Full wwPDB X-ray Structure Validation Report (i)

Dec 20, 2023 – 12:15 PM JST

PDB ID	:	5H8Y
Title	:	Crystal structure of the complex between maize sulfite reductase and ferredoxin in the form-2 crystal
Authors	:	Kurisu, G.; Nakayama, M.; Hase, T.
Deposited on	:	2015-12-25
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

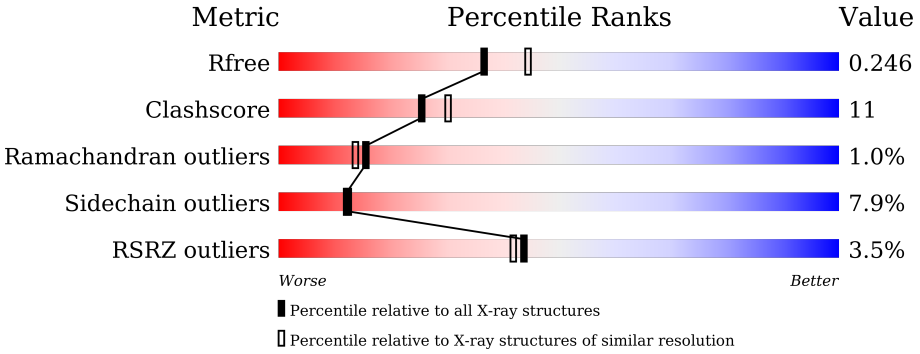
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	583	.% 76% 16% • • •
1	B	583	.% 78% 14% • • •
1	C	583	.% 77% 14% 5% • •
1	D	583	3% 77% 13% • • 5%
2	E	98	4% 78% 17% • •
2	F	98	51% 49% 23% •• 26%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SRM	A	702	X	-	-	-
4	SRM	B	702	X	-	-	-
4	SRM	C	702	X	-	-	-
4	SRM	D	702	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 19620 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.

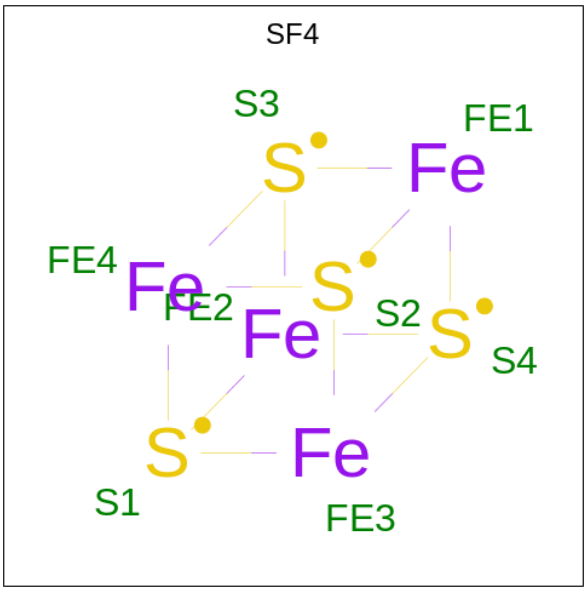
- Molecule 1 is a protein called Sulfite reductase [ferredoxin], chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	567	4458	2831	770	840	17	0	0	0
1	B	565	4455	2829	772	838	16	0	0	0
1	C	563	4429	2816	768	828	17	0	0	0
1	D	554	4365	2777	754	818	16	0	0	0

- Molecule 2 is a protein called Ferredoxin-1, chloroplastic.

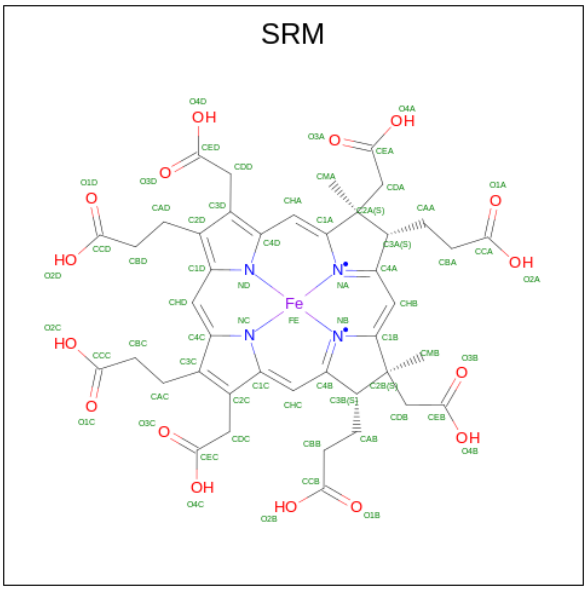
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	96	726	447	113	162	4	0	0	0
2	F	73	495	302	86	103	4	0	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 4 is SIROHEME (three-letter code: SRM) (formula: $C_{42}H_{44}FeN_4O_{16}$).



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

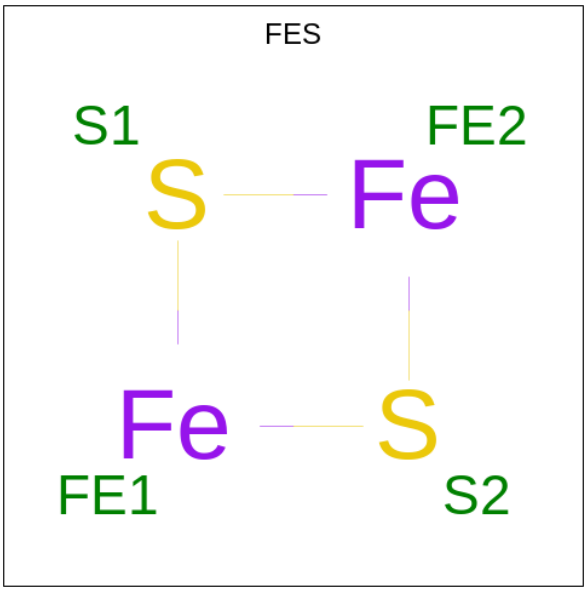
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0
5	B	1	1	1	0	0
5	C	1	1	1	0	0
5	D	1	1	1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
6	A	1	1	1	0	0
6	B	1	1	1	0	0
6	C	1	1	1	0	0
6	D	1	1	1	0	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
7	E	1	4	2	2	0	0
			Total	Fe	S		
7	F	1	4	2	2	0	0

- Molecule 8 is water.

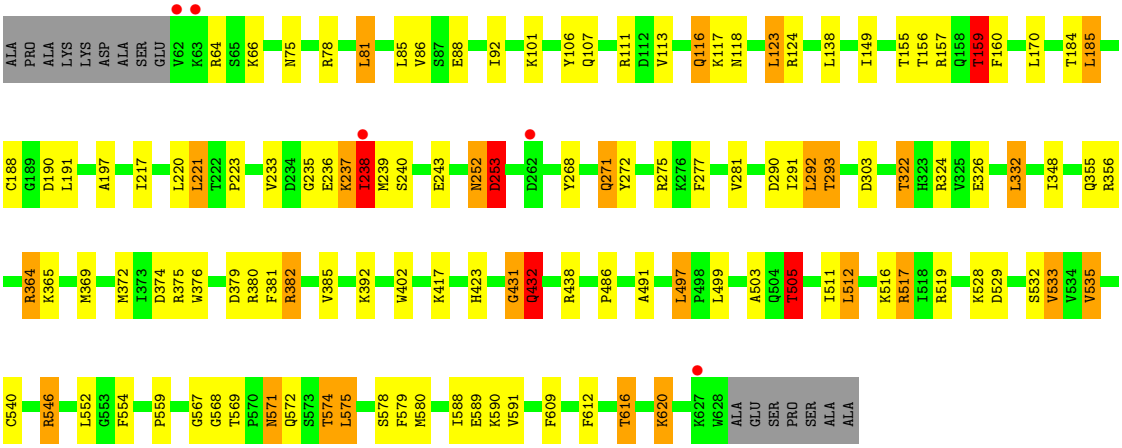
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	118	118	118	0	0
			Total	O		
8	B	124	124	124	0	0
			Total	O		
8	C	77	77	77	0	0
			Total	O		
8	D	66	66	66	0	0
			Total	O		
8	E	7	7	7	0	0

3 Residue-property plots (i)

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

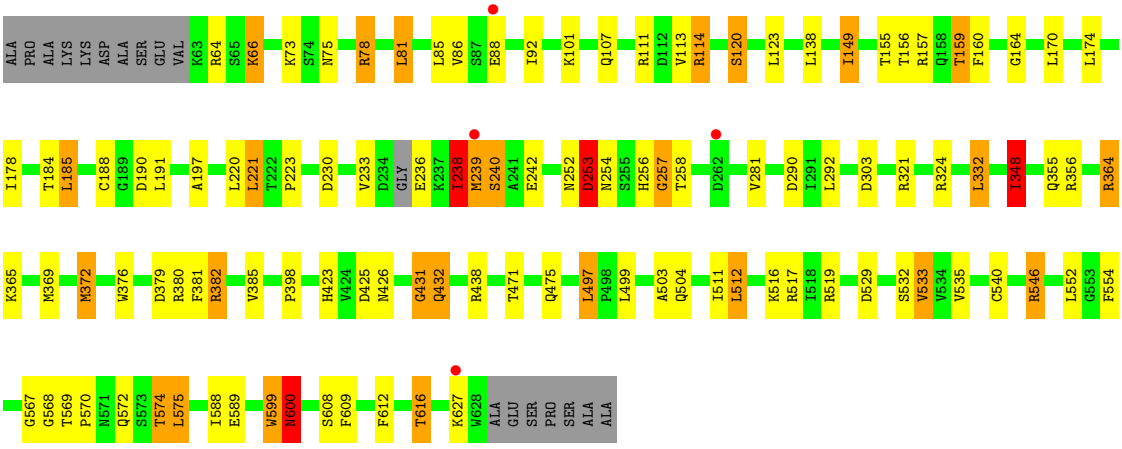
• Molecule 1: Sulfite reductase [ferredoxin], chloroplastic

Chain A:



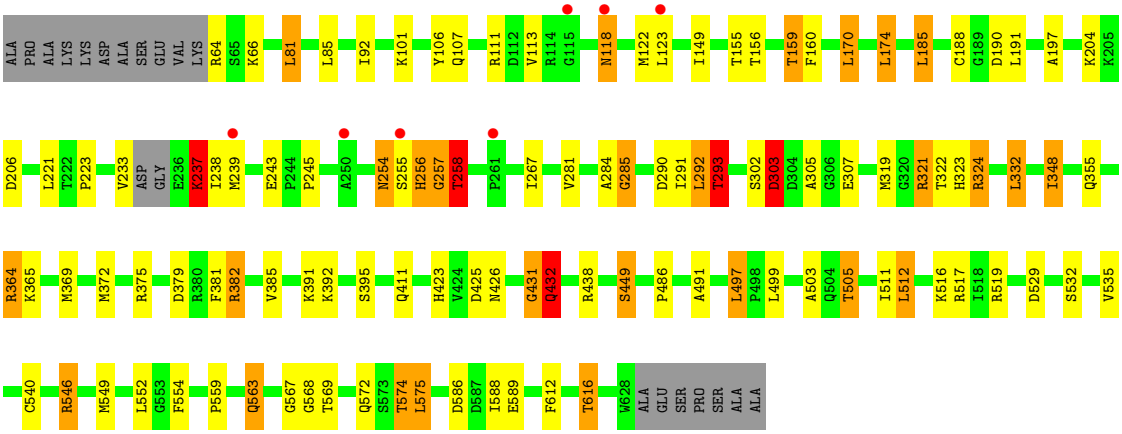
• Molecule 1: Sulfite reductase [ferredoxin], chloroplastic

Chain B:



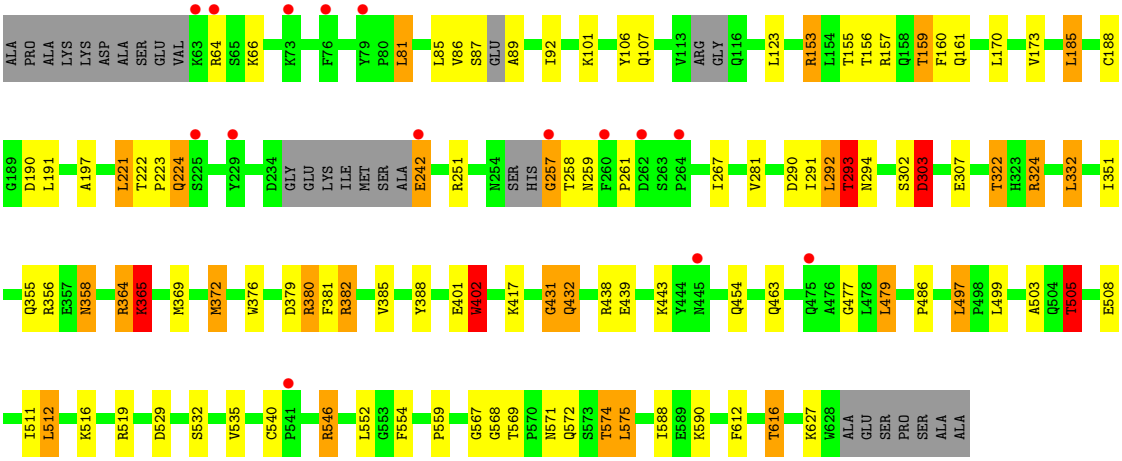
• Molecule 1: Sulfite reductase [ferredoxin], chloroplastic

Chain C:



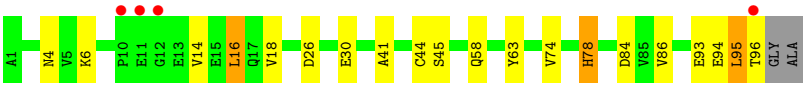
- Molecule 1: Sulfite reductase [ferredoxin], chloroplastic

Chain D:



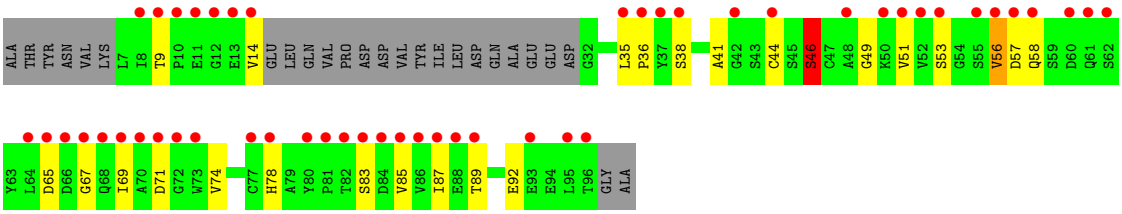
- Molecule 2: Ferredoxin-1, chloroplastic

Chain E:



- Molecule 2: Ferredoxin-1, chloroplastic

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	176.22Å 176.22Å 195.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.07 – 2.20 30.06 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.07-2.20) 100.0 (30.06-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.218 , 0.247 0.219 , 0.246	Depositor DCC
R_{free} test set	8681 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 15.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.229 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19620	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, SRM, FES, MG, SF4

