



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:14 pm BST

PDB ID : 3MMB
Title : Dissimilatory sulfite reductase in complex with the endproduct sulfide
Authors : Parey, K.; Warkentin, E.; Kroneck, P.M.H.; Ermler, U.
Deposited on : 2010-04-19
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

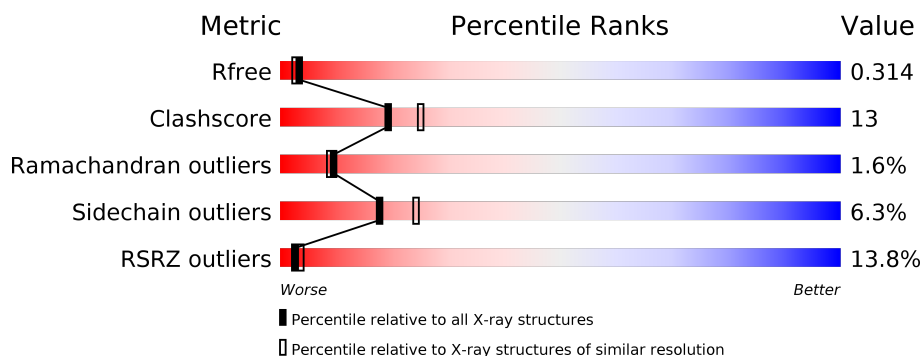
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	
1	D	418	
2	B	366	
2	E	366	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SRM	A	580	-	-	X	-
4	SF4	B	585	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12893 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.

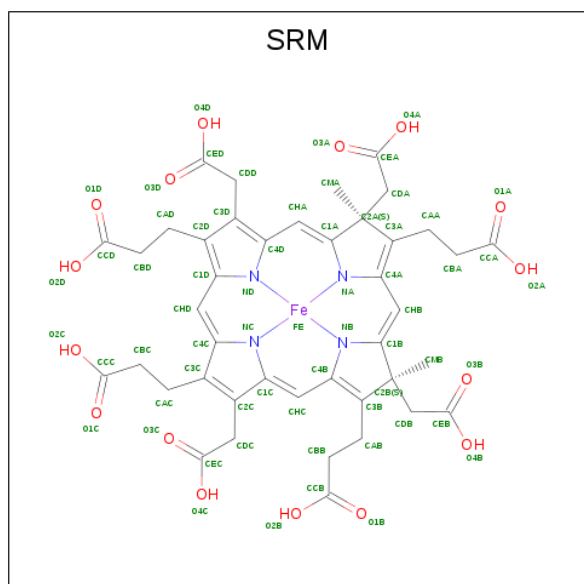
- Molecule 1 is a protein called Sulfite reductase, dissimilatory-type subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3330	2134	557	613	26			
1	D	417	Total	C	N	O	S	0	0	0
			3330	2134	557	613	26			

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

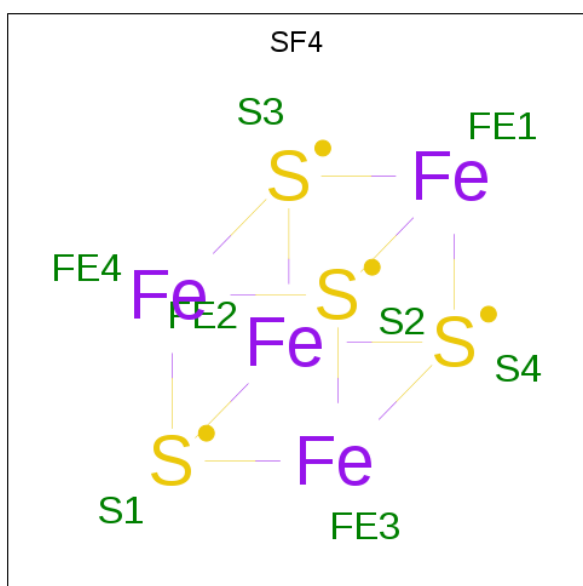
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			
2	E	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			

- Molecule 3 is SIROHEME (three-letter code: SRM) (formula: $C_{42}H_{42}FeN_4O_{16}$).



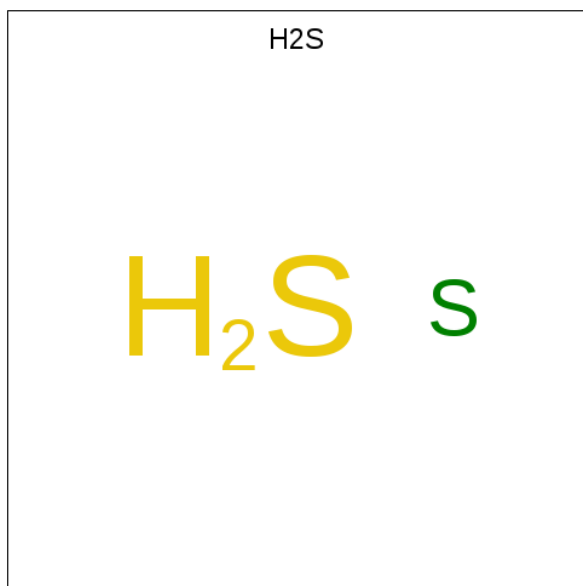
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	B	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	D	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	E	1	Total	C	Fe	N	O	
			63	42	1	4	16	

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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 HYDROSULFURIC ACID (three-letter code: H2S) (formula: H₂S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total S 1 1	0	0

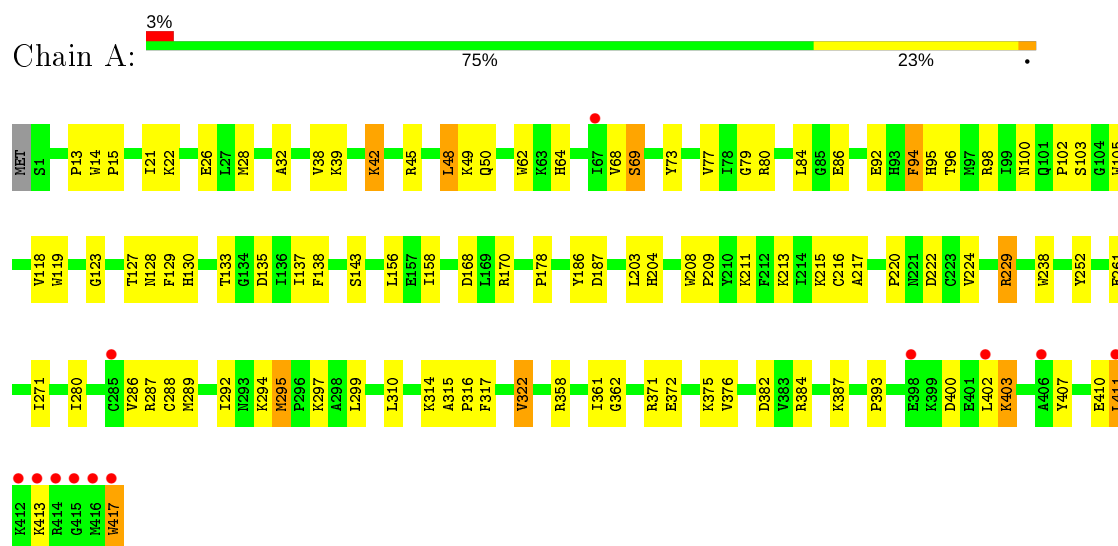
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	32	Total O 32 32	0	0
6	B	36	Total O 36 36	0	0
6	D	33	Total O 33 33	0	0
6	E	13	Total O 13 13	0	0

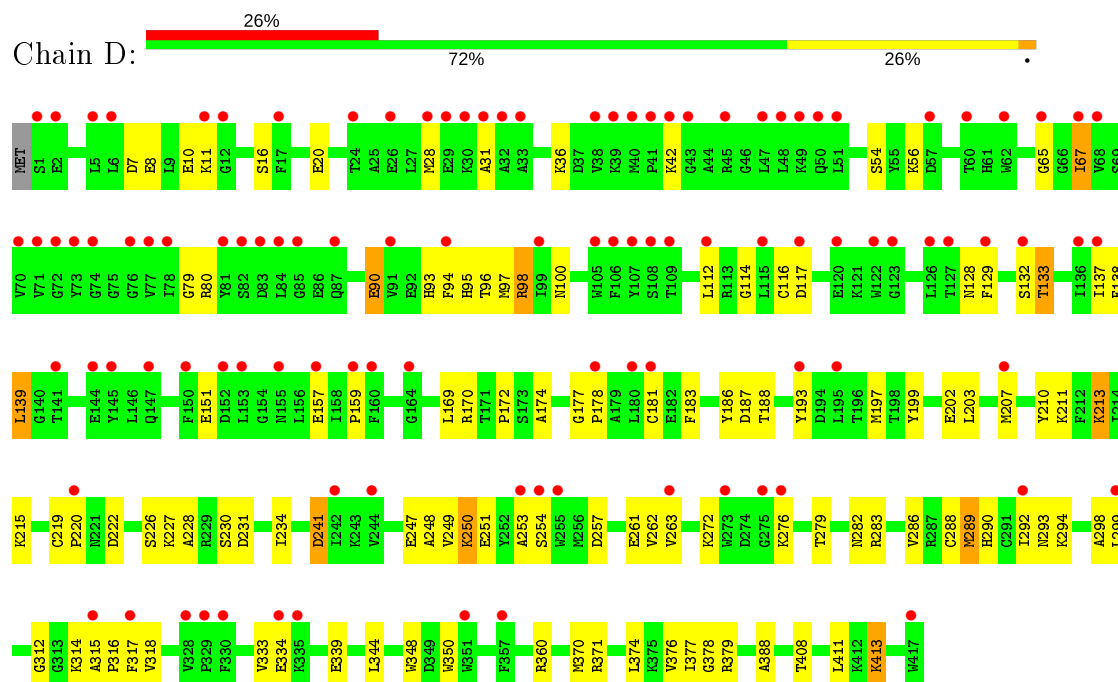
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

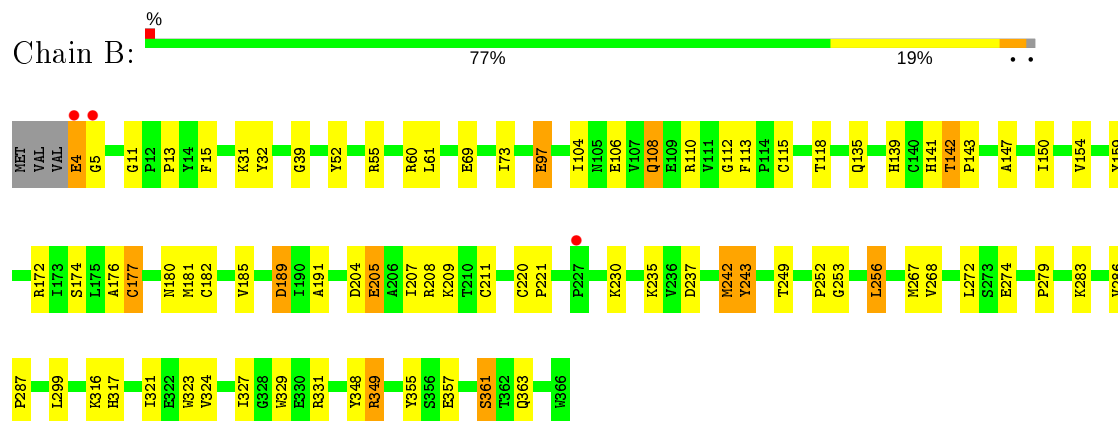
- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha



