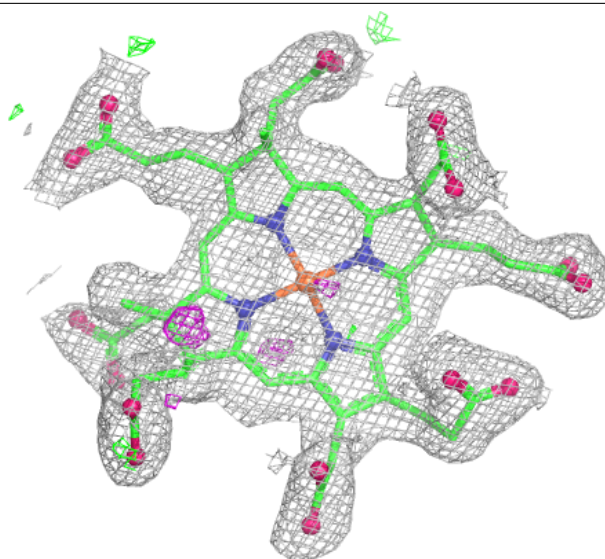
Electron density around SRM E 570:

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



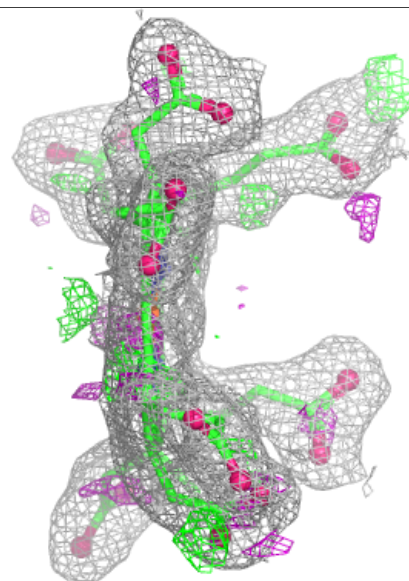
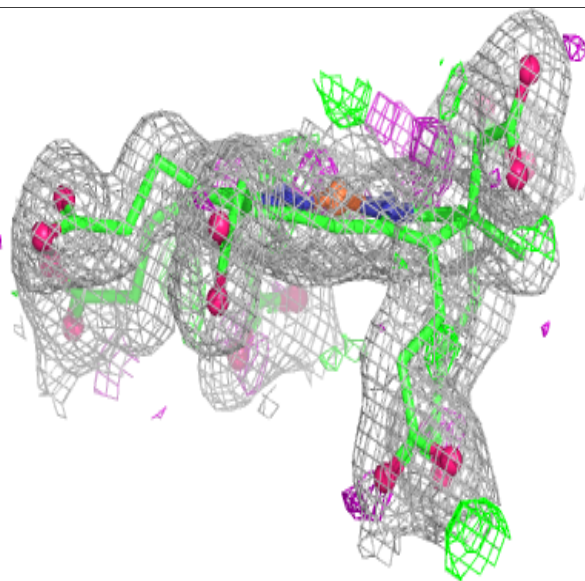
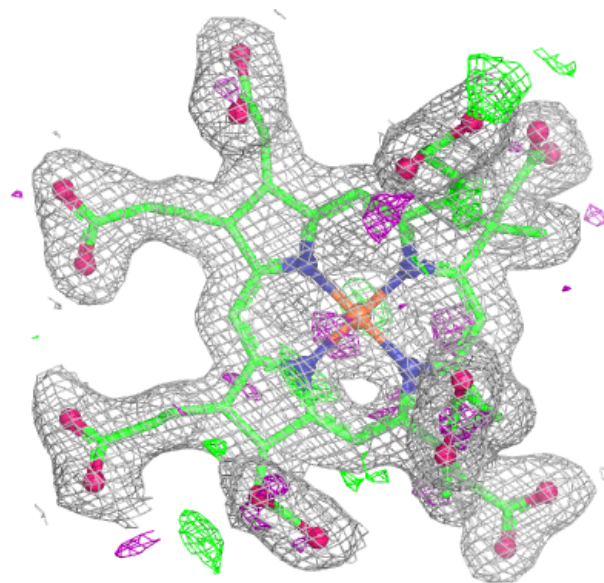
Electron density around SRM A 580:

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



Electron density around SRM B 570:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.