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	0.88	4/4554 (0.1%)	1.01	26/6173 (0.4%)
1	B	0.88	3/4550 (0.1%)	1.02	22/6165 (0.4%)
1	C	0.78	3/4524 (0.1%)	0.98	23/6131 (0.4%)
1	D	0.72	0/4456	0.95	19/6036 (0.3%)
2	E	0.71	0/738	0.80	0/1008
2	F	0.74	1/502 (0.2%)	0.79	0/684
All	All	0.81	11/19324 (0.1%)	0.98	90/26197 (0.3%)

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	2
1	B	0	4
1	C	0	5
1	D	0	2
2	F	0	1
All	All	0	14

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	285	GLY	N-CA	6.76	1.56	1.46
1	B	600	ASN	N-CA	5.86	1.58	1.46
1	A	578	SER	CB-OG	-5.84	1.34	1.42
1	A	111	ARG	CD-NE	-5.76	1.36	1.46
1	C	321	ARG	CD-NE	-5.53	1.37	1.46
2	F	46	SER	CB-OG	5.50	1.49	1.42
1	A	159	THR	CB-CG2	-5.28	1.34	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	449	SER	CB-OG	-5.23	1.35	1.42
1	B	532	SER	CB-OG	-5.12	1.35	1.42
1	B	253	ASP	CB-CG	5.11	1.62	1.51
1	A	432	GLN	N-CA	5.02	1.56	1.46

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	364	ARG	NE-CZ-NH2	-13.94	113.33	120.30
1	B	546	ARG	NE-CZ-NH2	-13.19	113.70	120.30
1	B	364	ARG	NE-CZ-NH2	-13.06	113.77	120.30
1	C	364	ARG	NE-CZ-NH2	-12.07	114.26	120.30
1	D	546	ARG	NE-CZ-NH2	-11.48	114.56	120.30
1	C	321	ARG	NE-CZ-NH2	-11.18	114.71	120.30
1	D	364	ARG	NE-CZ-NH2	-11.13	114.74	120.30
1	B	546	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	D	153	ARG	NE-CZ-NH1	-10.69	114.95	120.30
1	A	364	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	C	258	THR	N-CA-CB	9.63	128.61	110.30
1	B	364	ARG	NE-CZ-NH1	9.59	125.10	120.30
1	B	382	ARG	NE-CZ-NH2	-9.59	115.50	120.30
1	A	382	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	D	546	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	B	303	ASP	CB-CG-OD1	8.87	126.28	118.30
1	C	364	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	C	382	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	A	303	ASP	CB-CG-OD1	8.73	126.16	118.30
1	A	303	ASP	CB-CG-OD2	-8.43	110.71	118.30
1	B	303	ASP	CB-CG-OD2	-8.26	110.87	118.30
1	A	271	GLN	N-CA-C	-8.03	89.31	111.00
1	B	253	ASP	N-CA-CB	7.99	124.98	110.60
1	C	348	ILE	CG1-CB-CG2	-7.93	93.95	111.40
1	D	364	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	D	382	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	D	402	TRP	N-CA-CB	7.44	124.00	110.60
1	A	253	ASP	N-CA-CB	7.43	123.97	110.60
1	C	324	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	C	382	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	546	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	C	546	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	B	382	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	A	382	ARG	NE-CZ-NH1	6.72	123.66	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	321	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	C	321	ARG	CG-CD-NE	-6.64	97.86	111.80
1	A	375	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	C	324	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	D	401	GLU	N-CA-C	6.50	128.56	111.00
1	B	600	ASN	N-CA-CB	6.28	121.91	110.60
1	A	111	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	111	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	D	382	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	B	321	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	D	153	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	D	324	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	111	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	D	303	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	356	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	303	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	324	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	348	ILE	CG1-CB-CG2	5.68	123.89	111.40
1	C	284	ALA	C-N-CA	-5.67	110.38	122.30
1	A	160	PHE	CB-CA-C	-5.65	99.10	110.40
1	B	356	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	A	546	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	425	ASP	CB-CG-OD1	5.53	123.28	118.30
1	D	546	ARG	CG-CD-NE	-5.48	100.29	111.80
1	A	252	ASN	O-C-N	-5.46	113.97	122.70
1	A	364	ARG	CG-CD-NE	-5.45	100.35	111.80
1	B	240	SER	N-CA-C	-5.42	96.37	111.00
1	A	505	THR	CB-CA-C	-5.39	97.04	111.60
1	D	356	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	111	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	517	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	293	THR	N-CA-CB	-5.37	100.11	110.30
1	C	364	ARG	CG-CD-NE	-5.37	100.53	111.80
1	A	620	LYS	CB-CG-CD	5.36	125.53	111.60
1	A	356	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	571	ASN	N-CA-CB	-5.36	100.96	110.60
1	B	160	PHE	CB-CA-C	-5.31	99.78	110.40
1	B	599	TRP	C-N-CA	-5.30	108.45	121.70
1	A	571	ASN	CB-CA-C	-5.27	99.85	110.40
1	A	253	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	356	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	C	586	ASP	CB-CG-OD1	5.23	123.01	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	505	THR	CB-CA-C	-5.21	97.53	111.60
1	C	432	GLN	N-CA-CB	5.20	119.96	110.60
1	D	293	THR	N-CA-CB	-5.19	100.44	110.30
1	D	364	ARG	CB-CA-C	-5.17	100.06	110.40
1	B	364	ARG	CG-CD-NE	-5.14	101.01	111.80
1	A	431	GLY	C-N-CA	-5.12	108.89	121.70
1	C	160	PHE	CB-CA-C	-5.05	100.29	110.40
1	A	272	TYR	N-CA-C	-5.05	97.36	111.00
1	C	546	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	563	GLN	CB-CA-C	-5.04	100.32	110.40
1	C	111	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	C	425	ASP	CB-CG-OD1	5.03	122.83	118.30
1	D	160	PHE	CB-CA-C	-5.02	100.35	110.40
1	D	358	ASN	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	GLU	Peptide
1	A	238	ILE	Peptide
1	B	238	ILE	Peptide
1	B	239	MET	Peptide
1	B	256	HIS	Peptide
1	B	257	GLY	Peptide
1	C	237	LYS	Peptide
1	C	254	ASN	Peptide
1	C	257	GLY	Peptide
1	C	285	GLY	Peptide
1	C	302	SER	Peptide
1	D	257	GLY	Peptide
1	D	302	SER	Peptide
2	F	56	VAL	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	4458	0	4430	107	0
1	B	4455	0	4437	78	0
1	C	4429	0	4413	94	0
1	D	4365	0	4349	84	0
2	E	726	0	671	15	0
2	F	495	0	431	16	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
3	C	8	0	0	0	0
3	D	8	0	0	0	0
4	A	63	0	34	9	0
4	B	63	0	34	10	0
4	C	63	0	34	7	0
4	D	63	0	34	11	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	E	4	0	0	0	0
7	F	4	0	0	0	0
8	A	118	0	0	8	0
8	B	124	0	0	3	0
8	C	77	0	0	10	0
8	D	66	0	0	2	0
8	E	7	0	0	1	0
All	All	19620	0	18867	404	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 11.

All (404) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:TYR:HE1	1:A:188:CYS:SG	1.11	1.66
1:C:106:TYR:HE1	1:C:188:CYS:SG	1.17	1.65
1:D:106:TYR:HE1	1:D:188:CYS:SG	1.17	1.64
1:A:106:TYR:CE1	1:A:188:CYS:SG	2.03	1.50
1:C:255:SER:C	1:C:257:GLY:HA3	1.36	1.39