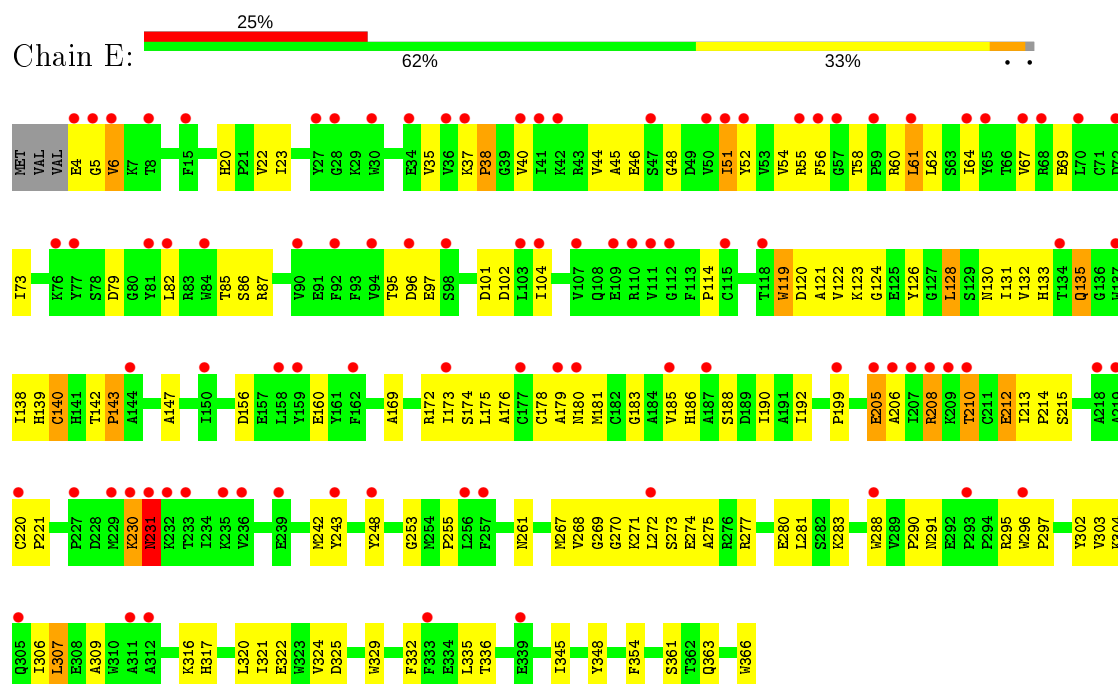
- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha



- 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	94.80Å 68.50Å 146.50Å 90.00° 107.50° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.30) 93.0 (19.96-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.255 , 0.302 0.269 , 0.314	Depositor DCC
R_{free} test set	3960 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 4.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.159 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12893	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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, H2S, 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	0.70	0/3417	0.77	2/4610 (0.0%)
1	D	0.49	0/3417	0.62	0/4610
2	B	0.74	1/2984 (0.0%)	0.80	0/4058
2	E	0.48	0/2984	0.67	1/4058 (0.0%)
All	All	0.61	1/12802 (0.0%)	0.72	3/17336 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	177	CYS	CB-SG	-7.84	1.69	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	61	LEU	CA-CB-CG	6.04	129.20	115.30
1	A	411	LEU	CA-CB-CG	5.88	128.82	115.30
1	A	84	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3330	0	3276	82	0
1	D	3330	0	3276	89	0
2	B	2901	0	2838	70	0
2	E	2901	0	2839	106	0
3	A	63	0	34	24	0
3	B	63	0	34	7	0
3	D	63	0	34	13	0
3	E	63	0	34	13	0
4	A	16	0	0	0	0
4	B	16	0	0	2	0
4	D	16	0	0	1	0
4	E	16	0	0	1	0
5	A	1	0	0	0	0
6	A	32	0	0	1	0
6	B	36	0	0	1	0
6	D	33	0	0	6	0
6	E	13	0	0	4	0
All	All	12893	0	12365	322	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 13.