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:PHE:CE2	1:A:580:MET:HE2	1.72	1.25
1:D:153:ARG:NH1	1:D:508:GLU:OE1	1.72	1.21
1:B:155:THR:HB	4:B:702:SRM:HAB2	1.22	1.18
1:C:204:LYS:HE2	1:C:206:ASP:OD2	1.49	1.11
1:C:319:MET:HE3	1:C:549:MET:HE2	1.11	1.10
1:C:155:THR:HB	4:C:702:SRM:HAB2	1.15	1.09
1:D:155:THR:HB	4:D:702:SRM:HAB2	1.15	1.07
1:A:155:THR:HB	4:A:702:SRM:HAB2	1.25	1.06
1:A:237:LYS:CB	1:A:238:ILE:O	2.04	1.05
1:A:431:GLY:O	1:A:432:GLN:HB3	1.56	1.05
1:C:255:SER:C	1:C:257:GLY:CA	2.25	1.05
1:B:254:ASN:OD1	1:B:257:GLY:HA3	1.57	1.04
1:C:106:TYR:CE1	1:C:188:CYS:SG	2.08	1.04
1:C:255:SER:O	1:C:257:GLY:HA3	1.61	1.01
1:C:257:GLY:HA2	1:C:258:THR:HG23	1.43	1.00
1:C:355:GLN:HB2	1:C:369:MET:HE3	1.02	1.00
1:A:123:LEU:HD21	1:A:184:THR:HG21	1.39	1.00
1:B:355:GLN:HB2	1:B:369:MET:CE	1.91	0.99
1:B:355:GLN:HB2	1:B:369:MET:HE3	1.01	0.99
1:C:319:MET:HE3	1:C:549:MET:CE	1.93	0.99
1:C:355:GLN:HB2	1:C:369:MET:CE	1.94	0.98
1:C:355:GLN:CB	1:C:369:MET:HE3	1.94	0.97
1:C:319:MET:CE	1:C:549:MET:HE2	1.93	0.97
1:A:431:GLY:O	1:A:432:GLN:CB	2.01	0.97
1:B:355:GLN:CB	1:B:369:MET:HE3	1.94	0.97
1:C:255:SER:O	1:C:257:GLY:CA	2.14	0.96
1:D:106:TYR:CE1	1:D:188:CYS:SG	2.08	0.95
1:B:66:LYS:H	1:B:66:LYS:HE3	1.31	0.95
1:A:580:MET:HE1	1:A:591:VAL:HG13	1.46	0.94
1:B:431:GLY:O	1:B:432:GLN:CB	2.11	0.94
1:C:572:GLN:OE1	8:C:801:HOH:O	1.86	0.94
1:A:355:GLN:HB2	1:A:369:MET:CE	1.99	0.92
1:A:579:PHE:CE2	1:A:580:MET:CE	2.51	0.92
1:A:579:PHE:HE2	1:A:580:MET:HE2	1.31	0.90
1:A:355:GLN:HB2	1:A:369:MET:HE2	1.51	0.90
1:B:599:TRP:O	1:B:600:ASN:CB	2.18	0.88
1:B:599:TRP:O	1:B:600:ASN:HB3	1.72	0.87
1:A:277:PHE:HE1	1:A:369:MET:CE	1.86	0.87
1:D:364:ARG:O	1:D:365:LYS:HB2	1.76	0.85
1:A:237:LYS:CA	1:A:238:ILE:O	2.24	0.84
1:B:431:GLY:O	1:B:432:GLN:HB2	1.74	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ILE:CD1	8:A:808:HOH:O	2.26	0.84
1:C:505:THR:HG23	1:C:559:PRO:O	1.78	0.83
1:C:255:SER:CA	1:C:257:GLY:HA3	2.08	0.83
1:C:204:LYS:CE	1:C:206:ASP:OD2	2.27	0.83
1:D:505:THR:HG23	1:D:559:PRO:O	1.81	0.81
1:C:303:ASP:O	1:C:305:ALA:O	1.98	0.80
1:A:505:THR:HG23	1:A:559:PRO:O	1.82	0.80
1:B:123:LEU:CD1	1:B:174:LEU:CD2	2.60	0.79
1:B:252:ASN:O	1:B:253:ASP:CB	2.29	0.78
1:A:252:ASN:O	1:A:253:ASP:CB	2.29	0.78
1:A:277:PHE:HE1	1:A:369:MET:HE3	1.48	0.78
1:C:612:PHE:O	1:C:616:THR:HG23	1.83	0.78
1:D:364:ARG:O	1:D:365:LYS:CB	2.25	0.78
1:C:572:GLN:CG	8:C:801:HOH:O	2.31	0.77
2:F:44:CYS:SG	2:F:46:SER:OG	2.32	0.77
1:B:612:PHE:O	1:B:616:THR:HG23	1.84	0.77
1:A:322:THR:HG22	8:A:914:HOH:O	1.84	0.77
1:A:579:PHE:HE2	1:A:580:MET:CE	1.95	0.77
1:B:123:LEU:CD1	1:B:174:LEU:HD21	2.15	0.77
1:C:303:ASP:HB3	1:C:307:GLU:O	1.86	0.76
1:D:155:THR:HB	4:D:702:SRM:CAB	2.08	0.76
1:D:303:ASP:HB3	1:D:307:GLU:O	1.86	0.76
1:C:155:THR:HB	4:C:702:SRM:CAB	2.08	0.76
2:E:94:GLU:C	2:E:95:LEU:HD23	2.06	0.75
1:D:612:PHE:O	1:D:616:THR:HG23	1.86	0.75
1:D:559:PRO:HG2	2:E:30:GLU:OE1	1.85	0.75
1:A:277:PHE:CE1	1:A:369:MET:HE1	2.22	0.74
1:B:114:ARG:H	1:B:114:ARG:HD3	1.52	0.74
1:A:252:ASN:O	1:A:253:ASP:HB3	1.86	0.74
1:B:155:THR:HB	4:B:702:SRM:CAB	2.11	0.74
1:C:149:ILE:HG22	8:C:825:HOH:O	1.88	0.74
1:A:612:PHE:O	1:A:616:THR:HG23	1.86	0.74
1:C:256:HIS:N	1:C:257:GLY:HA3	2.03	0.74
1:D:222:THR:O	1:D:224:GLN:OE1	2.05	0.74
1:A:580:MET:CE	1:A:591:VAL:HG13	2.18	0.74
1:B:252:ASN:O	1:B:253:ASP:HB3	1.88	0.73
4:D:702:SRM:HBB1	4:D:702:SRM:CHC	2.19	0.72
1:B:471:THR:O	1:B:475:GLN:HG3	1.90	0.72
1:A:155:THR:HB	4:A:702:SRM:CAB	2.14	0.71
1:B:66:LYS:H	1:B:66:LYS:CE	2.03	0.71
1:A:517:ARG:HD2	1:A:589:GLU:OE1	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:THR:O	1:D:546:ARG:NH2	2.23	0.71
1:B:123:LEU:HD13	1:B:174:LEU:CD2	2.20	0.71
1:A:277:PHE:CE1	1:A:369:MET:CE	2.73	0.70
2:E:16:LEU:HD12	2:E:18:VAL:CG2	2.22	0.70
1:B:379:ASP:OD1	1:B:382:ARG:NH2	2.25	0.69
1:A:616:THR:O	1:A:620:LYS:HD2	1.92	0.69
2:E:95:LEU:HD23	2:E:95:LEU:N	2.07	0.69
1:A:217:ILE:CD1	1:A:348:ILE:HD13	2.22	0.69
1:A:277:PHE:HE1	1:A:369:MET:HE1	1.57	0.69
1:B:572:GLN:HG3	8:B:914:HOH:O	1.93	0.69
1:C:257:GLY:HA2	1:C:258:THR:CG2	2.21	0.68
1:D:379:ASP:OD1	1:D:382:ARG:NH2	2.27	0.68
1:C:379:ASP:OD1	1:C:382:ARG:NH2	2.26	0.68
1:A:379:ASP:OD1	1:A:382:ARG:NH2	2.28	0.68
1:C:255:SER:O	1:C:257:GLY:N	2.27	0.68
1:C:431:GLY:O	1:C:432:GLN:CB	2.42	0.68
1:B:254:ASN:OD1	1:B:257:GLY:CA	2.40	0.67
1:B:120:SER:OG	1:B:164:GLY:HA2	1.95	0.67
1:A:365:LYS:NZ	8:A:802:HOH:O	2.27	0.67
1:B:512:LEU:HD12	1:B:512:LEU:H	1.59	0.67
1:D:431:GLY:O	1:D:432:GLN:CB	2.40	0.67
1:D:155:THR:CB	4:D:702:SRM:HAB2	2.09	0.66
1:C:118:ASN:O	1:C:118:ASN:OD1	2.12	0.66
1:D:221:LEU:HD12	1:D:267:ILE:CD1	2.25	0.66
1:B:123:LEU:HD13	1:B:174:LEU:HD21	1.74	0.66
1:A:355:GLN:HB2	1:A:369:MET:HE3	1.76	0.66
1:B:156:THR:O	1:B:546:ARG:NH2	2.29	0.66
1:C:319:MET:CE	1:C:549:MET:CE	2.65	0.66
1:C:323:HIS:O	1:C:324:ARG:HB2	1.94	0.66
1:A:237:LYS:HA	1:A:238:ILE:O	1.96	0.65
1:A:423:HIS:HD2	8:A:842:HOH:O	1.80	0.65
1:B:517:ARG:HD2	1:B:589:GLU:OE1	1.97	0.65
1:C:517:ARG:HD2	1:C:589:GLU:OE1	1.97	0.64
2:F:49:GLY:N	2:F:74:VAL:O	2.29	0.64
2:F:83:SER:O	2:F:85:VAL:HG23	1.99	0.63
1:C:431:GLY:O	1:C:432:GLN:HB3	1.99	0.62
2:F:38:SER:HB3	2:F:46:SER:OG	2.00	0.62
1:A:324:ARG:NH1	2:E:26:ASP:OD2	2.32	0.62
1:B:66:LYS:HE3	1:B:66:LYS:N	2.10	0.62
1:A:123:LEU:HD22	1:A:124:ARG:N	2.16	0.61
1:B:431:GLY:O	1:B:432:GLN:HB3	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:LYS:CB	1:C:238:ILE:HA	2.30	0.61
2:F:58:GLN:NE2	2:F:74:VAL:HG23	2.15	0.61
1:D:355:GLN:O	1:D:358:ASN:O	2.17	0.61
1:D:123:LEU:HD21	1:D:173:VAL:HG11	1.83	0.61
1:D:439:GLU:O	1:D:443:LYS:HG2	2.00	0.61
1:B:123:LEU:HD11	1:B:174:LEU:HD22	1.83	0.61
1:D:572:GLN:HG3	8:D:814:HOH:O	2.01	0.60
1:A:355:GLN:NE2	1:A:372:MET:HE1	2.16	0.60
1:A:355:GLN:CB	1:A:369:MET:HE2	2.27	0.60
1:B:423:HIS:HD2	8:B:827:HOH:O	1.84	0.60
1:D:257:GLY:HA3	1:D:258:THR:CG2	2.32	0.60
1:C:123:LEU:HD13	1:C:174:LEU:CD2	2.32	0.60
1:C:290:ASP:O	1:C:293:THR:HB	2.02	0.60
1:B:123:LEU:HD11	1:B:184:THR:HG21	1.84	0.59
1:D:612:PHE:CE1	1:D:616:THR:HG21	2.37	0.59
1:C:355:GLN:NE2	1:C:372:MET:HE1	2.17	0.59
1:D:567:GLY:O	1:D:574:THR:HG23	2.02	0.59
1:B:123:LEU:HD11	1:B:174:LEU:CD2	2.32	0.59
1:A:217:ILE:HD13	1:A:348:ILE:HD13	1.83	0.59
1:A:355:GLN:HE21	1:A:372:MET:CE	2.16	0.59
1:D:322:THR:HG21	1:D:365:LYS:HE3	1.85	0.59
1:A:355:GLN:CB	1:A:369:MET:CE	2.78	0.58
1:D:369:MET:HE1	1:D:381:PHE:HZ	1.68	0.58
1:A:567:GLY:O	1:A:574:THR:HG23	2.04	0.58
1:A:116:GLN:O	1:A:116:GLN:CG	2.51	0.58
1:D:290:ASP:O	1:D:293:THR:HB	2.03	0.58
1:D:569:THR:HG23	1:D:574:THR:HG21	1.86	0.58
1:C:554:PHE:CE1	1:C:588:ILE:HD13	2.38	0.57
4:C:702:SRM:HBB2	4:C:702:SRM:CHC	2.34	0.57
1:A:75:ASN:O	1:A:78:ARG:HD2	2.03	0.57
1:C:612:PHE:CE1	1:C:616:THR:HG21	2.40	0.57
4:D:702:SRM:HBB1	4:D:702:SRM:HHC	1.87	0.57
1:A:290:ASP:O	1:A:293:THR:HB	2.05	0.57
1:D:92:ILE:H	1:D:107:GLN:HE22	1.51	0.57
1:D:402:TRP:O	1:D:571:ASN:OD1	2.22	0.57
4:D:702:SRM:HHC	4:D:702:SRM:CBB	2.35	0.57
1:C:355:GLN:HE21	1:C:372:MET:CE	2.18	0.57
1:B:239:MET:CB	1:B:240:SER:CA	2.82	0.56
1:A:217:ILE:HD11	1:A:348:ILE:CD1	2.35	0.56
1:A:569:THR:HG23	1:A:574:THR:HG21	1.87	0.56
1:A:580:MET:HE1	1:A:591:VAL:CG1	2.29	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:GLN:HE21	1:B:372:MET:CE	2.19	0.56
1:D:355:GLN:HE21	1:D:372:MET:CE	2.19	0.56
1:D:224:GLN:NE2	1:D:251:ARG:CZ	2.69	0.56
1:D:87:SER:O	1:D:89:ALA:N	2.39	0.55
1:A:116:GLN:O	1:A:116:GLN:HG2	2.04	0.55
1:B:612:PHE:CE1	1:B:616:THR:HG21	2.40	0.55
1:D:257:GLY:CA	1:D:388:TYR:HD2	2.18	0.55
2:E:6:LYS:HD2	2:E:86:VAL:HG13	1.88	0.55
1:A:612:PHE:CE1	1:A:616:THR:HG21	2.42	0.55
1:B:567:GLY:O	1:B:574:THR:HG23	2.06	0.55
1:C:572:GLN:HG2	8:C:801:HOH:O	2.01	0.55
1:A:92:ILE:H	1:A:107:GLN:HE22	1.52	0.55
1:C:332:LEU:HD13	1:C:575:LEU:HG	1.88	0.55
1:A:580:MET:CE	1:A:591:VAL:CG1	2.85	0.55
1:B:92:ILE:H	1:B:107:GLN:HE22	1.52	0.55
1:C:567:GLY:O	1:C:574:THR:HG23	2.06	0.55
1:C:92:ILE:H	1:C:107:GLN:HE22	1.54	0.54
1:A:217:ILE:CD1	1:A:348:ILE:CD1	2.85	0.54
1:C:423:HIS:HD2	8:C:824:HOH:O	1.91	0.54
1:A:106:TYR:CD1	1:A:188:CYS:SG	2.89	0.54
1:B:569:THR:HG23	1:B:574:THR:HG21	1.90	0.54
1:C:375:ARG:NH1	8:C:804:HOH:O	2.40	0.54
1:D:157:ARG:HG3	4:D:702:SRM:HBB2	1.90	0.54
1:D:242:GLU:N	1:D:242:GLU:OE2	2.41	0.54
1:D:431:GLY:O	1:D:432:GLN:HB3	2.07	0.54
4:C:702:SRM:HBB2	4:C:702:SRM:HHC	1.89	0.54
1:D:257:GLY:HA3	1:D:258:THR:HG22	1.90	0.54
1:A:117:LYS:CG	2:E:96:THR:OG1	2.55	0.54
4:A:702:SRM:HHC	4:A:702:SRM:HBB2	1.89	0.53
1:D:486:PRO:HB2	1:D:532:SER:HB2	1.89	0.53
1:D:161:GLN:OE1	4:D:702:SRM:HMB3	2.09	0.53
1:A:497:LEU:HD13	1:A:503:ALA:HB3	1.91	0.53
1:D:454:GLN:NE2	8:D:802:HOH:O	2.36	0.53
2:F:67:GLY:O	2:F:71:ASP:CB	2.57	0.53
2:E:16:LEU:HD12	2:E:18:VAL:HG23	1.90	0.53
1:B:497:LEU:HD13	1:B:503:ALA:HB3	1.91	0.52
1:C:155:THR:CB	4:C:702:SRM:HAB2	2.10	0.52
1:A:238:ILE:HA	1:A:239:MET:C	2.29	0.52
1:A:376:TRP:HB3	1:A:380:ARG:HG2	1.92	0.52
1:B:156:THR:HB	1:B:546:ARG:NH2	2.25	0.52
1:C:254:ASN:CB	1:C:255:SER:CB	2.88	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:LEU:HD13	1:C:503:ALA:HB3	1.90	0.52
1:D:505:THR:HG23	1:D:559:PRO:C	2.30	0.51
1:A:185:LEU:HD13	1:A:223:PRO:HD2	1.92	0.51
1:A:332:LEU:HD13	1:A:575:LEU:HG	1.92	0.51
1:B:348:ILE:C	1:B:348:ILE:HD12	2.30	0.51
1:C:255:SER:O	1:C:256:HIS:C	2.47	0.51
1:C:569:THR:HG23	1:C:574:THR:HG21	1.92	0.51
1:D:332:LEU:HD13	1:D:575:LEU:HG	1.93	0.51
1:D:497:LEU:HD13	1:D:503:ALA:HB3	1.91	0.51
1:B:178:ILE:HG22	1:B:238:ILE:HD12	1.92	0.51
1:A:402:TRP:O	1:A:571:ASN:OD1	2.29	0.51
1:B:355:GLN:NE2	1:B:372:MET:HE2	2.26	0.51
1:C:159:THR:HG21	4:C:702:SRM:O1B	2.10	0.51
4:D:702:SRM:CHC	4:D:702:SRM:CBB	2.88	0.51
1:B:156:THR:OG1	4:B:702:SRM:HAB1	2.11	0.51
1:D:567:GLY:O	1:D:574:THR:CG2	2.59	0.51
4:B:702:SRM:HHA	4:B:702:SRM:O3A	2.11	0.51
1:A:505:THR:CG2	1:A:559:PRO:O	2.57	0.50
1:C:123:LEU:HD21	1:C:170:LEU:HD21	1.91	0.50
1:C:486:PRO:HB2	1:C:532:SER:HB2	1.93	0.50
1:A:431:GLY:O	1:A:432:GLN:HB2	2.07	0.50
1:A:486:PRO:HB2	1:A:532:SER:HB2	1.94	0.50
1:A:190:ASP:OD2	1:A:364:ARG:NH2	2.43	0.50
1:A:365:LYS:HD3	8:A:809:HOH:O	2.10	0.50
1:A:533:VAL:HG22	1:A:609:PHE:HB3	1.94	0.50
1:A:567:GLY:O	1:A:574:THR:CG2	2.60	0.50
1:C:355:GLN:HE21	1:C:372:MET:HE1	1.75	0.50
1:C:505:THR:CG2	1:C:559:PRO:O	2.56	0.50
1:D:355:GLN:NE2	1:D:372:MET:HE2	2.27	0.50
1:A:324:ARG:NH2	8:E:201:HOH:O	2.45	0.50
1:B:332:LEU:HD13	1:B:575:LEU:HG	1.94	0.50
1:B:376:TRP:HB3	1:B:380:ARG:HG2	1.93	0.50
1:C:185:LEU:HD13	1:C:223:PRO:HD2	1.93	0.50
1:B:567:GLY:O	1:B:574:THR:CG2	2.59	0.50
1:D:479:LEU:HD23	1:D:479:LEU:N	2.27	0.49
1:D:190:ASP:OD2	1:D:364:ARG:NH2	2.42	0.49
1:D:322:THR:HG21	1:D:365:LYS:CE	2.41	0.49
1:C:190:ASP:OD2	1:C:364:ARG:NH2	2.41	0.49
1:B:190:ASP:OD2	1:B:364:ARG:NH2	2.43	0.49
1:C:567:GLY:O	1:C:574:THR:CG2	2.61	0.49
4:B:702:SRM:HHC	4:B:702:SRM:HBB2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:TYR:CD1	1:C:188:CYS:SG	2.94	0.49
1:A:579:PHE:CD2	1:A:580:MET:CE	2.96	0.49
1:D:258:THR:OG1	1:D:259:ASN:OD1	2.27	0.49
1:C:355:GLN:NE2	1:C:372:MET:CE	2.76	0.49
1:D:81:LEU:HD22	1:D:85:LEU:HG	1.95	0.49
1:B:533:VAL:HG22	1:B:609:PHE:HB3	1.95	0.48
1:C:81:LEU:HD22	1:C:85:LEU:HG	1.95	0.48
1:D:369:MET:HE1	1:D:381:PHE:CZ	2.47	0.48
1:A:159:THR:HG21	4:A:702:SRM:O1B	2.14	0.48
1:B:81:LEU:HD22	1:B:85:LEU:HG	1.95	0.48
1:D:185:LEU:HD13	1:D:223:PRO:HD2	1.95	0.48
1:D:190:ASP:CG	1:D:364:ARG:HH22	2.16	0.48
1:B:355:GLN:NE2	1:B:372:MET:CE	2.76	0.48
1:C:293:THR:HG22	8:C:838:HOH:O	2.12	0.48
1:B:239:MET:CB	1:B:240:SER:HA	2.43	0.48
8:B:920:HOH:O	1:C:324:ARG:HD2	2.12	0.48
1:D:156:THR:HB	1:D:546:ARG:NH2	2.28	0.48
1:A:123:LEU:HD21	1:A:184:THR:CG2	2.28	0.48
1:B:233:VAL:HG21	1:B:238:ILE:HD11	1.96	0.48
1:D:505:THR:CG2	1:D:559:PRO:O	2.57	0.48
1:C:190:ASP:CG	1:C:364:ARG:HH22	2.16	0.48
1:A:268:TYR:O	1:A:271:GLN:O	2.31	0.47
1:A:355:GLN:HE21	1:A:372:MET:HE1	1.77	0.47
1:C:256:HIS:N	1:C:257:GLY:CA	2.68	0.47
1:D:376:TRP:HB3	1:D:380:ARG:HG2	1.96	0.47
1:B:554:PHE:HE1	1:B:588:ILE:HD12	1.80	0.47
1:D:568:GLY:HA2	1:D:574:THR:HG22	1.95	0.47
1:D:257:GLY:HA2	1:D:388:TYR:HD2	1.79	0.47
1:B:504:GLN:NE2	2:F:41:ALA:CB	2.78	0.47
4:B:702:SRM:CAB	4:B:702:SRM:O3B	2.63	0.47
1:A:275:ARG:NH2	4:A:702:SRM:O4D	2.37	0.47
1:C:505:THR:HG23	1:C:559:PRO:C	2.34	0.47
1:C:568:GLY:HA2	1:C:574:THR:HG22	1.95	0.47
1:A:81:LEU:HD22	1:A:85:LEU:HG	1.97	0.47
1:A:190:ASP:CG	1:A:364:ARG:HH22	2.18	0.47
1:B:159:THR:HG21	4:B:702:SRM:O1B	2.15	0.47
1:B:185:LEU:HD13	1:B:223:PRO:HD2	1.97	0.47
1:C:321:ARG:NH2	1:C:563:GLN:OE1	2.47	0.47
1:D:257:GLY:HA3	1:D:388:TYR:HD2	1.79	0.47
1:D:381:PHE:O	1:D:385:VAL:HG23	2.15	0.47
1:D:355:GLN:NE2	1:D:372:MET:CE	2.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:9:THR:HG22	2:F:89:THR:OG1	2.15	0.47
1:A:355:GLN:NE2	1:A:372:MET:CE	2.75	0.46
4:B:702:SRM:HAB2	4:B:702:SRM:O3B	2.15	0.46
1:C:156:THR:OG1	4:C:702:SRM:HAB1	2.15	0.46
1:D:156:THR:OG1	4:D:702:SRM:HAB1	2.15	0.46
2:E:4:ASN:O	2:E:84:ASP:HA	2.14	0.46
2:E:45:SER:HB3	2:E:63:TYR:CE1	2.50	0.46
1:B:190:ASP:CG	1:B:364:ARG:HH22	2.17	0.46
1:B:233:VAL:O	1:B:233:VAL:HG22	2.16	0.46
1:A:381:PHE:O	1:A:385:VAL:HG23	2.16	0.46
1:A:554:PHE:HE1	1:A:588:ILE:HD12	1.81	0.46
1:A:568:GLY:HA2	1:A:574:THR:HG22	1.98	0.46
1:C:293:THR:CG2	8:C:838:HOH:O	2.63	0.46
2:E:41:ALA:HA	2:E:78:HIS:CE1	2.51	0.46
1:A:505:THR:HG23	1:A:559:PRO:C	2.36	0.46
1:D:257:GLY:HA2	1:D:388:TYR:CD2	2.51	0.46
1:D:106:TYR:CD1	1:D:188:CYS:SG	2.96	0.46
1:A:197:ALA:HA	1:A:281:VAL:O	2.16	0.46
1:C:254:ASN:HA	1:C:255:SER:HA	1.78	0.46
1:C:381:PHE:O	1:C:385:VAL:HG23	2.15	0.46
1:C:511:ILE:HG23	1:C:512:LEU:HD13	1.98	0.46
1:A:572:GLN:HA	8:A:841:HOH:O	2.16	0.45
1:D:224:GLN:HE22	1:D:251:ARG:CZ	2.30	0.45
1:B:381:PHE:O	1:B:385:VAL:HG23	2.16	0.45
1:B:568:GLY:HA2	1:B:574:THR:HG22	1.99	0.45
2:E:95:LEU:N	2:E:95:LEU:CD2	2.78	0.45
1:D:159:THR:HG21	4:D:702:SRM:O1B	2.16	0.45
1:B:290:ASP:OD1	1:B:546:ARG:HD2	2.17	0.45
1:D:123:LEU:CD2	1:D:173:VAL:HG11	2.46	0.45
2:F:58:GLN:OE1	2:F:69:ILE:HG12	2.17	0.45
1:B:570:PRO:HG2	1:B:608:SER:OG	2.17	0.45
1:C:123:LEU:HD13	1:C:174:LEU:HD23	1.98	0.45
2:E:94:GLU:C	2:E:95:LEU:CD2	2.83	0.45
1:A:277:PHE:CZ	1:A:369:MET:HE1	2.52	0.44
2:F:58:GLN:HE22	2:F:74:VAL:HA	1.83	0.44
1:D:257:GLY:HA3	1:D:258:THR:HG23	1.99	0.44
1:D:477:GLY:O	1:D:479:LEU:HD23	2.17	0.44
2:F:49:GLY:C	2:F:74:VAL:HG12	2.38	0.44
1:A:293:THR:HG21	1:A:546:ARG:CD	2.48	0.44
1:A:511:ILE:HG23	1:A:512:LEU:HD13	1.99	0.44
1:D:293:THR:HG21	1:D:546:ARG:HD3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:CD1	1:A:223:PRO:HD2	2.47	0.44
1:C:257:GLY:HA2	1:C:258:THR:CB	2.47	0.44
1:D:290:ASP:OD1	1:D:546:ARG:HD2	2.17	0.44
1:C:101:LYS:O	1:C:188:CYS:HB2	2.18	0.43
1:A:123:LEU:HD22	1:A:123:LEU:C	2.38	0.43
1:D:554:PHE:HE1	1:D:588:ILE:HD12	1.82	0.43
1:A:291:ILE:HG23	1:A:292:LEU:HD13	1.99	0.43
1:A:519:ARG:NH1	1:A:529:ASP:HA	2.34	0.43
4:A:702:SRM:HBB2	4:A:702:SRM:CHC	2.49	0.43
1:C:426:ASN:HD21	1:C:511:ILE:HG21	1.83	0.43
1:D:511:ILE:HG23	1:D:512:LEU:HD13	2.00	0.43
4:B:702:SRM:HBB2	4:B:702:SRM:CHC	2.49	0.43
1:D:351:ILE:HG23	1:D:369:MET:HE1	2.00	0.43
1:A:293:THR:CG2	8:A:898:HOH:O	2.67	0.43
1:D:479:LEU:N	1:D:479:LEU:CD2	2.81	0.43
1:B:197:ALA:HA	1:B:281:VAL:O	2.19	0.42
1:C:293:THR:HG21	1:C:546:ARG:CD	2.49	0.42
1:C:612:PHE:O	1:C:616:THR:CG2	2.62	0.42
1:C:197:ALA:HA	1:C:281:VAL:O	2.19	0.42
2:F:85:VAL:CG1	2:F:87:ILE:HG13	2.49	0.42
1:A:612:PHE:O	1:A:616:THR:CG2	2.62	0.42
1:B:185:LEU:CD1	1:B:223:PRO:HD2	2.49	0.42
1:A:238:ILE:HA	1:A:239:MET:O	2.20	0.42
1:C:122:MET:C	1:C:123:LEU:HD23	2.40	0.42
1:D:291:ILE:HG23	1:D:292:LEU:HD13	2.01	0.42
2:E:44:CYS:SG	2:E:45:SER:N	2.91	0.42
1:B:612:PHE:O	1:B:616:THR:CG2	2.61	0.42
1:D:612:PHE:O	1:D:616:THR:CG2	2.62	0.42
2:F:35:LEU:HB3	2:F:36:PRO:HD2	2.01	0.42
2:F:46:SER:HA	2:F:92:GLU:OE1	2.19	0.42
1:C:426:ASN:ND2	8:C:814:HOH:O	2.53	0.42
1:A:101:LYS:O	1:A:188:CYS:HB2	2.20	0.42
1:B:75:ASN:O	1:B:78:ARG:HG2	2.18	0.42
1:C:254:ASN:CB	1:C:255:SER:CA	2.96	0.42
1:D:197:ALA:HA	1:D:281:VAL:O	2.19	0.42
2:F:69:ILE:C	2:F:71:ASP:H	2.23	0.42
2:E:58:GLN:HE22	2:E:74:VAL:HA	1.84	0.42
1:A:157:ARG:HB2	4:A:702:SRM:CCB	2.50	0.41
1:B:426:ASN:HD21	1:B:511:ILE:HG21	1.84	0.41
1:B:220:LEU:HG	1:B:221:LEU:HD13	2.02	0.41
1:D:519:ARG:NH1	1:D:529:ASP:HA	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:58:GLN:HE22	2:F:74:VAL:HG23	1.84	0.41
1:A:517:ARG:CD	1:A:589:GLU:OE1	2.63	0.41
1:B:149:ILE:HD13	1:B:164:GLY:HA3	2.02	0.41
1:C:291:ILE:HG23	1:C:292:LEU:HD13	2.02	0.41
1:C:303:ASP:CB	1:C:307:GLU:O	2.65	0.41
1:C:519:ARG:NH1	1:C:529:ASP:HA	2.35	0.41
1:C:491:ALA:HA	1:C:535:VAL:O	2.21	0.41
1:D:101:LYS:O	1:D:188:CYS:HB2	2.21	0.41
1:A:238:ILE:HG12	1:A:240:SER:OG	2.20	0.41
1:A:620:LYS:H	1:A:620:LYS:HG3	1.47	0.41
1:B:114:ARG:H	1:B:114:ARG:CD	2.24	0.41
1:B:157:ARG:HB2	4:B:702:SRM:CCB	2.50	0.41
1:B:519:ARG:NH1	1:B:529:ASP:HA	2.36	0.41
1:A:491:ALA:HA	1:A:535:VAL:O	2.21	0.41
1:B:78:ARG:NH1	1:B:230:ASP:OD1	2.50	0.41
1:B:101:LYS:O	1:B:188:CYS:HB2	2.20	0.41
1:C:568:GLY:HA2	1:C:574:THR:CG2	2.51	0.41
1:D:153:ARG:NH1	1:D:508:GLU:CD	2.64	0.41
1:A:149:ILE:HD13	8:A:808:HOH:O	2.10	0.41
1:A:355:GLN:CB	1:A:369:MET:HE3	2.46	0.41
4:A:702:SRM:CHC	4:A:702:SRM:CBB	2.99	0.40
1:B:233:VAL:O	1:B:236:GLU:HB3	2.21	0.40
1:C:517:ARG:CD	1:C:589:GLU:OE1	2.67	0.40
1:D:157:ARG:HH22	1:D:294:ASN:ND2	2.20	0.40
1:A:116:GLN:HG3	1:A:118:ASN:OD1	2.21	0.40
1:A:220:LEU:HG	1:A:221:LEU:HD13	2.02	0.40
1:C:572:GLN:HA	8:C:823:HOH:O	2.22	0.40
1:D:185:LEU:CD1	1:D:223:PRO:HD2	2.51	0.40
1:A:156:THR:OG1	4:A:702:SRM:HAB1	2.22	0.40
1:C:323:HIS:O	1:C:324:ARG:CB	2.61	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	565/583 (97%)	546 (97%)	14 (2%)	5 (1%)	17	16
1	B	561/583 (96%)	545 (97%)	10 (2%)	6 (1%)	14	12
1	C	559/583 (96%)	544 (97%)	9 (2%)	6 (1%)	14	12
1	D	544/583 (93%)	529 (97%)	10 (2%)	5 (1%)	17	16
2	E	94/98 (96%)	90 (96%)	4 (4%)	0	100	100
2	F	69/98 (70%)	61 (88%)	5 (7%)	3 (4%)	2	1
All	All	2392/2528 (95%)	2315 (97%)	52 (2%)	25 (1%)	15	14