All (322) 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)
4:D:575:SF4:S4	6:D:439:HOH:O	1.93	1.21
1:D:315:ALA:HB1	1:D:316:PRO:HD2	1.26	1.14
2:E:230:LYS:HB2	2:E:231:ASN:HB2	1.29	1.07
1:D:413:LYS:NZ	6:D:430:HOH:O	1.96	0.97
1:D:211:LYS:HD3	1:D:213:LYS:HE3	1.45	0.96
2:E:121:ALA:HB2	3:E:570:SRM:O3D	1.65	0.95
1:A:215:LYS:HE2	1:A:229:ARG:HD3	1.48	0.93
2:E:230:LYS:CB	2:E:231:ASN:HB2	1.99	0.93
1:A:80:ARG:NH2	3:A:580:SRM:O2A	2.02	0.92
2:E:55:ARG:HH22	3:E:570:SRM:HBA2	1.37	0.88
2:E:140:CYS:HG	4:E:585:SF4:FE2	0.79	0.87
2:E:176:ALA:HB2	2:E:185:VAL:HG21	1.58	0.84
2:B:274:GLU:OE1	2:B:363:GLN:NE2	2.10	0.84
3:A:580:SRM:O1A	2:B:139:HIS:HD2	1.60	0.84
1:D:183:PHE:HB2	6:D:439:HOH:O	1.79	0.82
1:D:170:ARG:HG3	1:D:213:LYS:HE2	1.62	0.81
3:E:570:SRM:O4D	3:E:570:SRM:HHA	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:230:LYS:HB2	2:E:231:ASN:CB	2.10	0.80
1:A:314:LYS:HG2	1:A:322:VAL:HG23	1.64	0.80
2:E:85:THR:HB	3:E:570:SRM:HAB2	1.64	0.79
1:D:262:VAL:HG22	1:D:294:LYS:HG2	1.63	0.79
2:B:177:CYS:HB2	4:B:585:SF4:S3	2.23	0.78
2:B:349:ARG:HG3	2:B:349:ARG:HH11	1.48	0.78
1:D:211:LYS:CD	1:D:213:LYS:HE3	2.14	0.77
2:B:185:VAL:HG12	2:B:191:ALA:HB1	1.67	0.77
2:B:349:ARG:HA	2:E:354:PHE:HE2	1.50	0.76
1:A:413:LYS:HG2	1:A:413:LYS:O	1.85	0.75
3:D:580:SRM:HHB	3:D:580:SRM:HBA2	1.68	0.75
2:E:309:ALA:HB3	2:E:336:THR:HG22	1.68	0.75
1:D:219:CYS:SG	6:D:439:HOH:O	2.44	0.74
2:E:86:SER:OG	3:E:570:SRM:HAB1	1.87	0.74
1:D:317:PHE:HE2	2:E:180:ASN:HD22	1.34	0.74
1:D:178:PRO:HG3	1:D:187:ASP:HA	1.71	0.73
2:E:126:TYR:CD1	2:E:169:ALA:HA	2.23	0.73
1:A:417:TRP:CD1	1:A:417:TRP:C	2.63	0.72
2:E:124:GLY:HA3	2:E:316:LYS:HD2	1.72	0.72
2:E:230:LYS:CA	2:E:231:ASN:HB2	2.19	0.72
2:B:349:ARG:HA	2:E:354:PHE:CE2	2.25	0.71
2:E:128:LEU:HD21	2:E:173:ILE:HD12	1.74	0.70
1:D:248:ALA:HB3	1:D:298:ALA:HB2	1.72	0.69
1:A:322:VAL:HG12	2:B:355:TYR:CZ	2.27	0.69
1:D:315:ALA:HB1	1:D:316:PRO:CD	2.14	0.69
1:A:403:LYS:HB3	2:E:261:ASN:OD1	1.93	0.68
1:D:215:LYS:HG3	1:D:230:SER:HB3	1.74	0.68
2:B:176:ALA:HB2	2:B:185:VAL:HG21	1.74	0.68
3:A:580:SRM:O1A	2:B:139:HIS:CD2	2.45	0.68
1:A:322:VAL:HG12	2:B:355:TYR:CE1	2.28	0.68
3:A:580:SRM:CBB	3:A:580:SRM:CMB	2.73	0.67
2:B:205:GLU:OE2	2:B:209:LYS:NZ	2.28	0.67
1:D:374:LEU:HB3	1:D:379:ARG:O	1.95	0.66
1:A:127:THR:O	2:B:61:LEU:HD12	1.95	0.66
2:E:199:PRO:HA	6:E:377:HOH:O	1.95	0.66
1:D:16:SER:O	1:D:20:GLU:HG2	1.96	0.66
3:E:570:SRM:HDA1	6:E:376:HOH:O	1.94	0.66
3:A:580:SRM:C4C	2:B:182:CYS:HA	2.27	0.65
3:D:580:SRM:CDD	3:D:580:SRM:HBD2	2.26	0.65
1:D:211:LYS:NZ	3:D:580:SRM:HDD2	2.12	0.64
1:D:133:THR:OG1	3:D:580:SRM:HAB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:O	1:A:69:SER:HB3	1.97	0.64
2:E:55:ARG:NH2	3:E:570:SRM:HBA2	2.11	0.64
1:A:62:TRP:HB3	1:A:80:ARG:HD2	1.80	0.63
3:A:580:SRM:CMB	3:A:580:SRM:HBB2	2.29	0.63
1:A:288:CYS:O	1:A:289:MET:HB2	1.98	0.62
3:B:570:SRM:HDD2	3:B:570:SRM:HBD2	1.81	0.62
1:D:65:GLY:H	1:D:80:ARG:NH1	1.98	0.62
1:A:186:TYR:OH	1:A:216:CYS:HB3	2.00	0.62
1:D:128:ASN:HB2	1:D:137:ILE:HB	1.81	0.62
1:D:249:VAL:HG23	1:D:298:ALA:HB1	1.82	0.62
2:E:206:ALA:O	2:E:210:THR:OG1	2.19	0.61
2:E:212:GLU:HB2	6:E:374:HOH:O	2.01	0.61
1:A:271:ILE:HD12	1:A:280:ILE:HG12	1.83	0.61
1:A:211:LYS:NZ	3:A:580:SRM:HAD1	2.15	0.60
2:B:189:ASP:O	2:B:268:VAL:HA	2.01	0.60
2:E:277:ARG:NH2	2:E:280:GLU:OE1	2.34	0.60
1:D:286:VAL:HB	2:E:363:GLN:HG3	1.84	0.59
1:A:94:PHE:O	2:B:139:HIS:HE1	1.86	0.59
1:A:68:VAL:HG13	1:A:77:VAL:HG12	1.83	0.59
2:E:291:ASN:HA	2:E:296:TRP:HE1	1.68	0.59
2:B:331:ARG:NH2	2:E:366:TRP:O	2.36	0.58
1:D:317:PHE:HE2	2:E:180:ASN:ND2	1.99	0.58
1:A:96:THR:HG23	2:B:139:HIS:NE2	2.18	0.58
3:A:580:SRM:HMB1	3:A:580:SRM:CBB	2.34	0.58
2:B:142:THR:N	2:B:143:PRO:CD	2.66	0.58
2:E:51:ILE:HD12	2:E:95:THR:HG22	1.84	0.58
1:D:315:ALA:CB	1:D:316:PRO:HD2	2.13	0.58
3:A:580:SRM:HMB3	3:A:580:SRM:HBB2	1.86	0.58
1:D:371:ARG:NH1	6:D:418:HOH:O	2.26	0.58
2:B:55:ARG:O	2:B:115:CYS:HA	2.04	0.58
3:D:580:SRM:HBD2	3:D:580:SRM:HDD1	1.87	0.57
3:D:580:SRM:O4D	3:D:580:SRM:HHA	2.04	0.57
1:D:292:ILE:HG23	1:D:299:LEU:O	2.05	0.57
2:B:349:ARG:HG3	2:B:349:ARG:NH1	2.17	0.57
1:A:292:ILE:HG23	1:A:299:LEU:O	2.04	0.56
2:E:175:LEU:HA	2:E:192:ILE:O	2.05	0.56
2:B:331:ARG:NH1	1:D:283:ARG:O	2.38	0.56
2:B:204:ASP:O	2:B:208:ARG:HG3	2.06	0.56
1:A:215:LYS:HE2	1:A:229:ARG:CD	2.30	0.56
1:A:64:HIS:HE1	2:B:249:THR:O	1.88	0.56
1:D:98:ARG:CZ	3:D:580:SRM:HMB3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:133:HIS:HB2	2:E:147:ALA:HB1	1.88	0.56
2:E:304:LYS:C	2:E:306:ILE:H	2.08	0.56
1:A:98:ARG:HH21	3:A:580:SRM:HMB3	1.69	0.55
2:E:119:TRP:HE1	3:E:570:SRM:HDD2	1.70	0.55
1:D:183:PHE:HE2	1:D:293:ASN:OD1	1.90	0.55
1:A:45:ARG:O	1:A:49:LYS:HG3	2.06	0.55
1:D:183:PHE:CB	6:D:439:HOH:O	2.46	0.55
1:D:228:ALA:HB2	2:E:272:LEU:CD2	2.36	0.55
2:B:348:TYR:O	2:E:354:PHE:HD2	1.90	0.55
1:A:252:TYR:CD2	1:A:295:MET:HG3	2.42	0.55
1:A:286:VAL:CG2	2:B:363:GLN:HG2	2.36	0.54
2:B:52:TYR:CE1	2:B:97:GLU:HB3	2.42	0.54
1:D:181:CYS:SG	1:D:183:PHE:HB2	2.48	0.54
1:D:248:ALA:CB	1:D:298:ALA:HB2	2.36	0.54
2:B:207:ILE:HG13	2:B:253:GLY:HA3	1.89	0.54
3:B:570:SRM:CBA	3:B:570:SRM:HMA3	2.37	0.54
2:E:316:LYS:O	2:E:317:HIS:HB2	2.07	0.54
1:D:65:GLY:HA3	1:D:79:GLY:O	2.07	0.54
2:B:349:ARG:CA	2:E:354:PHE:HE2	2.19	0.54
1:A:393:PRO:HG3	2:E:181:MET:HE3	1.88	0.54
2:E:172:ARG:HH21	3:E:570:SRM:C2C	2.21	0.54
3:A:580:SRM:HDA2	4:B:585:SF4:S1	2.49	0.53
1:D:316:PRO:HG3	2:E:179:ALA:O	2.09	0.53
2:B:147:ALA:HB2	2:B:177:CYS:SG	2.48	0.53
1:A:119:TRP:CH2	1:A:138:PHE:HB3	2.43	0.53
2:B:104:ILE:O	2:B:108:GLN:HG2	2.09	0.52
1:D:317:PHE:CE2	2:E:180:ASN:ND2	2.76	0.52
1:D:257:ASP:O	1:D:261:GLU:HB2	2.08	0.52
3:D:580:SRM:HDD2	3:D:580:SRM:HBD2	1.90	0.52
1:A:211:LYS:HZ2	3:A:580:SRM:HAD1	1.75	0.52
1:A:238:TRP:CZ2	1:A:287:ARG:HG2	2.44	0.52
1:D:211:LYS:HZ1	3:D:580:SRM:HDD2	1.75	0.52
1:D:288:CYS:O	1:D:289:MET:HB2	2.10	0.52
2:E:20:HIS:HB3	2:E:23:ILE:HD12	1.91	0.52
1:A:94:PHE:O	2:B:139:HIS:CE1	2.63	0.52
1:D:94:PHE:O	2:E:139:HIS:NE2	2.40	0.52
1:A:314:LYS:HG2	1:A:322:VAL:CG2	2.37	0.52
2:B:279:PRO:HD2	2:B:361:SER:HB2	1.92	0.52
1:A:21:ILE:HG21	1:A:48:LEU:HB2	1.91	0.51
1:D:199:TYR:HB3	1:D:202:GLU:HB2	1.92	0.51
2:E:156:ASP:OD2	2:E:295:ARG:NH1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:580:SRM:CHB	3:D:580:SRM:HBA2	2.39	0.51
2:B:272:LEU:HD12	3:B:570:SRM:HBC1	1.93	0.51
2:B:108:GLN:NE2	2:B:113:PHE:O	2.44	0.51
1:A:135:ASP:OD1	3:A:580:SRM:O1B	2.29	0.51
1:D:231:ASP:CG	1:D:360:ARG:HH21	2.14	0.51
2:B:150:ILE:O	2:B:154:VAL:HG23	2.10	0.51
1:D:241:ASP:OD2	1:D:282:ASN:ND2	2.44	0.51
2:E:304:LYS:C	2:E:306:ILE:N	2.64	0.51
1:D:312:GLY:O	1:D:314:LYS:HG2	2.11	0.50
2:E:20:HIS:CE1	2:E:22:VAL:HB	2.47	0.50
1:A:403:LYS:HB2	1:A:403:LYS:NZ	2.27	0.50
1:A:13:PRO:HB2	2:B:159:TYR:CD1	2.47	0.50
1:D:28:MET:SD	2:E:64:ILE:HD11	2.51	0.50
2:E:40:VAL:HG13	2:E:54:VAL:HG22	1.93	0.50
1:A:118:VAL:HG21	1:A:156:LEU:HD11	1.94	0.50
1:A:372:GLU:O	1:A:376:VAL:HG23	2.12	0.49
1:A:79:GLY:HA2	1:A:95:HIS:ND1	2.27	0.49
1:A:102:PRO:HG3	2:B:13:PRO:HG2	1.93	0.49
1:A:14:TRP:CD2	1:A:15:PRO:HD2	2.47	0.49
2:B:242:MET:C	2:B:243:TYR:CG	2.85	0.49
1:D:112:LEU:HD12	2:E:82:LEU:HD21	1.95	0.49
2:B:211:CYS:SG	2:B:252:PRO:HD2	2.53	0.49
1:D:8:GLU:HA	1:D:11:LYS:HZ2	1.78	0.49
1:A:203:LEU:HD23	1:A:203:LEU:C	2.33	0.49
1:A:417:TRP:HD1	1:A:417:TRP:O	1.95	0.49
2:E:212:GLU:HB3	2:E:215:SER:OG	2.13	0.49
1:A:168:ASP:OD1	1:A:170:ARG:HD3	2.11	0.49
1:A:314:LYS:CG	1:A:322:VAL:HG23	2.39	0.49
1:A:213:LYS:NZ	3:A:580:SRM:O1C	2.45	0.49
1:A:127:THR:O	2:B:61:LEU:CD1	2.61	0.49
1:A:103:SER:HB2	2:B:15:PHE:HB3	1.95	0.49
2:E:102:ASP:O	6:E:370:HOH:O	2.20	0.49
2:E:173:ILE:HA	2:E:190:ILE:O	2.12	0.49
1:A:220:PRO:HB3	2:B:274:GLU:HG3	1.95	0.48
1:A:417:TRP:HD1	1:A:417:TRP:C	2.13	0.48
2:E:132:VAL:HG22	2:E:174:SER:OG	2.13	0.48
2:E:205:GLU:HG3	2:E:208:ARG:NH1	2.27	0.48
2:E:69:GLU:O	2:E:73:ILE:HG13	2.13	0.48
2:E:296:TRP:N	2:E:297:PRO:HD3	2.28	0.48
1:A:68:VAL:O	1:A:69:SER:CB	2.61	0.48
1:D:186:TYR:CD1	1:D:333:VAL:HG11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:VAL:O	2:E:348:TYR:OH	2.27	0.48
2:E:51:ILE:HG13	2:E:52:TYR:H	1.78	0.48
1:D:377:ILE:HG13	1:D:379:ARG:HG2	1.96	0.48
2:B:141:HIS:O	6:B:382:HOH:O	2.20	0.48
2:B:108:GLN:O	2:B:112:GLY:HA2	2.13	0.47
2:B:256:LEU:H	2:B:256:LEU:HD23	1.79	0.47
2:E:142:THR:N	2:E:143:PRO:HD3	2.29	0.47
2:E:291:ASN:HA	2:E:296:TRP:NE1	2.28	0.47
1:A:252:TYR:CE2	1:A:295:MET:HG3	2.49	0.47
1:D:215:LYS:HB2	1:D:226:SER:CB	2.44	0.47
2:E:281:LEU:O	2:E:283:LYS:NZ	2.44	0.47
1:D:202:GLU:N	1:D:202:GLU:OE1	2.48	0.47
1:D:314:LYS:NZ	1:D:315:ALA:O	2.47	0.47
3:A:580:SRM:NC	2:B:182:CYS:HA	2.29	0.47
2:E:363:GLN:HB2	2:E:363:GLN:HE21	1.59	0.47
2:E:277:ARG:NH1	2:E:325:ASP:OD2	2.39	0.47
1:A:22:LYS:O	1:A:26:GLU:HG3	2.14	0.46
1:A:315:ALA:HB1	1:A:316:PRO:CD	2.45	0.46
1:A:382:ASP:OD1	1:A:384:ARG:HD2	2.14	0.46
2:E:37:LYS:HB2	2:E:38:PRO:HD2	1.97	0.46
2:E:176:ALA:CB	2:E:181:MET:HA	2.45	0.46
1:D:129:PHE:HB2	2:E:62:LEU:HD12	1.96	0.46
2:E:316:LYS:HG2	2:E:317:HIS:CD2	2.51	0.46
3:A:580:SRM:C3D	2:B:180:ASN:HB3	2.46	0.46
2:B:176:ALA:HB1	2:B:181:MET:HA	1.98	0.46
2:E:35:VAL:HG21	2:E:120:ASP:HB3	1.98	0.46
1:D:151:GLU:HG3	2:E:6:VAL:HG13	1.97	0.46
2:B:39:GLY:HA2	2:B:118:THR:HG23	1.98	0.46
1:D:213:LYS:O	1:D:230:SER:HB2	2.16	0.46
2:E:302:TYR:O	2:E:306:ILE:HG13	2.16	0.46
2:E:268:VAL:HG13	2:E:320:LEU:HD22	1.98	0.46
1:A:13:PRO:HB2	2:B:159:TYR:CE1	2.50	0.45
2:E:130:ASN:OD1	2:E:131:ILE:N	2.48	0.45
2:B:316:LYS:HG2	2:B:317:HIS:CD2	2.51	0.45
2:E:280:GLU:HG2	2:E:321:ILE:HG12	1.98	0.45
2:E:320:LEU:O	2:E:324:VAL:HG23	2.16	0.45
3:E:570:SRM:O2A	3:E:570:SRM:HMA3	2.16	0.45
2:E:274:GLU:OE1	2:E:361:SER:OG	2.34	0.45
1:D:116:CYS:SG	2:E:67:VAL:HB	2.56	0.45
3:B:570:SRM:C1A	3:B:570:SRM:HBA1	2.47	0.45
1:D:211:LYS:HZ2	3:D:580:SRM:HDD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:277:ARG:HG2	2:E:322:GLU:HG2	1.98	0.45
2:E:283:LYS:HD3	2:E:329:TRP:CZ2	2.51	0.45
1:A:158:ILE:HD11	6:A:427:HOH:O	2.15	0.45
1:D:317:PHE:HB2	3:D:580:SRM:O1D	2.16	0.45
1:A:73:TYR:CD1	1:A:204:HIS:HB3	2.52	0.45
1:A:286:VAL:HG23	2:B:363:GLN:HG2	1.98	0.45
2:E:270:GLY:HA2	2:E:280:GLU:O	2.17	0.45
2:B:69:GLU:O	2:B:73:ILE:HG13	2.17	0.45
1:D:90:GLU:H	1:D:90:GLU:CD	2.19	0.45
1:A:361:ILE:HG23	1:A:362:GLY:N	2.32	0.45
1:D:290:HIS:HB2	2:E:275:ALA:HB1	1.99	0.45
2:E:220:CYS:HA	2:E:221:PRO:HD3	1.82	0.45
3:E:570:SRM:HBA1	3:E:570:SRM:CHB	2.44	0.45
2:B:220:CYS:HA	2:B:221:PRO:HD3	1.83	0.45
2:E:40:VAL:HG22	2:E:54:VAL:HG13	1.99	0.45
2:B:4:GLU:HB3	2:B:5:GLY:H	1.64	0.44
1:D:339:GLU:OE2	1:D:379:ARG:NH2	2.41	0.44
1:A:208:TRP:HB3	1:A:209:PRO:HD2	1.99	0.44
1:A:387:LYS:N	2:B:357:GLU:O	2.49	0.44
2:B:237:ASP:C	2:B:237:ASP:OD1	2.56	0.44
2:E:55:ARG:NH2	3:E:570:SRM:HMB2	2.31	0.44
1:D:169:LEU:O	1:D:203:LEU:HG	2.17	0.44
1:A:42:LYS:HB2	1:A:42:LYS:HE3	1.51	0.44
1:D:170:ARG:O	1:D:172:PRO:HD3	2.17	0.44
1:D:250:LYS:O	1:D:253:ALA:N	2.39	0.44
1:A:168:ASP:OD2	1:A:203:LEU:O	2.35	0.43
2:E:183:GLY:O	2:E:186:HIS:CE1	2.71	0.43
2:E:44:VAL:HG13	2:E:48:GLY:HA2	2.00	0.43
2:E:135:GLN:O	2:E:138:ILE:HB	2.18	0.43
2:E:142:THR:HG22	2:E:248:TYR:HD2	1.83	0.43
2:E:101:ASP:HA	2:E:104:ILE:HD12	1.99	0.43
2:E:248:TYR:CD1	2:E:255:PRO:HA	2.53	0.43
1:A:261:GLU:OE1	1:A:294:LYS:NZ	2.48	0.43
2:B:172:ARG:HH21	3:B:570:SRM:C2C	2.31	0.43
1:D:169:LEU:O	1:D:203:LEU:HA	2.17	0.43
1:D:67:ILE:HG13	1:D:67:ILE:H	1.68	0.43
2:E:316:LYS:O	2:E:317:HIS:CB	2.67	0.43
1:D:286:VAL:CB	2:E:363:GLN:HG3	2.49	0.43
1:D:96:THR:HG22	1:D:139:LEU:HA	2.01	0.43
1:D:8:GLU:HG2	1:D:11:LYS:HZ2	1.82	0.43
1:A:393:PRO:HG3	2:E:181:MET:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ALA:HB1	1:A:222:ASP:HA	2.01	0.43
1:D:228:ALA:CB	2:E:272:LEU:HD21	2.48	0.43
1:A:105:TRP:HD1	1:A:130:HIS:CD2	2.37	0.43
1:D:7:ASP:O	1:D:10:GLU:HB2	2.18	0.43
1:A:64:HIS:CE1	2:B:249:THR:O	2.71	0.43
1:D:222:ASP:OD1	1:D:227:LYS:HG2	2.19	0.43
2:E:253:GLY:C	2:E:255:PRO:HD3	2.39	0.43
1:D:262:VAL:O	1:D:263:VAL:C	2.58	0.42
1:A:371:ARG:CG	1:A:372:GLU:N	2.81	0.42
1:A:297:LYS:HE2	2:B:32:TYR:CD1	2.54	0.42
1:D:31:ALA:HB1	1:D:36:LYS:HB2	2.00	0.42
2:E:213:ILE:N	2:E:214:PRO:HD2	2.35	0.42
3:B:570:SRM:HHA	3:B:570:SRM:O4D	2.20	0.42
1:D:114:GLY:O	1:D:117:ASP:HB2	2.19	0.42
1:A:32:ALA:HB2	1:A:38:VAL:HB	2.00	0.42
1:D:177:GLY:HA3	1:D:178:PRO:HD2	1.85	0.42
1:D:228:ALA:CB	2:E:272:LEU:CD2	2.97	0.42
2:E:288:TRP:CH2	2:E:290:PRO:HB3	2.55	0.42
1:A:317:PHE:CE2	2:B:180:ASN:OD1	2.73	0.42
1:D:174:ALA:HB1	1:D:188:THR:HB	2.01	0.42
1:D:374:LEU:O	1:D:378:GLY:N	2.53	0.42
1:D:193:TYR:O	1:D:197:MET:HG2	2.19	0.42
1:D:370:MET:O	1:D:374:LEU:HG	2.20	0.42
1:A:28:MET:HE2	1:A:123:GLY:O	2.19	0.42
2:B:191:ALA:HB3	2:B:267:MET:HB2	2.01	0.42
1:D:408:THR:HA	1:D:411:LEU:HD12	2.01	0.42
1:A:98:ARG:NH2	3:A:580:SRM:HMB3	2.34	0.41
3:A:580:SRM:C1C	2:B:182:CYS:HA	2.50	0.41
2:E:269:GLY:O	2:E:321:ILE:HB	2.20	0.41
2:E:303:VAL:O	2:E:307:LEU:HB2	2.20	0.41
2:B:286:VAL:HA	2:B:287:PRO:HD3	1.93	0.41
1:D:93:HIS:HB3	1:D:95:HIS:NE2	2.35	0.41
1:A:229:ARG:HG3	3:A:580:SRM:O4C	2.21	0.41
2:E:56:PHE:HD2	2:E:114:PRO:O	2.04	0.41
1:A:129:PHE:HA	1:A:130:HIS:HA	1.80	0.41
3:B:570:SRM:HHA	3:B:570:SRM:CED	2.50	0.41
1:A:178:PRO:HG3	1:A:187:ASP:HA	2.02	0.41
2:B:324:VAL:HG11	2:B:329:TRP:CZ2	2.55	0.41
1:D:344:LEU:HB3	1:D:348:TRP:CH2	2.56	0.41
1:A:407:TYR:OH	2:E:199:PRO:O	2.30	0.41
1:A:358:ARG:NH2	3:A:580:SRM:O3D	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:176:ALA:HB1	2:E:181:MET:HA	2.03	0.41
2:B:324:VAL:HG11	2:B:329:TRP:CE2	2.56	0.41
2:E:135:GLN:HB3	2:E:139:HIS:HB3	2.02	0.41
1:A:128:ASN:HB2	1:A:137:ILE:CG1	2.51	0.40
1:A:211:LYS:HZ1	3:A:580:SRM:HAD1	1.84	0.40
1:A:315:ALA:HB3	3:A:580:SRM:HBD1	2.03	0.40
1:D:132:SER:N	3:D:580:SRM:HBB1	2.36	0.40
1:D:97:MET:HB2	1:D:138:PHE:HB2	2.02	0.40
2:E:87:ARG:O	2:E:130:ASN:HB3	2.19	0.40
1:D:96:THR:HG23	2:E:139:HIS:CE1	2.57	0.40
3:A:580:SRM:HHB	3:A:580:SRM:HBA1	2.03	0.40
2:B:106:GLU:HG2	2:B:110:ARG:HD3	2.03	0.40
2:B:323:TRP:O	2:B:327:ILE:HG12	2.21	0.40
1:D:350:TRP:CG	1:D:376:VAL:HG21	2.56	0.40
2:E:142:THR:O	2:E:178:CYS:SG	2.79	0.40
3:A:580:SRM:O3B	2:B:135:GLN:HG2	2.22	0.40
1:D:8:GLU:HG2	1:D:11:LYS:NZ	2.37	0.40
2:E:121:ALA:CB	3:E:570:SRM:O3D	2.52	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%)	392 (94%)	22 (5%)	1 (0%)	47	58
1	D	415/418 (99%)	380 (92%)	28 (7%)	7 (2%)	9	8
2	B	361/366 (99%)	331 (92%)	27 (8%)	3 (1%)	19	23
2	E	361/366 (99%)	308 (85%)	39 (11%)	14 (4%)	3	1
All	All	1552/1568 (99%)	1411 (91%)	116 (8%)	25 (2%)	9	9