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	432	GLN
1	B	238	ILE
1	B	432	GLN
1	B	600	ASN
1	C	256	HIS
1	C	258	THR
1	C	432	GLN
1	D	432	GLN
2	F	57	ASP
1	A	238	ILE
1	A	253	ASP
1	B	253	ASP
1	B	431	GLY
1	C	303	ASP
1	C	431	GLY
1	D	303	ASP
1	D	365	LYS
1	D	402	TRP
2	F	65	ASP
1	A	235	GLY
1	B	258	THR
1	C	237	LYS
1	A	237	LYS
2	F	56	VAL
1	D	431	GLY

5.3.2 Protein sidechains (i)

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	479/493 (97%)	440 (92%)	39 (8%)	11	12
1	B	480/493 (97%)	443 (92%)	37 (8%)	13	13
1	C	475/493 (96%)	437 (92%)	38 (8%)	12	12
1	D	470/493 (95%)	433 (92%)	37 (8%)	12	12
2	E	83/83 (100%)	78 (94%)	5 (6%)	19	22
2	F	49/83 (59%)	44 (90%)	5 (10%)	7	6
All	All	2036/2138 (95%)	1875 (92%)	161 (8%)	12	12

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	66	LYS
1	A	81	LEU
1	A	86	VAL
1	A	88	GLU
1	A	113	VAL
1	A	116	GLN
1	A	123	LEU
1	A	138	LEU
1	A	159	THR
1	A	170	LEU
1	A	185	LEU
1	A	191	LEU
1	A	221	LEU
1	A	233	VAL
1	A	243	GLU
1	A	292	LEU
1	A	293	THR
1	A	322	THR
1	A	326	GLU
1	A	332	LEU
1	A	374	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	392	LYS
1	A	417	LYS
1	A	438	ARG
1	A	497	LEU
1	A	499	LEU
1	A	505	THR
1	A	512	LEU
1	A	516	LYS
1	A	528	LYS
1	A	533	VAL
1	A	535	VAL
1	A	540	CYS
1	A	552	LEU
1	A	574	THR
1	A	575	LEU
1	A	590	LYS
1	A	616	THR
1	B	64	ARG
1	B	66	LYS
1	B	73	LYS
1	B	78	ARG
1	B	81	LEU
1	B	86	VAL
1	B	88	GLU
1	B	113	VAL
1	B	114	ARG
1	B	120	SER
1	B	138	LEU
1	B	149	ILE
1	B	159	THR
1	B	170	LEU
1	B	185	LEU
1	B	191	LEU
1	B	221	LEU
1	B	242	GLU
1	B	292	LEU
1	B	332	LEU
1	B	348	ILE
1	B	365	LYS
1	B	372	MET
1	B	398	PRO
1	B	438	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	497	LEU
1	B	499	LEU
1	B	512	LEU
1	B	516	LYS
1	B	533	VAL
1	B	535	VAL
1	B	540	CYS
1	B	552	LEU
1	B	574	THR
1	B	575	LEU
1	B	616	THR
1	B	627	LYS
1	C	64	ARG
1	C	66	LYS
1	C	81	LEU
1	C	113	VAL
1	C	118	ASN
1	C	159	THR
1	C	170	LEU
1	C	174	LEU
1	C	185	LEU
1	C	191	LEU
1	C	221	LEU
1	C	233	VAL
1	C	239	MET
1	C	243	GLU
1	C	245	PRO
1	C	267	ILE
1	C	292	LEU
1	C	293	THR
1	C	322	THR
1	C	332	LEU
1	C	348	ILE
1	C	365	LYS
1	C	391	LYS
1	C	392	LYS
1	C	395	SER
1	C	411	GLN
1	C	438	ARG
1	C	449	SER
1	C	497	LEU
1	C	499	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	505	THR
1	C	512	LEU
1	C	516	LYS
1	C	540	CYS
1	C	552	LEU
1	C	574	THR
1	C	575	LEU
1	C	616	THR
1	D	64	ARG
1	D	66	LYS
1	D	81	LEU
1	D	86	VAL
1	D	159	THR
1	D	170	LEU
1	D	185	LEU
1	D	191	LEU
1	D	221	LEU
1	D	224	GLN
1	D	242	GLU
1	D	261	PRO
1	D	292	LEU
1	D	293	THR
1	D	322	THR
1	D	324	ARG
1	D	332	LEU
1	D	365	LYS
1	D	372	MET
1	D	380	ARG
1	D	417	LYS
1	D	438	ARG
1	D	463	GLN
1	D	479	LEU
1	D	497	LEU
1	D	499	LEU
1	D	505	THR
1	D	512	LEU
1	D	516	LYS
1	D	535	VAL
1	D	540	CYS
1	D	552	LEU
1	D	574	THR
1	D	575	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	590	LYS
1	D	616	THR
1	D	627	LYS
2	E	14	VAL
2	E	16	LEU
2	E	78	HIS
2	E	93	GLU
2	E	95	LEU
2	F	14	VAL
2	F	46	SER
2	F	51	VAL
2	F	53	SER
2	F	78	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	107	GLN
1	A	135	GLN
1	A	192	ASN
1	A	211	GLN
1	A	224	GLN
1	A	252	ASN
1	A	294	ASN
1	A	355	GLN
1	A	403	GLN
1	A	423	HIS
1	A	426	ASN
1	A	454	GLN
1	A	463	GLN
1	A	542	ASN
1	B	98	GLN
1	B	107	GLN
1	B	118	ASN
1	B	192	ASN
1	B	211	GLN
1	B	252	ASN
1	B	294	ASN
1	B	355	GLN
1	B	403	GLN
1	B	423	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	426	ASN
1	B	454	GLN
1	B	504	GLN
1	B	542	ASN
1	B	572	GLN
1	C	98	GLN
1	C	107	GLN
1	C	211	GLN
1	C	224	GLN
1	C	252	ASN
1	C	294	ASN
1	C	355	GLN
1	C	403	GLN
1	C	423	HIS
1	C	426	ASN
1	C	454	GLN
1	C	542	ASN
1	C	572	GLN
1	D	98	GLN
1	D	107	GLN
1	D	118	ASN
1	D	192	ASN
1	D	211	GLN
1	D	252	ASN
1	D	271	GLN
1	D	294	ASN
1	D	355	GLN
1	D	403	GLN
1	D	426	ASN
1	D	454	GLN
1	D	542	ASN
1	D	572	GLN
2	E	58	GLN
2	F	58	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
4	SRM	D	702	1	68,70,70	2.87	24 (35%)	81,112,112	3.52	35 (43%)
7	FES	E	101	2	0,4,4	-	-	-		
4	SRM	C	702	1	68,70,70	3.12	23 (33%)	81,112,112	3.72	39 (48%)
3	SF4	C	701	1	0,12,12	-	-	-		
4	SRM	B	702	1	68,70,70	2.76	25 (36%)	81,112,112	3.92	40 (49%)
3	SF4	D	701	1	0,12,12	-	-	-		
3	SF4	A	701	1	0,12,12	-	-	-		
4	SRM	A	702	1	68,70,70	2.90	25 (36%)	81,112,112	4.01	44 (54%)
7	FES	F	101	2	0,4,4	-	-	-		
3	SF4	B	701	1	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SRM	D	702	1	3/3/19/23	12/38/126/126	-
7	FES	E	101	2	-	-	0/1/1/1
4	SRM	C	702	1	3/3/19/23	10/38/126/126	-
3	SF4	C	701	1	-	-	0/6/5/5
4	SRM	B	702	1	3/3/19/23	13/38/126/126	-
3	SF4	D	701	1	-	-	0/6/5/5
3	SF4	A	701	1	-	-	0/6/5/5
4	SRM	A	702	1	3/3/19/23	13/38/126/126	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FES	F	101	2	-	-	0/1/1/1
3	SF4	B	701	1	-	-	0/6/5/5

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	702	SRM	C4B-NB	-14.43	1.25	1.35
4	D	702	SRM	C4B-NB	-11.26	1.27	1.35
4	A	702	SRM	C4B-NB	-10.53	1.27	1.35
4	C	702	SRM	CHD-C4C	8.89	1.47	1.35
4	D	702	SRM	CHD-C4C	8.85	1.47	1.35
4	A	702	SRM	CHD-C4C	8.75	1.47	1.35
4	B	702	SRM	C4B-NB	-8.45	1.29	1.35
4	B	702	SRM	CHD-C4C	7.25	1.45	1.35
4	D	702	SRM	CHA-C1A	6.98	1.47	1.35
4	B	702	SRM	CHA-C1A	6.66	1.47	1.35
4	A	702	SRM	CAB-C3B	-6.47	1.39	1.54
4	B	702	SRM	CAB-CBB	6.36	1.72	1.52
4	D	702	SRM	CHC-C1C	6.29	1.50	1.38
4	C	702	SRM	CHA-C1A	5.98	1.46	1.35
4	C	702	SRM	CAB-CBB	5.70	1.70	1.52
4	A	702	SRM	CAB-CBB	5.58	1.70	1.52
4	A	702	SRM	CBB-CCB	5.57	1.63	1.50
4	A	702	SRM	CHA-C1A	5.34	1.44	1.35
4	A	702	SRM	CDC-CEC	-5.30	1.43	1.51
4	C	702	SRM	CAB-C3B	-5.29	1.42	1.54
4	B	702	SRM	CAB-C3B	-5.25	1.42	1.54
4	C	702	SRM	C3B-C4B	-5.13	1.40	1.51
4	B	702	SRM	C3B-C4B	-5.03	1.40	1.51
4	B	702	SRM	C2B-C3B	-5.00	1.41	1.55
4	C	702	SRM	CHC-C1C	5.00	1.48	1.38
4	B	702	SRM	CHC-C1C	4.89	1.47	1.38
4	B	702	SRM	C3C-C2C	4.87	1.47	1.36
4	D	702	SRM	C3B-C4B	-4.78	1.41	1.51
4	C	702	SRM	C3C-C2C	4.73	1.46	1.36
4	C	702	SRM	CDC-CEC	-4.67	1.43	1.51
4	A	702	SRM	C3B-C4B	-4.65	1.41	1.51
4	C	702	SRM	C2B-C3B	-4.61	1.42	1.55
4	B	702	SRM	CBB-CCB	4.53	1.61	1.50
4	D	702	SRM	CAB-C3B	-4.46	1.44	1.54
4	D	702	SRM	C3C-C2C	4.41	1.46	1.36
4	B	702	SRM	C3D-C2D	4.26	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	702	SRM	C2B-C3B	-4.20	1.43	1.55
4	D	702	SRM	CDC-CEC	-4.07	1.44	1.51
4	A	702	SRM	CHC-C1C	4.06	1.46	1.38
4	C	702	SRM	C1C-NC	-4.00	1.32	1.39
4	A	702	SRM	C2B-C3B	-4.00	1.44	1.55
4	D	702	SRM	C3D-C2D	3.89	1.48	1.39
4	A	702	SRM	C4C-NC	-3.86	1.32	1.39
4	C	702	SRM	C3D-C2D	3.79	1.48	1.39
4	A	702	SRM	C3C-C2C	3.72	1.44	1.36
4	B	702	SRM	C1C-NC	-3.69	1.32	1.39
4	B	702	SRM	C3A-C4A	-3.57	1.43	1.51
4	D	702	SRM	CAB-CBB	3.54	1.63	1.52
4	A	702	SRM	C1D-CHD	3.51	1.50	1.41
4	C	702	SRM	CBB-CCB	3.44	1.58	1.50
4	A	702	SRM	C3D-C2D	3.40	1.47	1.39
4	A	702	SRM	C1C-NC	-3.37	1.33	1.39
4	C	702	SRM	C4D-CHA	3.37	1.50	1.41
4	D	702	SRM	C4C-NC	-3.28	1.33	1.39
4	A	702	SRM	C4A-NA	-3.14	1.33	1.35
4	B	702	SRM	C1D-CHD	3.14	1.49	1.41
4	C	702	SRM	C4C-NC	-3.09	1.33	1.39
4	B	702	SRM	FE-NC	3.00	2.07	1.95
4	D	702	SRM	C1C-NC	-2.99	1.34	1.39
4	D	702	SRM	CHB-C4A	2.97	1.47	1.39
4	A	702	SRM	FE-NC	2.93	2.07	1.95
4	D	702	SRM	C3A-C4A	-2.87	1.45	1.51
4	B	702	SRM	C4D-CHA	2.80	1.48	1.41
4	B	702	SRM	C4C-NC	-2.76	1.34	1.39
4	D	702	SRM	FE-NC	2.75	2.06	1.95
4	C	702	SRM	CMB-C2B	-2.74	1.49	1.54
4	D	702	SRM	CBB-CCB	2.72	1.56	1.50
4	D	702	SRM	C2A-C3A	-2.60	1.48	1.55
4	D	702	SRM	C1D-CHD	2.52	1.48	1.41
4	A	702	SRM	CAD-C2D	-2.48	1.48	1.52
4	A	702	SRM	C4D-CHA	2.46	1.47	1.41
4	A	702	SRM	C1D-ND	-2.46	1.31	1.36
4	D	702	SRM	C4D-CHA	2.45	1.47	1.41
4	B	702	SRM	CHB-C4A	2.40	1.46	1.39
4	B	702	SRM	O4A-CEA	-2.36	1.22	1.30
4	B	702	SRM	C4A-NA	-2.35	1.33	1.35
4	A	702	SRM	C2A-C3A	-2.34	1.48	1.55
4	A	702	SRM	O3A-CEA	2.33	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	702	SRM	C3A-C4A	-2.32	1.46	1.51
4	B	702	SRM	CDC-CEC	-2.31	1.47	1.51
4	C	702	SRM	C1D-CHD	2.29	1.47	1.41
4	D	702	SRM	CHB-C1B	2.28	1.44	1.37
4	C	702	SRM	CHB-C4A	2.25	1.45	1.39
4	D	702	SRM	C1C-C2C	2.22	1.49	1.45
4	B	702	SRM	C2A-C3A	-2.22	1.49	1.55
4	A	702	SRM	O4D-CED	-2.21	1.23	1.30
4	B	702	SRM	CAD-C2D	-2.21	1.48	1.52
4	B	702	SRM	O4D-CED	-2.19	1.23	1.30
4	C	702	SRM	CDC-C2C	-2.18	1.47	1.51
4	A	702	SRM	CHB-C4A	2.14	1.45	1.39
4	D	702	SRM	FE-NA	2.10	2.08	1.97
4	B	702	SRM	O1B-CCB	2.10	1.29	1.22
4	C	702	SRM	C2A-C3A	-2.07	1.49	1.55
4	D	702	SRM	O4D-CED	-2.06	1.23	1.30
4	C	702	SRM	FE-NA	2.05	2.08	1.97
4	C	702	SRM	O4A-CEA	-2.03	1.23	1.30
4	A	702	SRM	O2B-CCB	-2.01	1.24	1.30