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	251	GLU
2	E	6	VAL
2	E	160	GLU
2	E	231	ASN
1	D	250	LYS
2	E	79	ASP
2	E	122	VAL
2	E	5	GLY
2	E	45	ALA
2	E	135	GLN
2	E	332	PHE
1	A	69	SER
2	B	11	GLY
1	D	67	ILE
1	D	220	PRO
1	D	388	ALA
2	E	38	PRO
2	B	60	ARG
1	D	247	GLU
2	E	119	TRP
1	D	289	MET
2	E	60	ARG
2	E	143	PRO
2	E	208	ARG
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%)	331 (94%)	22 (6%)	18	25
1	D	353/354 (100%)	332 (94%)	21 (6%)	19	27
2	B	314/317 (99%)	297 (95%)	17 (5%)	22	30
2	E	314/317 (99%)	290 (92%)	24 (8%)	13	16
All	All	1334/1342 (99%)	1250 (94%)	84 (6%)	18	24

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	42	LYS
1	A	48	LEU
1	A	50	GLN
1	A	86	GLU
1	A	92	GLU
1	A	94	PHE
1	A	100	ASN
1	A	133	THR
1	A	143	SER
1	A	224	VAL
1	A	229	ARG
1	A	295	MET
1	A	310	LEU
1	A	322	VAL
1	A	375	LYS
1	A	400	ASP
1	A	402	LEU
1	A	403	LYS
1	A	410	GLU
1	A	411	LEU
1	A	417	TRP
2	B	4	GLU
2	B	31	LYS
2	B	97	GLU
2	B	108	GLN
2	B	174	SER
2	B	189	ASP
2	B	205	GLU
2	B	230	LYS
2	B	235	LYS
2	B	242	MET
2	B	243	TYR
2	B	256	LEU
2	B	283	LYS
2	B	299	LEU
2	B	321	ILE
2	B	349	ARG
2	B	361	SER
1	D	42	LYS
1	D	54	SER
1	D	56	LYS

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Mol	Chain	Res	Type
1	D	90	GLU
1	D	98	ARG
1	D	100	ASN
1	D	133	THR
1	D	139	LEU
1	D	157	GLU
1	D	159	PRO
1	D	207	MET
1	D	210	TYR
1	D	213	LYS
1	D	234	ILE
1	D	241	ASP
1	D	254	SER
1	D	272	LYS
1	D	276	LYS
1	D	279	THR
1	D	334	GLU
1	D	413	LYS
2	E	4	GLU
2	E	46	GLU
2	E	51	ILE
2	E	58	THR
2	E	61	LEU
2	E	96	ASP
2	E	97	GLU
2	E	123	LYS
2	E	128	LEU
2	E	140	CYS
2	E	188	SER
2	E	205	GLU
2	E	210	THR
2	E	212	GLU
2	E	230	LYS
2	E	231	ASN
2	E	242	MET
2	E	243	TYR
2	E	267	MET
2	E	271	LYS
2	E	273	SER
2	E	307	LEU
2	E	335	LEU
2	E	345	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	100	ASN
1	A	147	GLN
2	B	108	GLN
2	B	139	HIS
1	D	100	ASN
1	D	282	ASN
2	E	180	ASN
2	E	363	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is modelled with single atom - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SRM	D	580	-	34,70,70	2.15	10 (29%)	38,112,112	3.83	17 (44%)
4	SF4	A	575	1	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SF4	B	585	2	0,12,12	0.00	-	-		
4	SF4	E	585	2	0,12,12	0.00	-	-		
4	SF4	D	576	1	0,12,12	0.00	-	-		
4	SF4	A	576	1	0,12,12	0.00	-	-		
4	SF4	B	586	2	0,12,12	0.00	-	-		
4	SF4	E	586	2	0,12,12	0.00	-	-		
3	SRM	A	580	2,5	34,70,70	2.11	8 (23%)	38,112,112	3.71	20 (52%)
3	SRM	B	570	1	34,70,70	2.37	10 (29%)	38,112,112	3.82	21 (55%)
4	SF4	D	575	1,6	0,12,12	0.00	-	-		
3	SRM	E	570	1	34,70,70	2.26	9 (26%)	38,112,112	4.17	18 (47%)