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	702	SRM	CMB-C2B-C3B	12.55	135.28	112.08
4	A	702	SRM	CMB-C2B-C3B	12.29	134.79	112.08
4	A	702	SRM	C2B-C3B-C4B	12.10	116.39	100.90
4	B	702	SRM	C2B-C3B-C4B	11.97	116.23	100.90
4	D	702	SRM	C2B-C3B-C4B	11.91	116.14	100.90
4	C	702	SRM	C2B-C3B-C4B	11.69	115.86	100.90
4	C	702	SRM	CMB-C2B-C3B	11.57	133.46	112.08
4	B	702	SRM	CAB-CBB-CCB	11.30	142.48	112.51
4	A	702	SRM	CAA-C3A-C4A	10.71	130.08	111.19
4	A	702	SRM	CAB-CBB-CCB	10.66	140.79	112.51
4	D	702	SRM	CAA-C3A-C4A	10.59	129.86	111.19
4	C	702	SRM	CAA-C3A-C4A	10.46	129.63	111.19
4	C	702	SRM	CAB-CBB-CCB	10.45	140.25	112.51
4	B	702	SRM	CAA-C3A-C4A	9.78	128.43	111.19
4	D	702	SRM	CAB-CBB-CCB	9.64	138.09	112.51
4	D	702	SRM	CMB-C2B-C3B	9.56	129.74	112.08
4	C	702	SRM	CBB-CAB-C3B	-9.29	87.92	114.73
4	A	702	SRM	O2B-CCB-O1B	-7.88	103.65	123.30
4	B	702	SRM	CBB-CAB-C3B	-7.82	92.17	114.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	702	SRM	CMB-C2B-CDB	-7.52	98.41	110.80
4	A	702	SRM	CMA-C2A-C3A	-7.33	98.52	112.08
4	B	702	SRM	CAB-C3B-C4B	7.04	123.61	111.19
4	A	702	SRM	CAB-C3B-C4B	7.00	123.54	111.19
4	B	702	SRM	CBD-CAD-C2D	-6.91	100.83	112.62
4	A	702	SRM	CBB-CAB-C3B	-6.87	94.89	114.73
4	D	702	SRM	CBD-CAD-C2D	-6.58	101.38	112.62
4	A	702	SRM	CBD-CAD-C2D	-6.50	101.53	112.62
4	A	702	SRM	C2B-C1B-CHB	-6.30	117.79	123.54
4	B	702	SRM	C2B-C1B-CHB	-6.13	117.94	123.54
4	D	702	SRM	CAC-CBC-CCC	-6.06	100.56	113.60
4	D	702	SRM	C3B-C2B-C1B	-6.03	90.57	100.92
4	B	702	SRM	CMA-C2A-C3A	-6.03	100.93	112.08
4	D	702	SRM	CAB-C3B-C4B	6.03	121.82	111.19
4	C	702	SRM	CBD-CAD-C2D	-5.99	102.39	112.62
4	B	702	SRM	CMB-C2B-CDB	-5.95	100.99	110.80
4	C	702	SRM	CAB-C3B-C4B	5.92	121.64	111.19
4	A	702	SRM	C3D-CDD-CED	-5.92	107.14	114.21
4	C	702	SRM	C2A-C3A-C4A	5.88	108.43	100.90
4	A	702	SRM	C3B-C2B-C1B	-5.67	91.19	100.92
4	B	702	SRM	O2B-CCB-O1B	-5.63	109.26	123.30
4	D	702	SRM	CMA-C2A-C3A	-5.62	101.70	112.08
4	A	702	SRM	CDB-C2B-C3B	-5.53	93.56	108.39
4	B	702	SRM	C3C-C4C-NC	5.52	115.69	110.32
4	C	702	SRM	C3B-C2B-C1B	-5.48	91.51	100.92
4	D	702	SRM	CBB-CAB-C3B	-5.47	98.93	114.73
4	B	702	SRM	C3B-C2B-C1B	-5.44	91.58	100.92
4	A	702	SRM	CDA-C2A-C3A	5.43	122.94	108.39
4	D	702	SRM	C3C-C4C-NC	5.41	115.59	110.32
4	D	702	SRM	C2A-C3A-C4A	5.36	107.76	100.90
4	C	702	SRM	O2B-CCB-O1B	-5.35	109.96	123.30
4	A	702	SRM	C2C-C1C-NC	5.32	115.50	110.32
4	C	702	SRM	CMA-C2A-C3A	-5.31	102.27	112.08
4	B	702	SRM	CDB-C2B-C3B	-5.30	94.20	108.39
4	B	702	SRM	CAC-CBC-CCC	-5.26	102.28	113.60
4	B	702	SRM	CDA-C2A-C3A	4.98	121.74	108.39
4	A	702	SRM	CHC-C1C-NC	-4.94	119.10	124.44
4	D	702	SRM	CDA-C2A-C3A	4.86	121.40	108.39
4	D	702	SRM	C4C-C3C-C2C	-4.75	101.36	106.86
4	C	702	SRM	CDB-C2B-C3B	-4.73	95.72	108.39
4	B	702	SRM	C4C-C3C-C2C	-4.73	101.39	106.86
4	A	702	SRM	C2A-C3A-C4A	4.52	106.69	100.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	702	SRM	CDA-C2A-C3A	4.51	120.48	108.39
4	B	702	SRM	C2A-C3A-C4A	4.50	106.67	100.90
4	A	702	SRM	C3C-C4C-NC	4.43	114.64	110.32
4	D	702	SRM	CDB-C2B-C3B	-4.35	96.75	108.39
4	B	702	SRM	CHC-C1C-NC	-4.25	119.84	124.44
4	C	702	SRM	CDA-C2A-C1A	4.20	120.34	107.12
4	C	702	SRM	CAC-CBC-CCC	-4.17	104.64	113.60
4	A	702	SRM	C1C-C2C-C3C	-3.98	102.26	106.86
4	D	702	SRM	C2B-C1B-CHB	-3.96	119.93	123.54
4	A	702	SRM	C4A-CHB-C1B	-3.93	120.08	125.88
4	D	702	SRM	CHC-C1C-NC	-3.87	120.25	124.44
4	C	702	SRM	C4C-C3C-C2C	-3.80	102.46	106.86
4	B	702	SRM	CDA-C2A-C1A	3.80	119.05	107.12
4	D	702	SRM	CDA-C2A-C1A	3.78	119.01	107.12
4	D	702	SRM	CEC-CDC-C2C	3.76	123.56	113.79
4	C	702	SRM	CMB-C2B-C1B	3.75	128.33	109.57
4	C	702	SRM	C2A-C1A-NA	3.73	117.21	111.21
4	C	702	SRM	C2B-C1B-CHB	-3.70	120.16	123.54
4	A	702	SRM	CDA-C2A-C1A	3.68	118.68	107.12
4	D	702	SRM	C2B-C1B-NB	3.57	116.94	111.21
4	A	702	SRM	O3C-CEC-CDC	-3.45	112.00	122.08
4	C	702	SRM	CHC-C1C-NC	-3.42	120.74	124.44
4	A	702	SRM	C2A-C1A-NA	3.41	116.69	111.21
4	B	702	SRM	C2B-C1B-NB	3.38	116.65	111.21
4	D	702	SRM	O1C-CCC-CBC	-3.37	112.25	123.08
4	A	702	SRM	CAC-CBC-CCC	-3.37	106.36	113.60
4	A	702	SRM	CDD-C3D-C2D	3.34	132.45	126.49
4	B	702	SRM	C4D-CHA-C1A	-3.26	123.67	130.12
4	C	702	SRM	C3D-CDD-CED	3.22	118.06	114.21
4	B	702	SRM	CAA-C3A-C2A	3.20	122.96	114.14
4	B	702	SRM	C2C-C1C-NC	3.18	113.42	110.32
4	A	702	SRM	CHD-C4C-NC	-3.14	121.03	124.43
4	B	702	SRM	O1A-CCA-CBA	-3.12	113.07	123.08
4	C	702	SRM	C3A-C2A-C1A	-3.09	95.62	100.92
4	A	702	SRM	C4C-C3C-C2C	-3.04	103.34	106.86
4	A	702	SRM	O2B-CCB-CBB	3.03	123.77	114.03
4	A	702	SRM	CMB-C2B-CDB	-3.02	105.83	110.80
4	C	702	SRM	C3C-C4C-NC	3.01	113.25	110.32
4	B	702	SRM	CMB-C2B-C1B	3.01	124.59	109.57
4	B	702	SRM	C4A-CHB-C1B	-3.00	121.45	125.88
4	C	702	SRM	CAB-C3B-C2B	3.00	122.41	114.14
4	C	702	SRM	C2B-C1B-NB	2.98	116.01	111.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	702	SRM	O2B-CCB-O1B	-2.96	115.92	123.30
4	D	702	SRM	O4C-CEC-O3C	2.96	130.66	123.30
4	A	702	SRM	O1B-CCB-CBB	2.95	132.54	123.08
4	A	702	SRM	O4C-CEC-O3C	2.94	130.62	123.30
4	B	702	SRM	CAC-C3C-C4C	2.84	130.26	124.89
4	A	702	SRM	C4B-NB-C1B	2.84	108.45	105.23
4	C	702	SRM	C2C-C1C-NC	2.80	113.05	110.32
4	D	702	SRM	CAB-C3B-C2B	2.76	121.73	114.14
4	A	702	SRM	CEC-CDC-C2C	2.74	120.90	113.79
4	B	702	SRM	CEC-CDC-C2C	2.70	120.79	113.79
4	A	702	SRM	C2B-C1B-NB	2.66	115.48	111.21
4	A	702	SRM	CAA-C3A-C2A	2.63	121.38	114.14
4	C	702	SRM	C1C-C2C-C3C	-2.62	103.83	106.86
4	D	702	SRM	C2C-C1C-NC	2.60	112.85	110.32
4	B	702	SRM	O4A-CEA-CDA	2.57	122.60	114.35
4	D	702	SRM	C2A-C1A-NA	2.56	115.32	111.21
4	B	702	SRM	O1C-CCC-CBC	-2.52	115.00	123.08
4	B	702	SRM	C3D-CDD-CED	-2.49	111.24	114.21
4	D	702	SRM	O3C-CEC-CDC	-2.49	114.82	122.08
4	A	702	SRM	C4D-CHA-C1A	-2.48	125.20	130.12
4	D	702	SRM	C3D-CDD-CED	-2.48	111.25	114.21
4	D	702	SRM	CAA-C3A-C2A	2.46	120.92	114.14
4	A	702	SRM	CMB-C2B-C1B	2.44	121.76	109.57
4	B	702	SRM	CHD-C4C-C3C	-2.41	121.04	124.93
4	B	702	SRM	C1C-C2C-C3C	-2.40	104.08	106.86
4	D	702	SRM	CMB-C2B-C1B	2.37	121.43	109.57
4	D	702	SRM	O3D-CED-CDD	-2.32	116.42	123.04
4	D	702	SRM	CHD-C4C-C3C	-2.31	121.20	124.93
4	B	702	SRM	O1B-CCB-CBB	2.31	130.50	123.08
4	B	702	SRM	O3C-CEC-CDC	-2.31	115.34	122.08
4	C	702	SRM	O4A-CEA-O3A	-2.30	117.57	123.30
4	C	702	SRM	O4C-CEC-O3C	2.30	129.02	123.30
4	B	702	SRM	CDD-C3D-C2D	2.26	130.52	126.49
4	C	702	SRM	O2B-CCB-CBB	2.24	121.23	114.03
4	B	702	SRM	O4A-CEA-O3A	-2.21	117.80	123.30
4	A	702	SRM	O4B-CEB-O3B	-2.18	117.87	123.30
4	B	702	SRM	CAB-C3B-C2B	2.17	120.12	114.14
4	C	702	SRM	CHD-C4C-C3C	-2.17	121.43	124.93
4	C	702	SRM	C4A-CHB-C1B	-2.16	122.69	125.88
4	C	702	SRM	O4A-CEA-CDA	2.15	121.25	114.35
4	A	702	SRM	C3A-C2A-C1A	-2.14	97.26	100.92
4	C	702	SRM	CAA-C3A-C2A	2.13	120.02	114.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	702	SRM	CAB-C3B-C2B	2.13	120.02	114.14
4	C	702	SRM	C4D-CHA-C1A	-2.13	125.90	130.12
4	D	702	SRM	CAC-C3C-C4C	2.11	128.88	124.89
4	B	702	SRM	O2A-CCA-CBA	2.10	120.78	114.03
4	A	702	SRM	CBA-CAA-C3A	2.09	120.76	114.73
4	C	702	SRM	O3C-CEC-CDC	-2.09	115.98	122.08
4	C	702	SRM	O3D-CED-CDD	-2.08	117.11	123.04
4	A	702	SRM	C3B-C4B-NB	-2.07	106.78	110.85
4	A	702	SRM	C3A-C4A-CHB	-2.06	118.86	123.32
4	A	702	SRM	CAD-C2D-C3D	2.04	131.33	124.90
4	C	702	SRM	O2A-CCA-CBA	2.02	120.52	114.03
4	D	702	SRM	C1C-C2C-C3C	-2.01	104.53	106.86
4	D	702	SRM	C4A-CHB-C1B	-2.00	122.93	125.88

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	702	SRM	C3A
4	A	702	SRM	C3B
4	A	702	SRM	NC
4	B	702	SRM	C3A
4	B	702	SRM	C3B
4	B	702	SRM	NC
4	C	702	SRM	C3A
4	C	702	SRM	C3B
4	C	702	SRM	NC
4	D	702	SRM	C3A
4	D	702	SRM	C3B
4	D	702	SRM	NC

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	702	SRM	C1A-C2A-CDA-CEA
4	A	702	SRM	CMA-C2A-CDA-CEA
4	A	702	SRM	C2A-C3A-CAA-CBA
4	B	702	SRM	C1A-C2A-CDA-CEA
4	B	702	SRM	CMA-C2A-CDA-CEA
4	B	702	SRM	C2A-C3A-CAA-CBA
4	C	702	SRM	C1A-C2A-CDA-CEA
4	C	702	SRM	CMA-C2A-CDA-CEA
4	C	702	SRM	C2A-C3A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	702	SRM	C1A-C2A-CDA-CEA
4	D	702	SRM	CMA-C2A-CDA-CEA
4	D	702	SRM	C2A-C3A-CAA-CBA
4	D	702	SRM	C2B-C3B-CAB-CBB
4	A	702	SRM	C2B-C3B-CAB-CBB
4	B	702	SRM	C2B-C3B-CAB-CBB
4	A	702	SRM	C3A-C2A-CDA-CEA
4	C	702	SRM	C3A-C2A-CDA-CEA
4	D	702	SRM	C3A-C2A-CDA-CEA
4	D	702	SRM	C3B-CAB-CBB-CCB
4	C	702	SRM	C2B-C3B-CAB-CBB
4	A	702	SRM	C3B-CAB-CBB-CCB
4	D	702	SRM	C3C-CAC-CBC-CCC
4	B	702	SRM	C3C-CAC-CBC-CCC
4	C	702	SRM	C3C-CAC-CBC-CCC
4	B	702	SRM	C3B-CAB-CBB-CCB
4	A	702	SRM	C3B-C2B-CDB-CEB
4	D	702	SRM	C3B-C2B-CDB-CEB
4	A	702	SRM	C2D-CAD-CBD-CCD
4	A	702	SRM	C3C-CAC-CBC-CCC
4	B	702	SRM	C3D-CDD-CED-O3D
4	B	702	SRM	C3B-C2B-CDB-CEB
4	B	702	SRM	C3D-CDD-CED-O4D
4	B	702	SRM	CAA-CBA-CCA-O2A
4	A	702	SRM	CAA-CBA-CCA-O1A
4	B	702	SRM	CAA-CBA-CCA-O1A
4	A	702	SRM	CAC-CBC-CCC-O2C
4	D	702	SRM	CAC-CBC-CCC-O1C
4	A	702	SRM	CAA-CBA-CCA-O2A
4	B	702	SRM	CAC-CBC-CCC-O1C
4	C	702	SRM	CAC-CBC-CCC-O2C
4	D	702	SRM	CAC-CBC-CCC-O2C
4	A	702	SRM	CAC-CBC-CCC-O1C
4	C	702	SRM	CAC-CBC-CCC-O1C
4	B	702	SRM	CAC-CBC-CCC-O2C
4	C	702	SRM	CAA-CBA-CCA-O1A
4	C	702	SRM	CAA-CBA-CCA-O2A
4	D	702	SRM	CAA-CBA-CCA-O1A
4	D	702	SRM	CAA-CBA-CCA-O2A

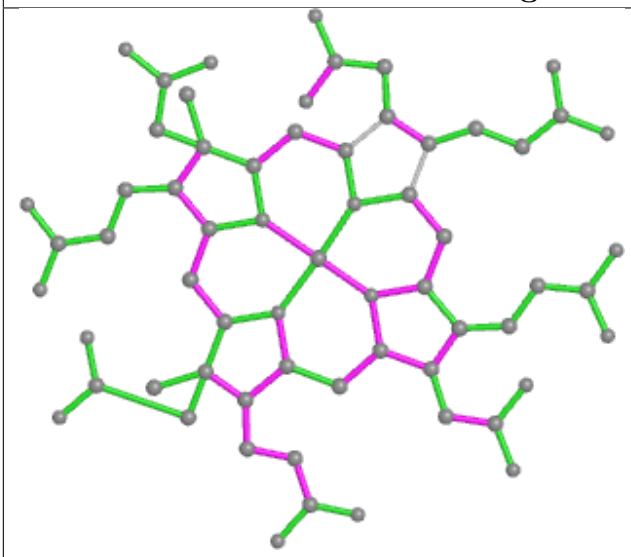
There are no ring outliers.

4 monomers are involved in 37 short contacts:

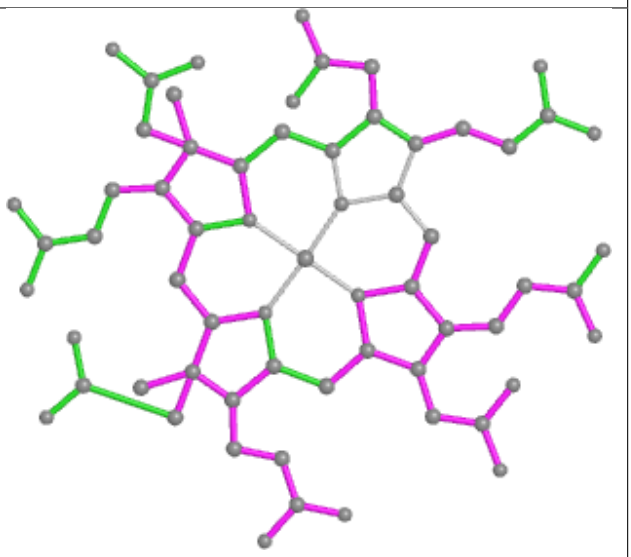
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	702	SRM	11	0
4	C	702	SRM	7	0
4	B	702	SRM	10	0
4	A	702	SRM	9	0

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 then 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.

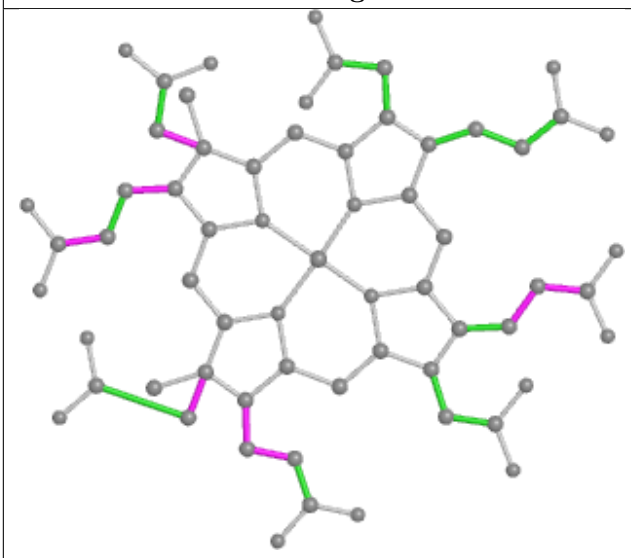
Ligand SRM D 702



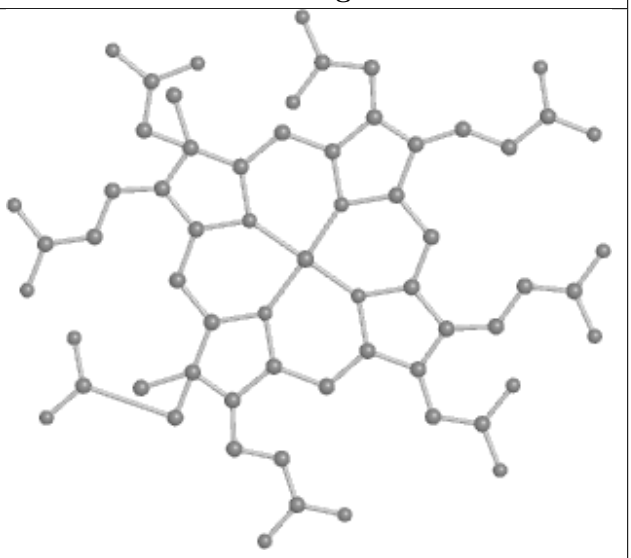
Bond lengths



Bond angles

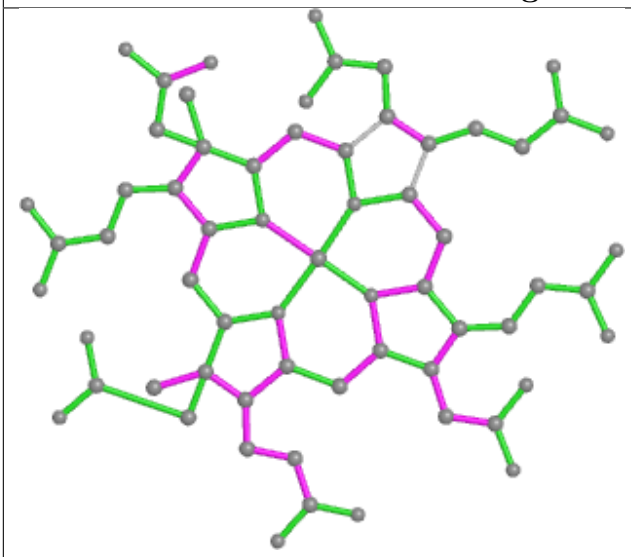


Torsions

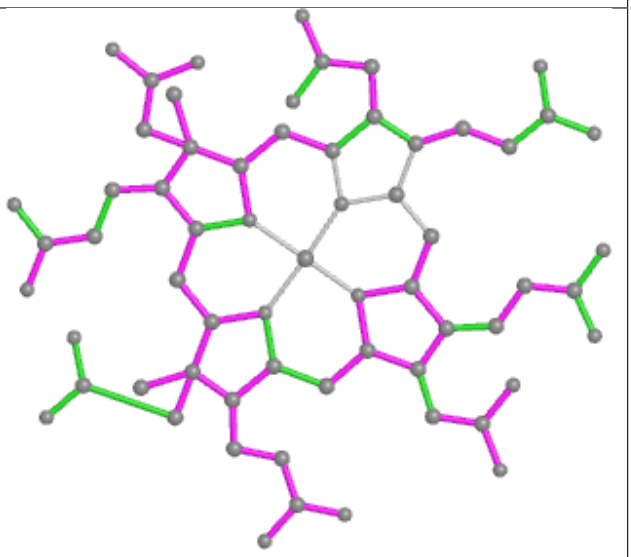


Rings

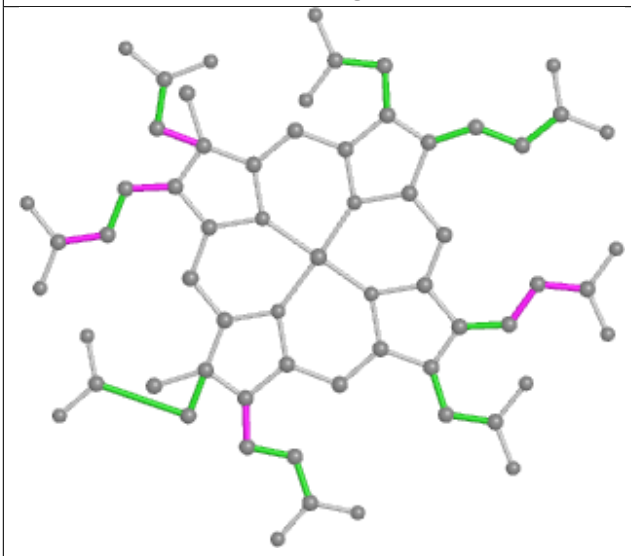
Ligand SRM C 702



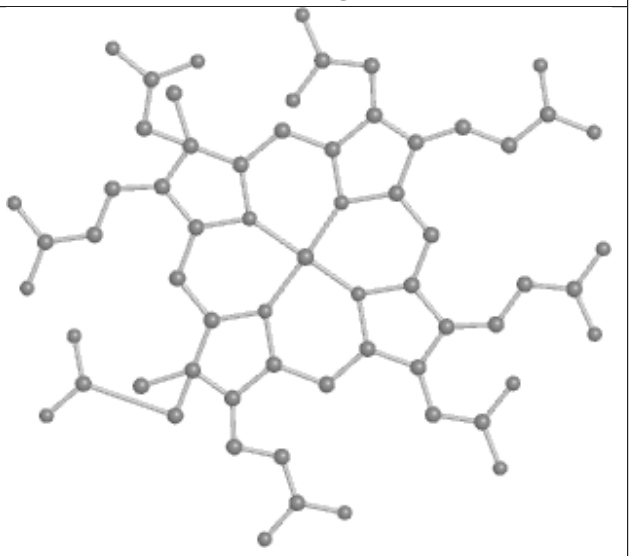
Bond lengths



Bond angles

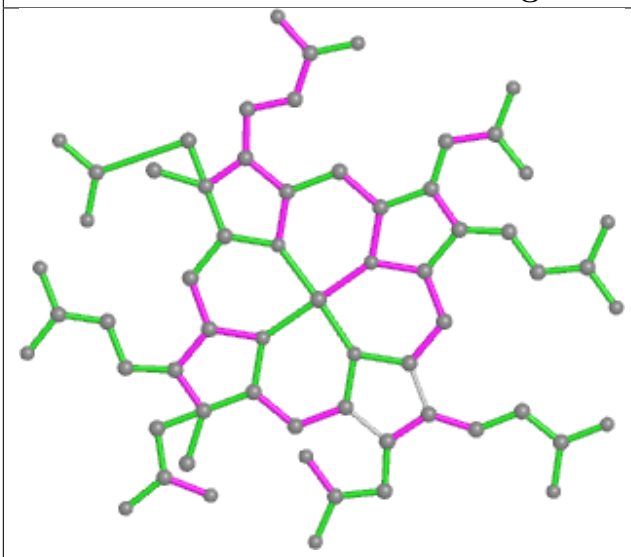


Torsions

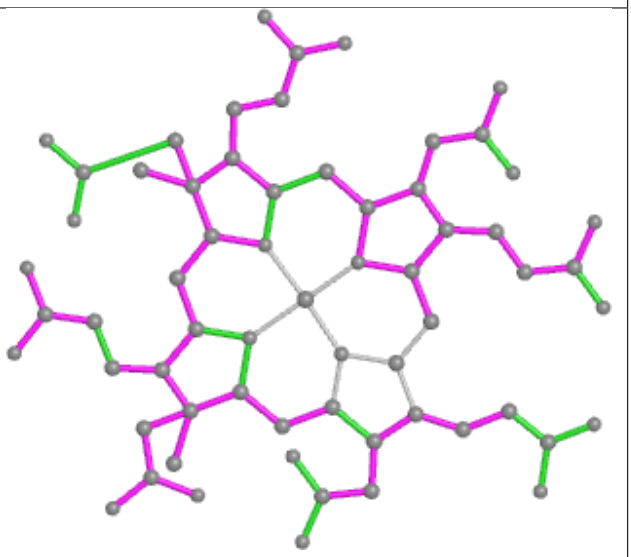


Rings

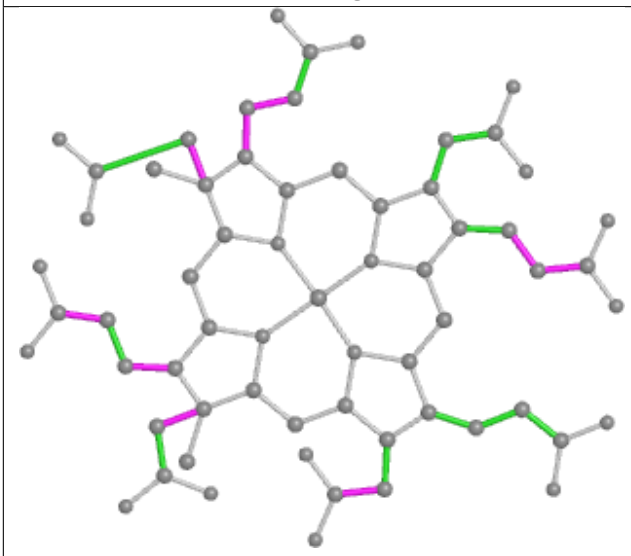
Ligand SRM B 702



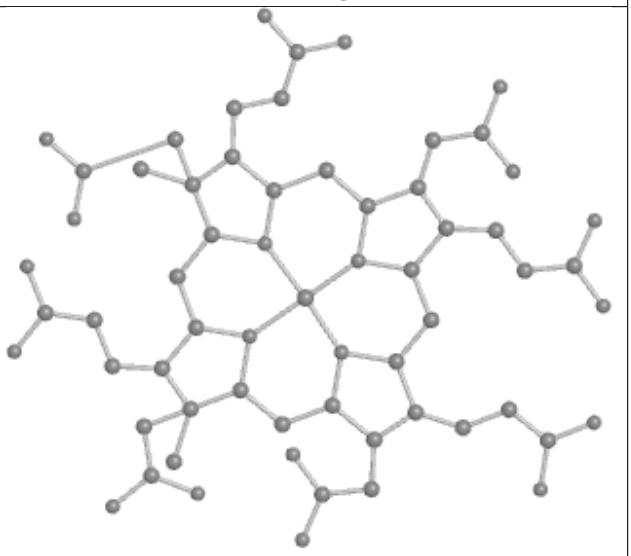
Bond lengths



Bond angles

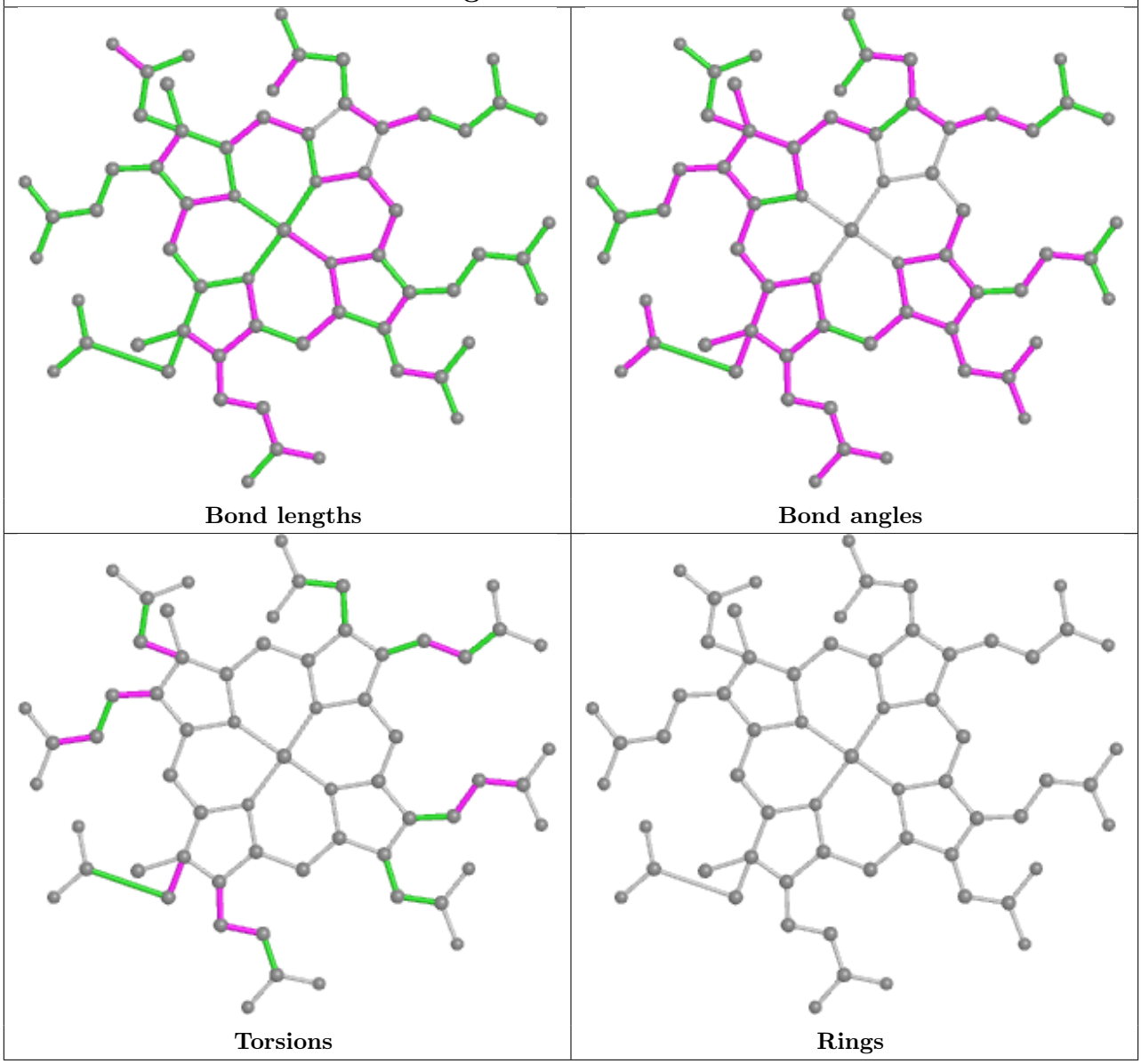


Torsions



Rings

Ligand SRM A 702



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	567/583 (97%)	-0.56	5 (0%)	84	83	17, 27, 43, 77	0
1	B	565/583 (96%)	-0.54	4 (0%)	87	86	17, 27, 43, 66	0
1	C	563/583 (96%)	-0.37	7 (1%)	79	77	18, 35, 61, 84	0
1	D	554/583 (95%)	-0.22	15 (2%)	54	52	20, 43, 70, 90	0
2	E	96/98 (97%)	0.13	4 (4%)	36	34	32, 47, 72, 86	0
2	F	73/98 (74%)	3.38	50 (68%)	0	0	48, 75, 104, 119	0
All	All	2418/2528 (95%)	-0.29	85 (3%)	44	42	17, 32, 67, 119	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	69	ILE	9.5
2	F	51	VAL	9.4
2	F	70	ALA	9.2
2	E	96	THR	8.2
2	F	48	ALA	8.1
2	F	80	TYR	7.8
2	F	96	THR	7.5
2	F	52	VAL	7.4
2	F	84	ASP	7.4
2	F	66	ASP	6.5
2	F	87	ILE	6.2
2	F	37	TYR	5.9
2	F	58	GLN	5.3
2	F	78	HIS	5.2
2	F	42	GLY	5.1
2	F	14	VAL	5.1
2	F	93	GLU	5.0
2	F	86	VAL	4.9
2	F	67	GLY	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	239	MET	4.7
2	F	12	GLY	4.6
2	F	61	GLN	4.6
1	A	62	VAL	4.2
2	F	73	TRP	4.1
2	F	88	GLU	4.1
1	D	257	GLY	4.1
1	C	255	SER	4.1
2	F	13	GLU	4.0
2	F	81	PRO	4.0
1	B	627	LYS	3.7
2	E	11	GLU	3.6
2	F	83	SER	3.5
1	D	225	SER	3.5
2	F	57	ASP	3.5
2	F	9	THR	3.4
2	F	35	LEU	3.3
1	D	242	GLU	3.3
1	A	627	LYS	3.2
1	D	64	ARG	3.2
2	F	53	SER	3.2
2	F	82	THR	3.1
2	F	62	SER	3.1
1	D	79	TYR	3.1
2	F	44	CYS	3.0
2	F	10	PRO	3.0
1	C	115	GLY	3.0
2	F	55	SER	3.0
2	F	50	LYS	3.0
2	E	10	PRO	2.9
2	F	85	VAL	2.9
2	F	72	GLY	2.9
2	F	60	ASP	2.9
2	F	68	GLN	2.8
2	F	77	CYS	2.8
2	F	65	ASP	2.7
1	D	264	PRO	2.6
1	B	88	GLU	2.6
2	F	71	ASP	2.6
1	D	541	PRO	2.5
2	F	56	VAL	2.5