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	D	580	-	-	10/22/126/126	-
4	SF4	A	575	1	-	-	0/6/5/5
4	SF4	B	585	2	-	-	0/6/5/5
4	SF4	E	585	2	-	-	0/6/5/5
4	SF4	D	576	1	-	-	0/6/5/5
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
3	SRM	A	580	2,5	-	9/22/126/126	-
3	SRM	B	570	1	-	10/22/126/126	-
4	SF4	D	575	1,6	-	-	0/6/5/5
3	SRM	E	570	1	-	11/22/126/126	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	570	SRM	C3D-C2D	6.84	1.55	1.39
3	D	580	SRM	C3D-C2D	6.43	1.54	1.39
3	A	580	SRM	C3D-C2D	6.41	1.54	1.39
3	B	570	SRM	C4A-NA	-6.09	1.28	1.39
3	E	570	SRM	C4A-NA	-5.99	1.28	1.39
3	E	570	SRM	C3D-C2D	5.59	1.52	1.39
3	E	570	SRM	C3C-C2C	4.90	1.52	1.37
3	B	570	SRM	C3C-C2C	4.68	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	570	SRM	C1B-NB	-4.63	1.29	1.37
3	A	580	SRM	C1C-C2C	4.33	1.52	1.42
3	B	570	SRM	C1B-NB	-4.29	1.30	1.37
3	D	580	SRM	C3C-C2C	4.20	1.50	1.37
3	A	580	SRM	FE-NA	4.19	2.12	1.95
3	D	580	SRM	C1C-C2C	3.79	1.51	1.42
3	D	580	SRM	FE-NB	3.69	2.10	1.95
3	B	570	SRM	C4C-C3C	3.63	1.50	1.42
3	A	580	SRM	C3C-C2C	3.58	1.48	1.37
3	A	580	SRM	FE-NB	3.57	2.09	1.95
3	E	570	SRM	C4C-C3C	3.56	1.50	1.42
3	D	580	SRM	C4A-NA	-3.50	1.33	1.39
3	A	580	SRM	C4A-NA	-3.40	1.33	1.39
3	D	580	SRM	FE-NA	3.38	2.08	1.95
3	A	580	SRM	CAD-C2D	3.35	1.57	1.52
3	E	570	SRM	C1C-C2C	3.27	1.50	1.42
3	D	580	SRM	C4C-C3C	3.12	1.49	1.42
3	D	580	SRM	CAD-C2D	3.08	1.56	1.52
3	B	570	SRM	C1C-C2C	3.05	1.49	1.42
3	B	570	SRM	CAD-C2D	3.02	1.56	1.52
3	B	570	SRM	CAA-C3A	2.70	1.56	1.51
3	E	570	SRM	C4B-NB	-2.44	1.35	1.39
3	B	570	SRM	C1D-CHD	-2.41	1.34	1.41
3	E	570	SRM	CHC-C4B	-2.37	1.34	1.39
3	D	580	SRM	C1A-NA	-2.31	1.33	1.37
3	A	580	SRM	C4C-C3C	2.30	1.47	1.42
3	B	570	SRM	C4B-NB	-2.19	1.35	1.39
3	E	570	SRM	C1A-NA	-2.10	1.34	1.37
3	D	580	SRM	C4B-NB	-2.10	1.35	1.39

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	580	SRM	CAB-C3B-C2B	-13.56	108.19	123.52
3	B	570	SRM	CAA-C3A-C2A	-12.75	109.11	123.52
3	E	570	SRM	CDC-C2C-C1C	-11.63	109.84	127.39
3	D	580	SRM	CAB-C3B-C2B	-11.40	110.64	123.52
3	E	570	SRM	CDD-C3D-C4D	-11.32	110.20	127.36
3	D	580	SRM	CDD-C3D-C4D	-10.62	111.26	127.36
3	E	570	SRM	CAA-C3A-C2A	-10.15	112.05	123.52
3	D	580	SRM	C4A-NA-C1A	8.31	111.00	106.28
3	D	580	SRM	CDD-C3D-C2D	-7.62	112.89	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	580	SRM	CDD-C3D-C4D	-7.34	116.24	127.36
3	E	570	SRM	CDD-C3D-C2D	-7.30	113.45	126.49
3	E	570	SRM	C3A-C4A-NA	7.24	118.22	110.14
3	D	580	SRM	CAA-C3A-C2A	-6.26	116.45	123.52
3	A	580	SRM	CBB-CAB-C3B	6.26	128.12	113.40
3	B	570	SRM	C3A-C4A-NA	6.20	117.06	110.14
3	B	570	SRM	CEC-CDC-C2C	-6.08	104.12	115.96
3	B	570	SRM	CBD-CAD-C2D	6.06	123.67	112.49
3	B	570	SRM	CDD-C3D-C4D	-5.86	118.47	127.36
3	A	580	SRM	C4A-NA-C1A	5.85	109.61	106.28
3	A	580	SRM	CAA-C3A-C2A	-5.76	117.01	123.52
3	E	570	SRM	C4A-NA-C1A	-5.39	103.21	106.28
3	D	580	SRM	CMA-C2A-CDA	5.22	117.32	109.96
3	B	570	SRM	C4D-CHA-C1A	-5.19	119.84	130.12
3	B	570	SRM	CBC-CAC-C3C	-4.84	103.56	112.48
3	B	570	SRM	C3B-C2B-C1B	-4.79	93.09	101.20
3	E	570	SRM	C4D-CHA-C1A	-4.59	121.03	130.12
3	A	580	SRM	CBA-CAA-C3A	4.57	124.16	113.40
3	B	570	SRM	C4A-NA-C1A	-4.51	103.72	106.28
3	B	570	SRM	CAA-CBA-CCA	4.46	120.16	112.67
3	D	580	SRM	CBD-CAD-C2D	4.44	120.67	112.49
3	B	570	SRM	CAB-CBB-CCB	4.37	120.00	112.67
3	A	580	SRM	C3A-C2A-C1A	-4.27	93.96	101.20
3	A	580	SRM	CDC-C2C-C1C	4.21	133.75	127.39
3	B	570	SRM	CMA-C2A-CDA	-4.06	104.23	109.96
3	B	570	SRM	C2B-CDB-CEB	4.03	121.19	115.29
3	E	570	SRM	CMA-C2A-CDA	-3.99	104.34	109.96
3	A	580	SRM	CBD-CAD-C2D	3.93	119.73	112.49
3	D	580	SRM	CBB-CAB-C3B	3.92	122.62	113.40
3	E	570	SRM	CDC-C2C-C3C	-3.85	119.61	126.49
3	B	570	SRM	CDC-C2C-C1C	-3.69	121.82	127.39
3	E	570	SRM	CAD-C2D-C3D	-3.63	113.45	124.90
3	A	580	SRM	C2A-CDA-CEA	3.60	120.56	115.29
3	D	580	SRM	C3A-C2A-C1A	-3.56	95.17	101.20
3	A	580	SRM	CBC-CAC-C3C	3.44	118.82	112.48
3	E	570	SRM	CHB-C4A-C3A	-3.40	117.90	125.36
3	E	570	SRM	C2B-CDB-CEB	3.33	120.17	115.29
3	D	580	SRM	CBA-CAA-C3A	3.33	121.23	113.40
3	E	570	SRM	C3B-C2B-C1B	-3.29	95.62	101.20
3	A	580	SRM	CDD-C3D-C2D	-3.27	120.65	126.49
3	A	580	SRM	CAD-C2D-C3D	-3.25	114.66	124.90
3	A	580	SRM	CDC-C2C-C3C	-3.20	120.77	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	SRM	CHB-C4A-C3A	-3.16	118.43	125.36
3	E	570	SRM	CAA-CBA-CCA	3.11	117.90	112.67
3	E	570	SRM	CBC-CAC-C3C	-3.05	106.85	112.48
3	B	570	SRM	CED-CDD-C3D	2.86	121.52	115.96
3	A	580	SRM	CAC-CBC-CCC	-2.71	108.12	112.67
3	D	580	SRM	C3B-C2B-C1B	-2.69	96.63	101.20
3	E	570	SRM	CAC-C3C-C2C	-2.62	116.64	124.90
3	B	570	SRM	CAC-C3C-C2C	-2.57	116.81	124.90
3	B	570	SRM	CHB-C1B-NB	-2.53	120.49	124.20
3	D	580	SRM	C3B-C4B-NB	2.50	112.92	110.14
3	D	580	SRM	CHA-C1A-NA	-2.42	120.66	124.20
3	D	580	SRM	C3A-C4A-NA	-2.40	107.45	110.14
3	E	570	SRM	CEC-CDC-C2C	-2.30	111.49	115.96
3	B	570	SRM	CBB-CAB-C3B	2.28	118.76	113.40
3	B	570	SRM	CDC-C2C-C3C	-2.28	122.42	126.49
3	D	580	SRM	C2B-CDB-CEB	-2.26	111.98	115.29
3	D	580	SRM	C4B-NB-C1B	-2.22	105.02	106.28
3	D	580	SRM	CDC-C2C-C1C	2.21	130.73	127.39
3	A	580	SRM	C3B-C4B-NB	2.21	112.60	110.14
3	A	580	SRM	CHA-C1A-NA	-2.20	120.97	124.20
3	A	580	SRM	CHB-C4A-C3A	2.17	130.11	125.36
3	B	570	SRM	CHC-C4B-NB	2.15	127.82	123.84
3	A	580	SRM	CAB-CBB-CCB	-2.05	109.24	112.67
3	E	570	SRM	C2A-C1A-CHA	-2.01	116.86	123.83
3	A	580	SRM	C3A-C4A-NA	-2.01	107.89	110.14

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	580	SRM	C1A-C2A-CDA-CEA
3	D	580	SRM	C4A-C3A-CAA-CBA
3	D	580	SRM	C3A-CAA-CBA-CCA
3	D	580	SRM	C4B-C3B-CAB-CBB
3	D	580	SRM	C2C-C3C-CAC-CBC
3	A	580	SRM	C4A-C3A-CAA-CBA
3	A	580	SRM	C2B-C3B-CAB-CBB
3	A	580	SRM	C3D-C2D-CAD-CBD
3	A	580	SRM	C2D-CAD-CBD-CCD
3	B	570	SRM	C4A-C3A-CAA-CBA
3	B	570	SRM	C4C-C3C-CAC-CBC
3	B	570	SRM	C3C-CAC-CBC-CCC

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Mol	Chain	Res	Type	Atoms
3	B	570	SRM	C3D-C2D-CAD-CBD
3	E	570	SRM	C3A-CAA-CBA-CCA
3	E	570	SRM	C1B-C2B-CDB-CEB
3	E	570	SRM	CMB-C2B-CDB-CEB
3	E	570	SRM	C4C-C3C-CAC-CBC
3	E	570	SRM	C1D-C2D-CAD-CBD
3	A	580	SRM	C4B-C3B-CAB-CBB
3	B	570	SRM	C4B-C3B-CAB-CBB
3	E	570	SRM	C4A-C3A-CAA-CBA
3	E	570	SRM	C4B-C3B-CAB-CBB
3	E	570	SRM	C2D-C3D-CDD-CED
3	D	580	SRM	C2D-C3D-CDD-CED
3	B	570	SRM	C3B-CAB-CBB-CCB
3	E	570	SRM	C3B-CAB-CBB-CCB
3	B	570	SRM	C3A-CAA-CBA-CCA
3	D	580	SRM	CMA-C2A-CDA-CEA
3	A	580	SRM	CMA-C2A-CDA-CEA
3	A	580	SRM	CMB-C2B-CDB-CEB
3	B	570	SRM	CMB-C2B-CDB-CEB
3	D	580	SRM	C4C-C3C-CAC-CBC
3	A	580	SRM	C1A-C2A-CDA-CEA
3	A	580	SRM	C3B-C2B-CDB-CEB
3	D	580	SRM	C3C-CAC-CBC-CCC
3	B	570	SRM	C4D-C3D-CDD-CED
3	E	570	SRM	C3C-CAC-CBC-CCC
3	D	580	SRM	CMB-C2B-CDB-CEB
3	B	570	SRM	CMA-C2A-CDA-CEA
3	E	570	SRM	CMA-C2A-CDA-CEA