2	F	38	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	260	PHE	2.4
1	D	445	ASN	2.4
1	B	262	ASP	2.4
1	C	118	ASN	2.4
2	F	36	PRO	2.4
2	F	95	LEU	2.4
1	D	229	TYR	2.3
2	E	12	GLY	2.3
1	D	262	ASP	2.3
1	B	239	MET	2.3
1	A	238	ILE	2.3
1	C	250	ALA	2.3
1	A	262	ASP	2.2
2	F	89	THR	2.2
2	F	64	LEU	2.2
1	C	261	PRO	2.2
2	F	11	GLU	2.2
1	D	475	GLN	2.2
1	D	73	LYS	2.1
1	D	76	PHE	2.1
1	C	123	LEU	2.0
1	A	63	LYS	2.0
1	D	63	LYS	2.0
2	F	8	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

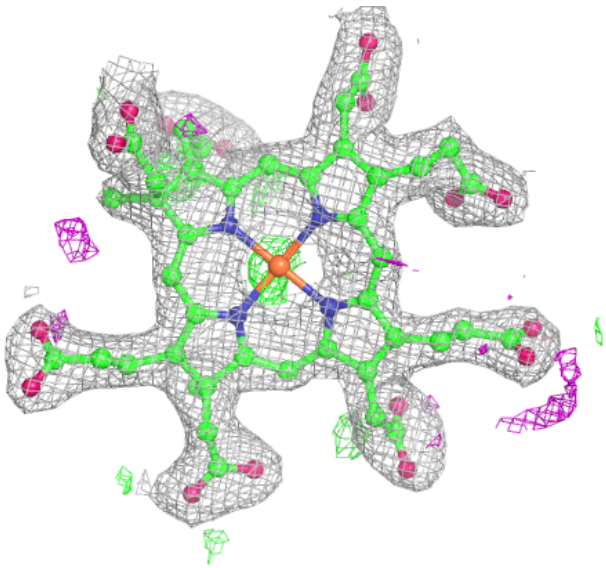
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

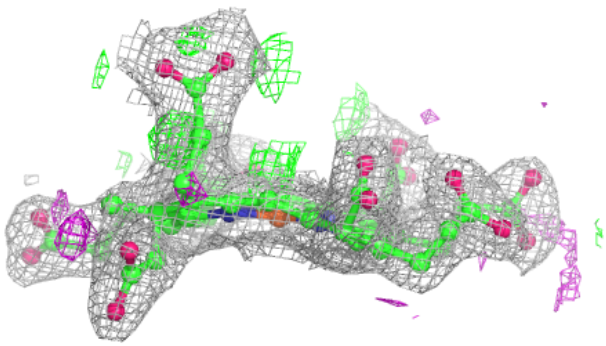
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SRM	C	702	63/63	0.95	0.13	23,28,36,44	0
4	SRM	D	702	63/63	0.95	0.11	24,34,41,46	0
4	SRM	B	702	63/63	0.96	0.11	18,22,29,43	0
6	CL	A	704	1/1	0.96	0.14	34,34,34,34	0
3	SF4	D	701	8/8	0.97	0.05	25,27,29,29	0
4	SRM	A	702	63/63	0.97	0.12	17,23,29,40	0
6	CL	C	704	1/1	0.97	0.25	44,44,44,44	0
7	FES	F	101	4/4	0.97	0.06	41,42,47,47	0
6	CL	B	704	1/1	0.98	0.19	40,40,40,40	0
3	SF4	A	701	8/8	0.98	0.06	19,20,23,23	0
6	CL	D	704	1/1	0.98	0.23	43,43,43,43	0
3	SF4	C	701	8/8	0.98	0.06	22,24,24,25	0
5	MG	C	703	1/1	0.99	0.20	12,12,12,12	0
7	FES	E	101	4/4	0.99	0.04	31,34,35,37	0
3	SF4	B	701	8/8	0.99	0.05	20,21,22,22	0
5	MG	B	703	1/1	1.00	0.14	8,8,8,8	0
5	MG	A	703	1/1	1.00	0.17	8,8,8,8	0
5	MG	D	703	1/1	1.00	0.21	16,16,16,16	0

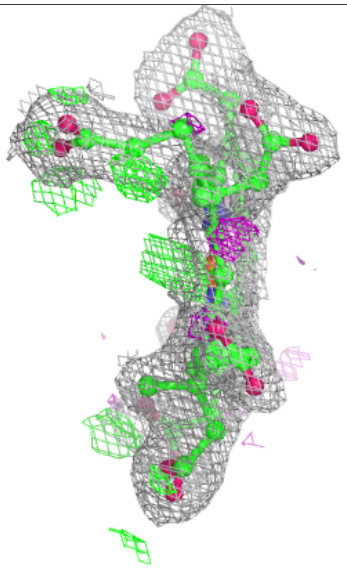
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SRM C 702:

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

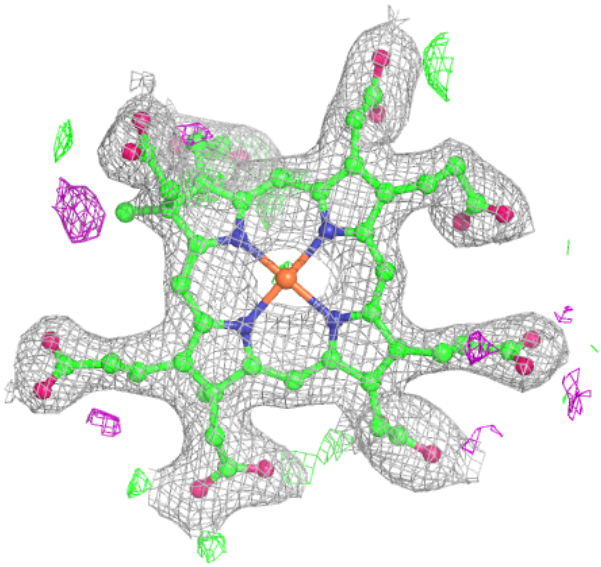


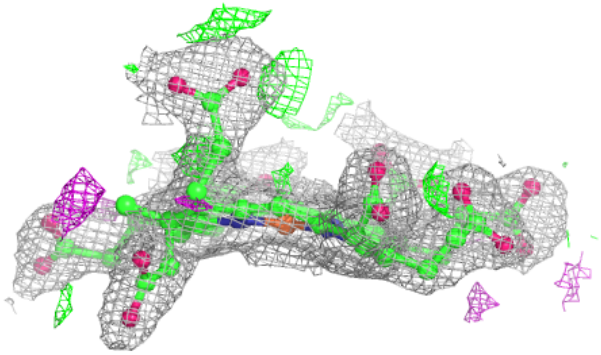


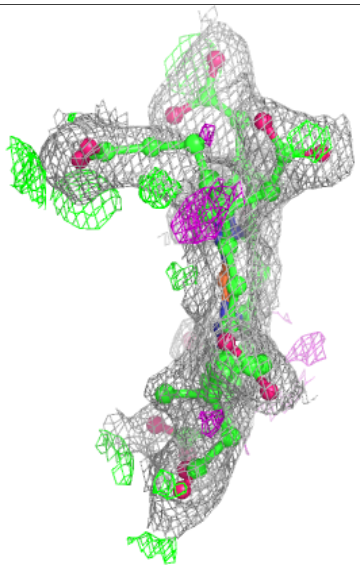


Electron density around SRM D 702:

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

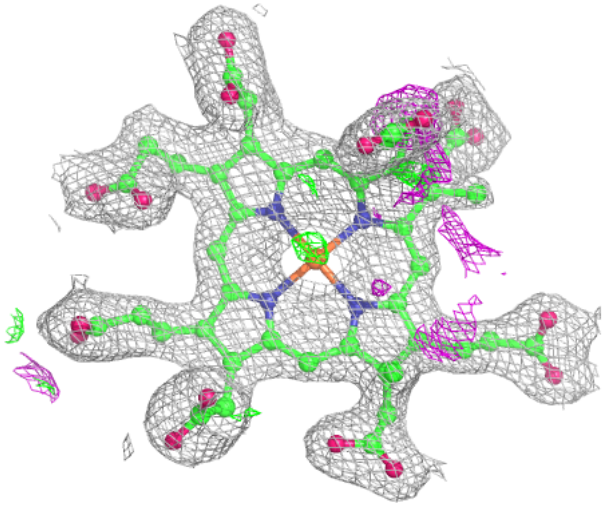


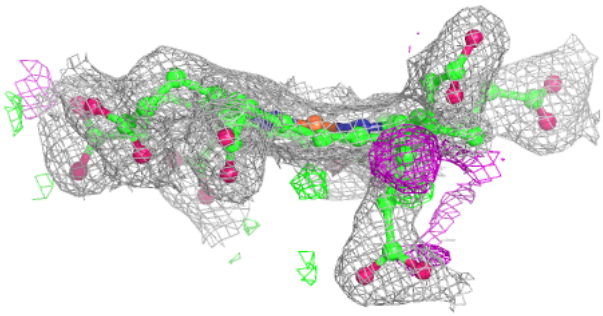


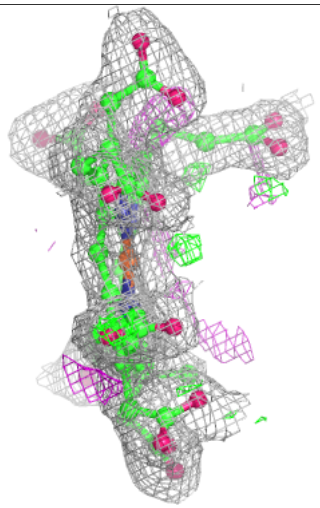


Electron density around SRM B 702:

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

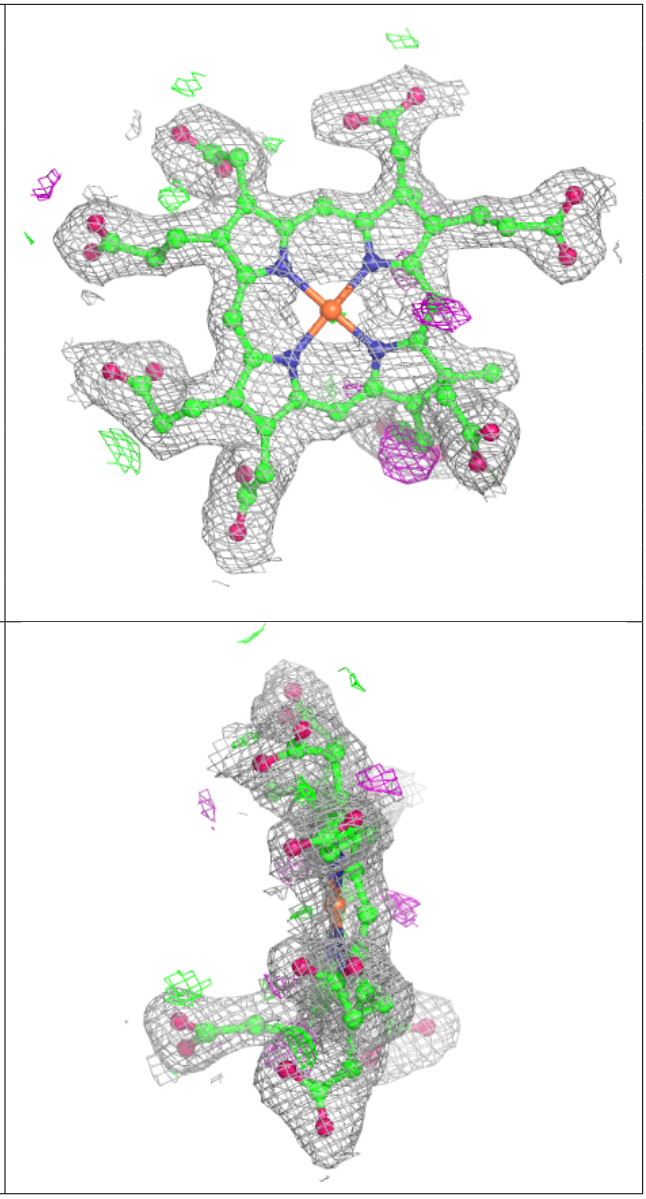






Electron density around SRM A 702:

$2mF_o$-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.