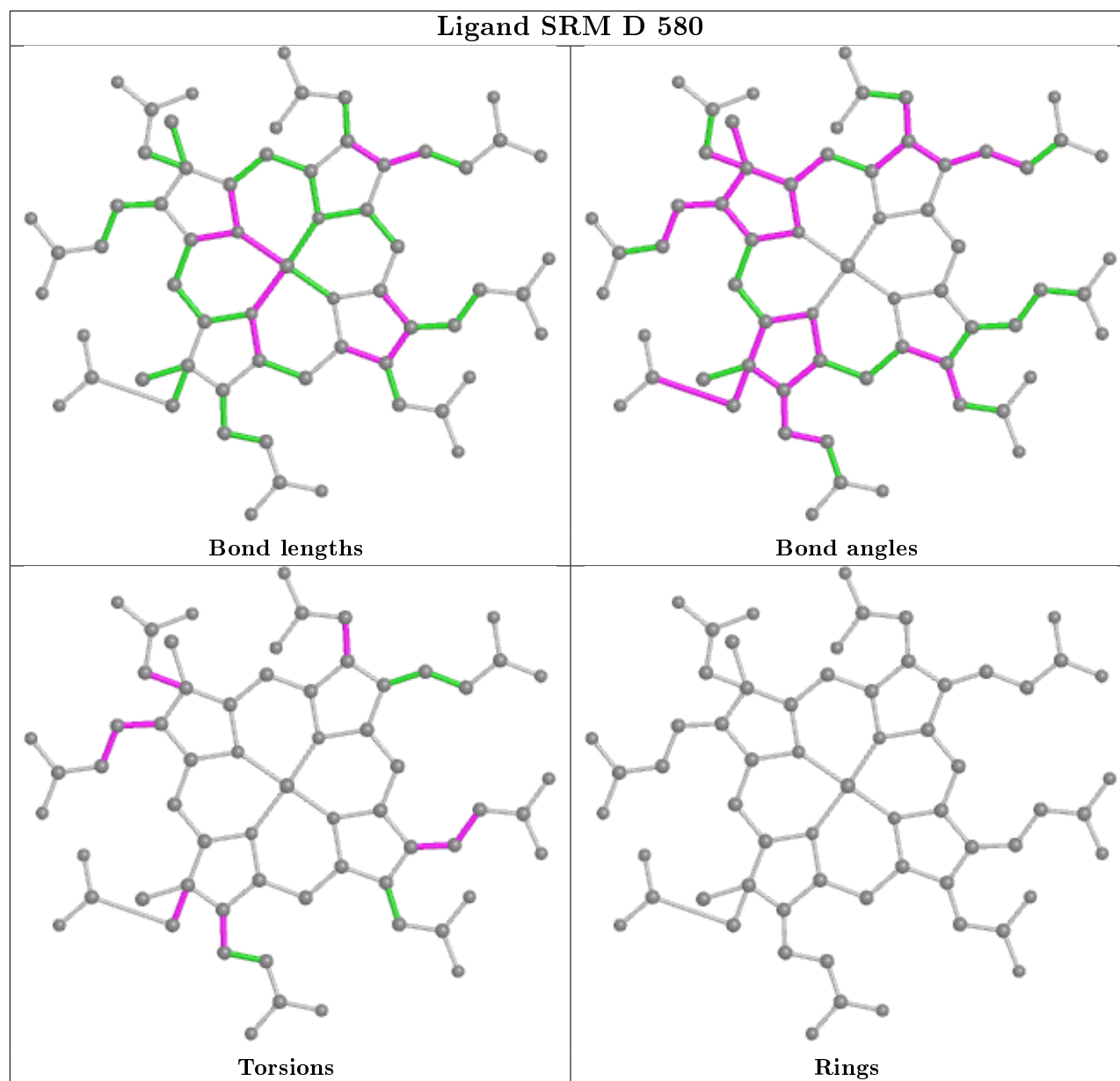
There are no ring outliers.

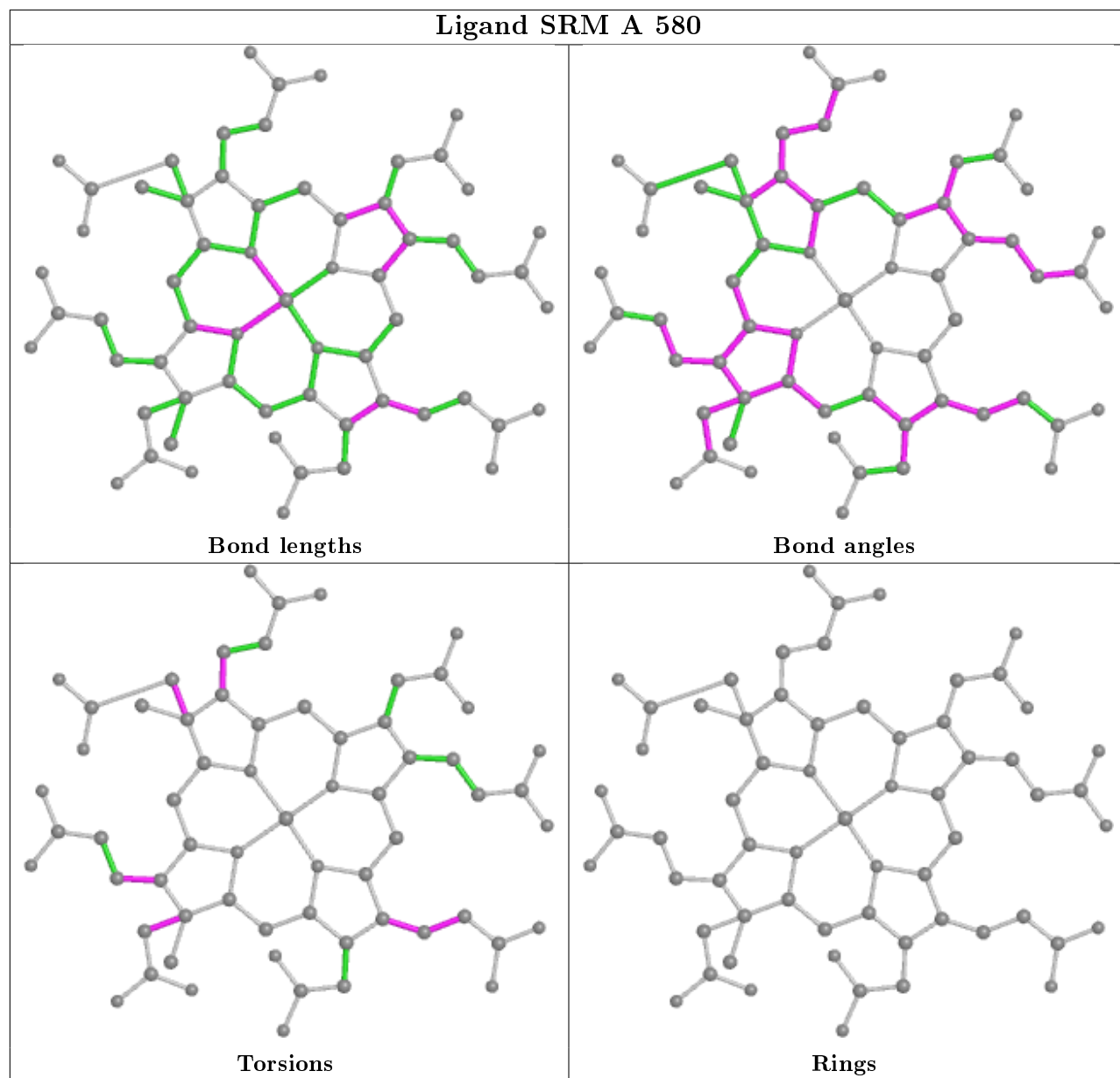
7 monomers are involved in 60 short contacts:

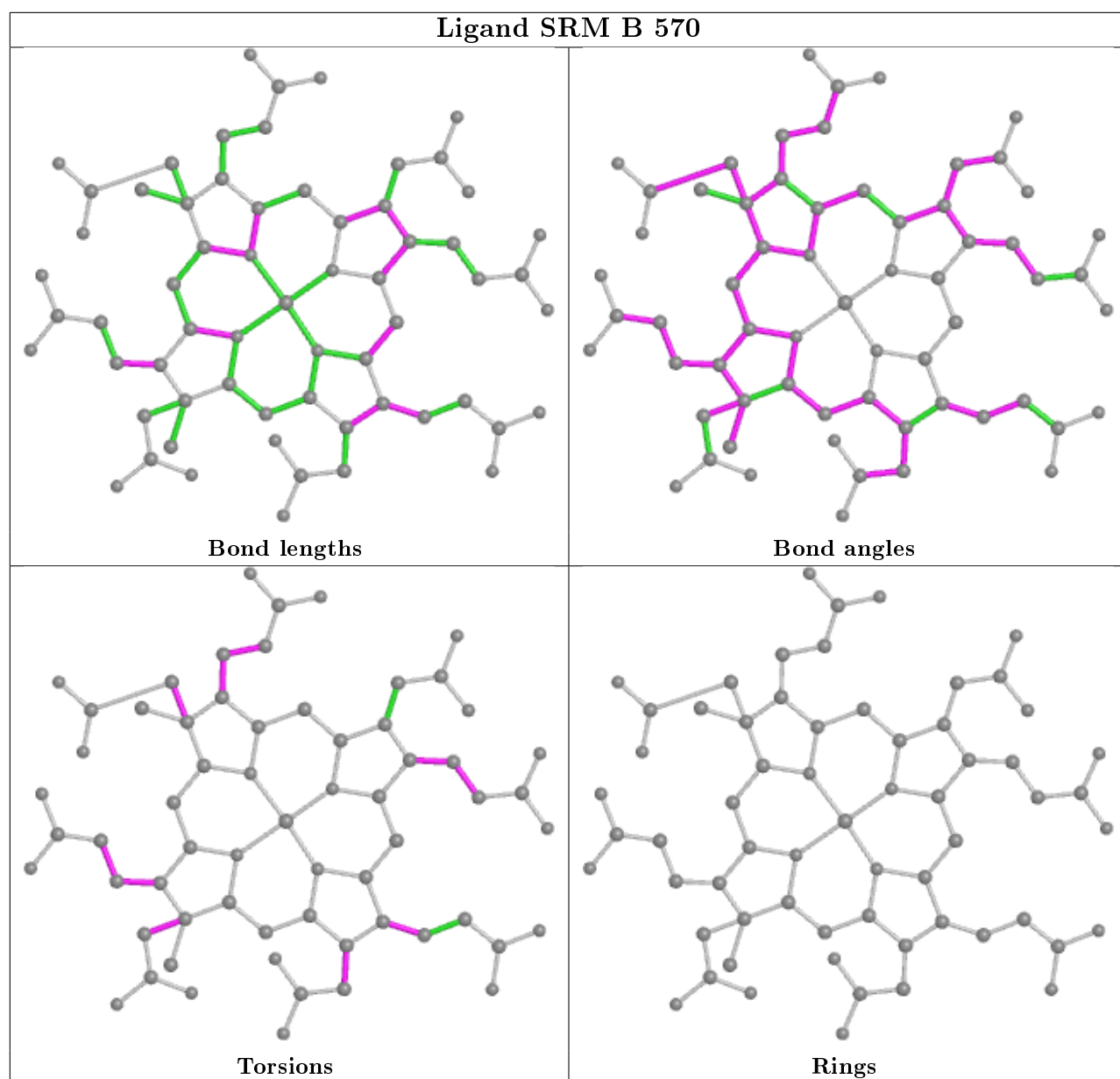
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	580	SRM	13	0
4	B	585	SF4	2	0
4	E	585	SF4	1	0
3	A	580	SRM	24	0
3	B	570	SRM	7	0
4	D	575	SF4	1	0
3	E	570	SRM	13	0

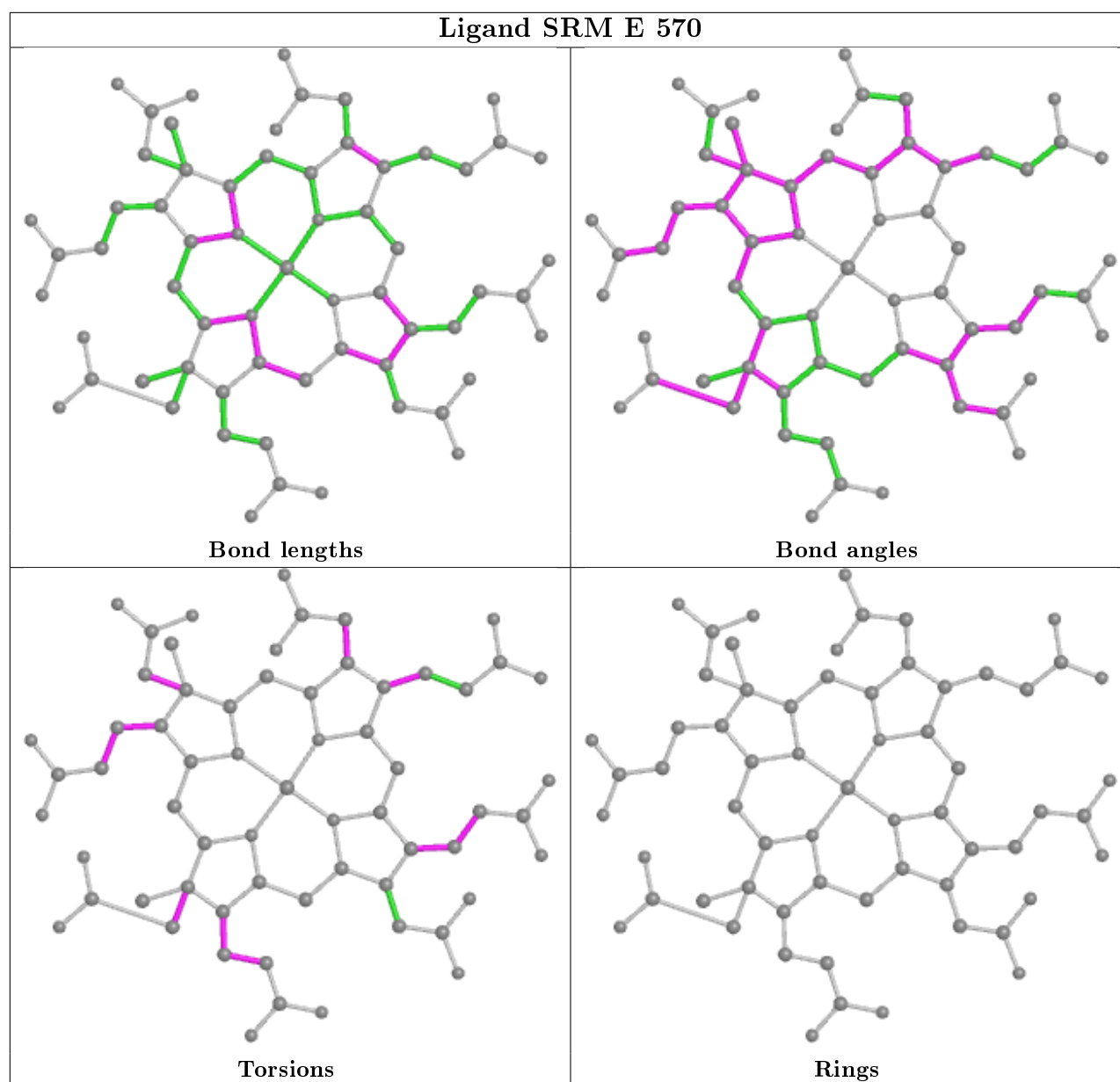
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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%)	0.32	12 (2%) 51 58	3, 7, 15, 31	0
1	D	417/418 (99%)	1.46	107 (25%) 0 0	2, 7, 13, 19	0
2	B	363/366 (99%)	0.17	3 (0%) 86 89	2, 6, 11, 20	0
2	E	363/366 (99%)	1.52	93 (25%) 0 0	2, 5, 23, 40	0
All	All	1560/1568 (99%)	0.87	215 (13%) 2 4	2, 6, 15, 40	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	40	MET	8.5
2	E	231	ASN	8.4
1	D	81	TYR	8.1
2	E	229	MET	8.0
1	D	87	GLN	7.3
1	D	1	SER	6.6
2	E	230	LYS	6.3
1	D	94	PHE	6.3
1	D	106	PHE	6.2
1	D	67	ILE	6.2
2	E	210	THR	5.9
1	D	12	GLY	5.8
2	E	82	LEU	5.5
2	E	236	VAL	5.4
2	E	4	GLU	5.1
2	E	27	TYR	5.1
1	D	91	VAL	5.1
1	D	115	LEU	4.9
2	E	67	VAL	4.9
1	D	47	LEU	4.8
1	D	39	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
2	E	296	TRP	4.7
1	D	145	TYR	4.7
2	E	150	ILE	4.6
1	D	417	TRP	4.6
1	A	417	TRP	4.5
1	D	68	VAL	4.4
1	D	29	GLU	4.4
1	D	43	GLY	4.4
1	D	42	LYS	4.2
1	D	72	GLY	4.0
1	A	413	LYS	4.0
2	E	28	GLY	4.0
2	E	81	TYR	3.9
1	D	38	VAL	3.9
1	D	70	VAL	3.9
1	D	74	GLY	3.9
2	E	56	PHE	3.9
1	D	144	GLU	3.9
2	E	92	PHE	3.8
1	D	126	LEU	3.8
1	D	76	GLY	3.8
1	D	65	GLY	3.8
2	E	6	VAL	3.8
2	E	179	ALA	3.8
2	E	233	THR	3.8
1	D	24	THR	3.7
1	D	5	LEU	3.7
2	E	47	SER	3.7
2	E	70	LEU	3.6
1	D	136	ILE	3.6
1	D	147	GLN	3.6
1	D	31	ALA	3.6
2	E	51	ILE	3.5
1	D	160	PHE	3.5
2	E	227	PRO	3.5
1	D	33	ALA	3.5
2	E	109	GLU	3.5
1	D	99	ILE	3.4
2	E	57	GLY	3.4
1	D	41	PRO	3.4
2	E	232	LYS	3.4
1	A	414	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	273	TRP	3.4
2	E	305	GLN	3.4
1	D	132	SER	3.4
2	E	36	VAL	3.3
2	E	209	LYS	3.3
2	E	185	VAL	3.3
2	E	110	ARG	3.3
1	A	402	LEU	3.3
1	D	122	TRP	3.2
1	D	276	LYS	3.2
2	E	40	VAL	3.2
2	E	61	LEU	3.2
1	D	193	TYR	3.1
2	E	134	THR	3.1
1	D	32	ALA	3.1
2	E	55	ARG	3.1
1	D	84	LEU	3.0
1	D	207	MET	3.0
1	D	335	LYS	3.0
2	E	206	ALA	3.0
1	D	164	GLY	3.0
2	E	173	ILE	3.0
2	E	218	ALA	2.9
1	A	415	GLY	2.9
1	D	328	VAL	2.9
1	D	60	THR	2.9
2	B	5	GLY	2.9
2	E	41	ILE	2.9
1	D	108	SER	2.9
1	D	30	LYS	2.9
1	D	2	GLU	2.9
1	D	49	LYS	2.9
2	E	52	TYR	2.9
2	E	34	GLU	2.9
2	E	107	VAL	2.9
1	D	180	LEU	2.9
2	E	235	LYS	2.9
2	E	64	ILE	2.8
2	E	98	SER	2.8
1	D	78	ILE	2.8
1	D	85	GLY	2.8
1	D	45	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	50	VAL	2.8
1	D	62	TRP	2.8
2	E	208	ARG	2.8
2	E	256	LEU	2.7
1	D	105	TRP	2.7
2	E	30	TRP	2.7
1	D	263	VAL	2.7
1	D	28	MET	2.7
1	D	242	ILE	2.7
2	E	207	ILE	2.7
2	E	77	TYR	2.7
1	D	77	VAL	2.7
1	D	244	VAL	2.7
2	E	15	PHE	2.7
1	D	83	ASP	2.7
1	D	157	GLU	2.7
1	D	159	PRO	2.6
2	E	76	LYS	2.6
2	E	257	PHE	2.6
1	A	406	ALA	2.6
1	A	411	LEU	2.6
2	E	248	TYR	2.6
2	E	243	TYR	2.6
1	D	26	GLU	2.6
2	E	205	GLU	2.6
2	B	4	GLU	2.5
2	E	288	TRP	2.5
2	E	159	TYR	2.5
1	D	220	PRO	2.5
1	D	51	LEU	2.5
1	D	195	LEU	2.5
1	D	330	PHE	2.5
2	E	162	PHE	2.5
2	E	180	ASN	2.5
1	D	292	ILE	2.5
2	E	103	LEU	2.5
1	D	82	SER	2.5
1	D	120	GLU	2.5
2	E	239	GLU	2.5
1	D	71	VAL	2.4
2	E	144	ALA	2.4
1	D	254	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	153	LEU	2.4
1	D	155	ASN	2.4
1	D	181	CYS	2.4
1	D	48	LEU	2.4
1	D	275	GLY	2.4
1	D	137	ILE	2.3
2	E	118	THR	2.3
1	D	357	PHE	2.3
2	E	65	TYR	2.3
1	D	127	THR	2.3
2	E	111	VAL	2.3
1	D	255	TRP	2.3
1	D	351	TRP	2.3
2	E	219	ALA	2.3
1	D	329	PRO	2.3
2	E	59	PRO	2.3
1	D	299	LEU	2.3
2	E	5	GLY	2.3
2	E	339	GLU	2.3
2	E	72	ASP	2.3
1	D	129	PHE	2.2
2	E	104	ILE	2.2
1	D	152	ASP	2.2
2	B	227	PRO	2.2
2	E	112	GLY	2.2
1	D	57	ASP	2.2
1	D	315	ALA	2.2
2	E	96	ASP	2.2
1	A	416	MET	2.2
1	D	107	TYR	2.2
2	E	293	PRO	2.2
1	D	123	GLY	2.2
2	E	177	CYS	2.2
1	D	141	THR	2.2
1	D	11	LYS	2.2
1	D	6	LEU	2.2
2	E	94	VAL	2.2
1	D	112	LEU	2.2
2	E	90	VAL	2.1
1	D	317	PHE	2.1
1	D	17	PHE	2.1
1	D	109	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	150	PHE	2.1
2	E	42	LYS	2.1
1	A	412	LYS	2.1
1	D	73	TYR	2.1
2	E	311	ALA	2.1
1	A	285	CYS	2.1
1	A	398	GLU	2.1
1	D	334	GLU	2.1
2	E	333	PHE	2.1
1	A	67	ILE	2.1
2	E	272	LEU	2.1
2	E	68	ARG	2.1
2	E	84	TRP	2.1
1	D	117	ASP	2.1
2	E	115	CYS	2.1
2	E	220	CYS	2.1
2	E	199	PRO	2.1
2	E	312	ALA	2.0
1	D	50	GLN	2.0
1	D	178	PRO	2.0
2	E	8	THR	2.0
1	D	253	ALA	2.0
2	E	37	LYS	2.0
2	E	137	TRP	2.0
2	E	158	LEU	2.0
2	E	187	ALA	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 carbohydrates in this entry.

6.4 Ligands [i](#)

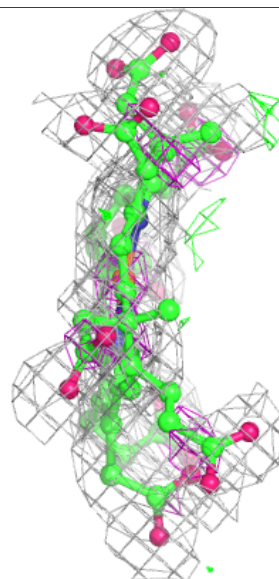
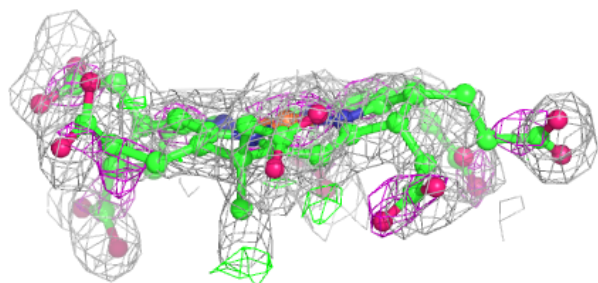
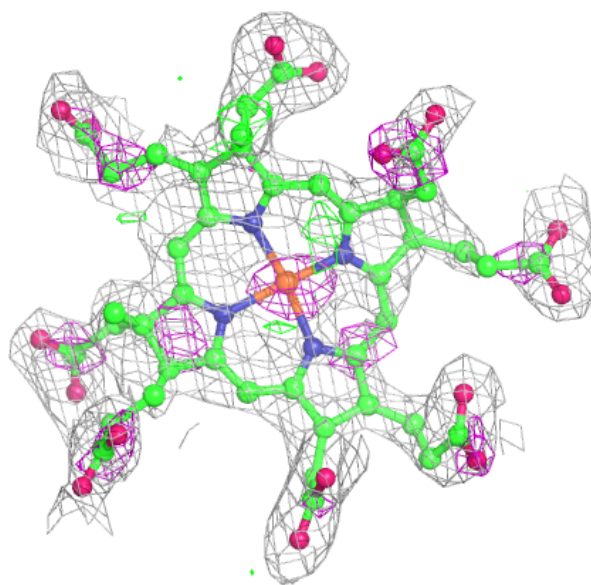
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SRM	D	580	63/63	0.84	0.28	18,21,24,30	0
5	H2S	A	590	1/1	0.92	0.11	20,20,20,20	0
3	SRM	E	570	63/63	0.92	0.24	5,5,6,6	0
4	SF4	D	576	8/8	0.93	0.08	7,7,8,8	0
3	SRM	A	580	63/63	0.95	0.13	7,10,14,17	0
3	SRM	B	570	63/63	0.95	0.13	3,4,6,7	0
4	SF4	D	575	8/8	0.95	0.10	3,3,3,3	0
4	SF4	E	585	8/8	0.95	0.13	19,20,21,21	0
4	SF4	E	586	8/8	0.96	0.06	13,15,15,16	0
4	SF4	A	576	8/8	0.97	0.06	5,6,6,6	0
4	SF4	B	585	8/8	0.97	0.05	10,11,12,16	0
4	SF4	B	586	8/8	0.98	0.06	2,3,3,3	0
4	SF4	A	575	8/8	0.98	0.07	6,6,7,7	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.

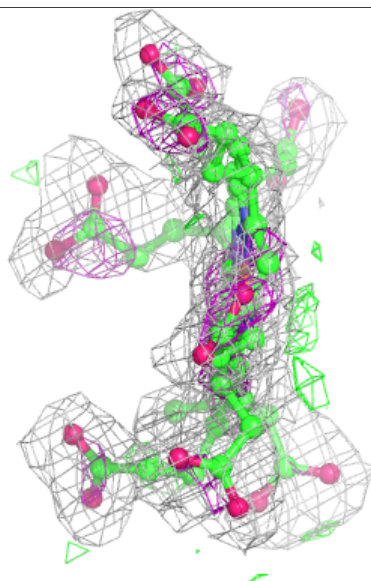
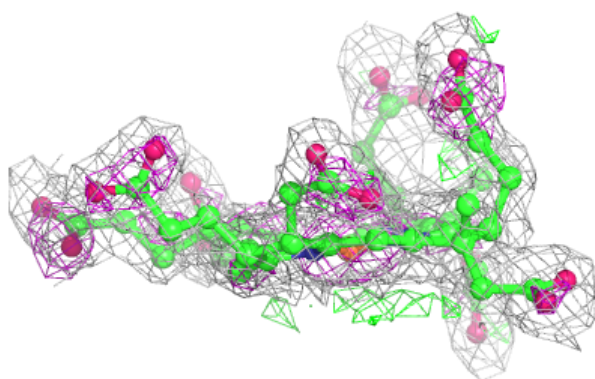
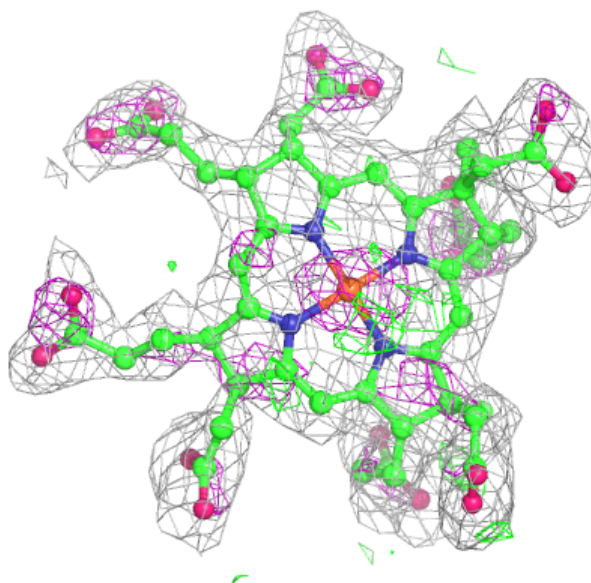
Electron density around SRM D 580:

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



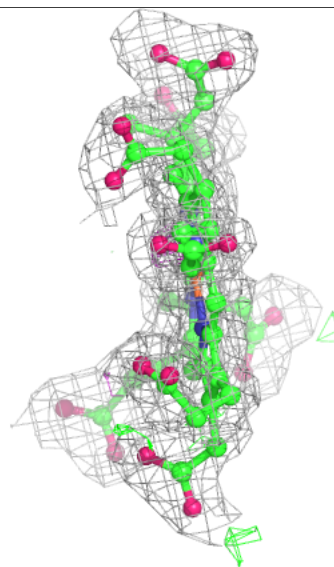
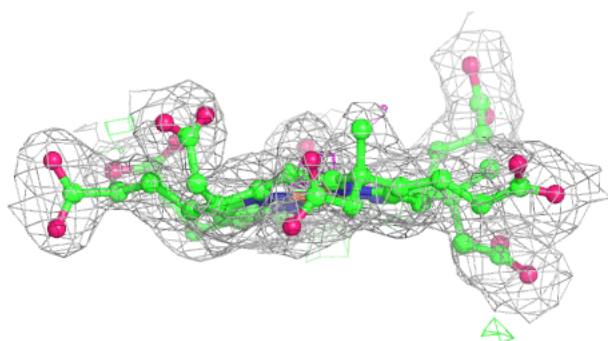
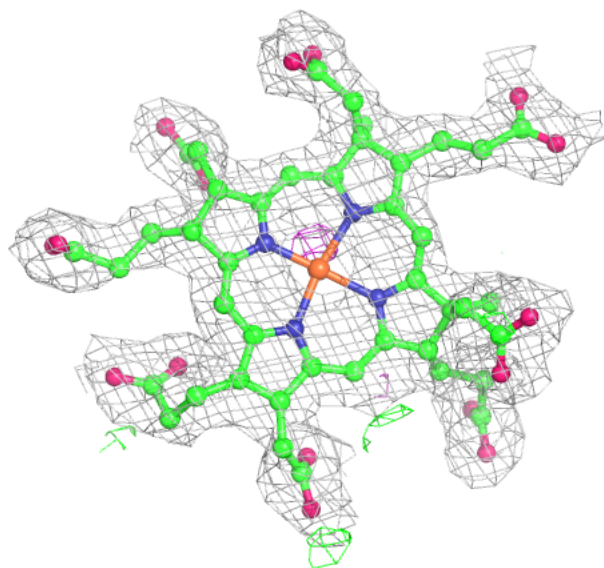
Electron density around SRM E 570:

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



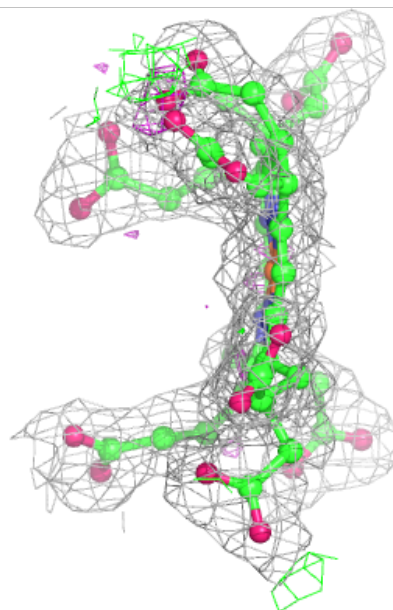
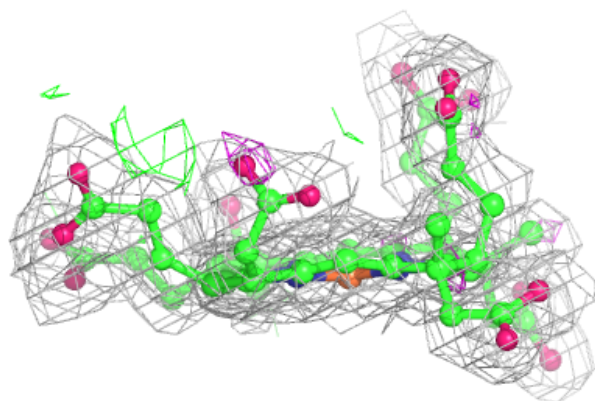
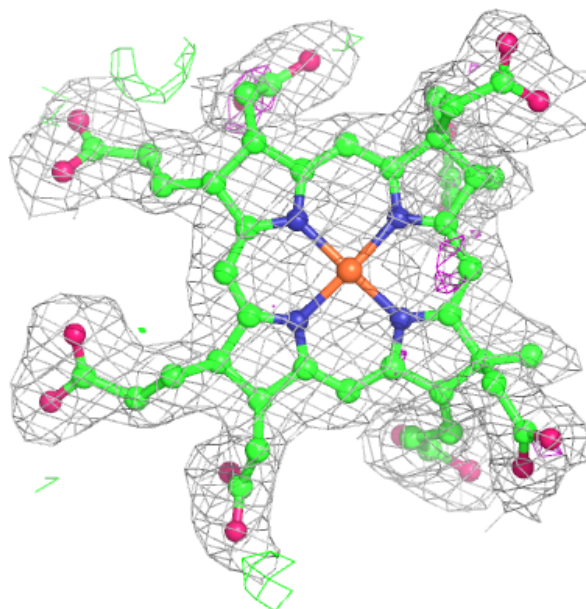
Electron density around SRM A 580:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.