Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 05:26 PM JST

PDB ID	:	7C3F / pdb_00007c3f
Title	:	Crystal structure of ferredoxin: thioredoxin reductase and thioredoxin m2 complex
Authors	:	Kurisu, G.; Juniar, L.; Tanaka, H.
Deposited on	:	2020-05-12
Resolution	:	2.40 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:

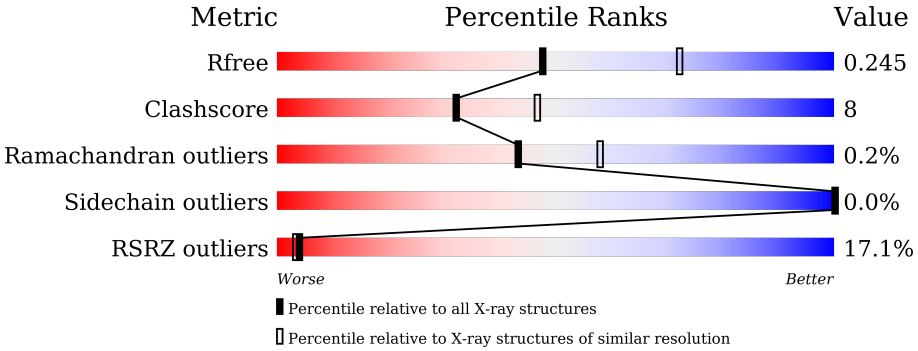
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	115	2% 85% 13% •
1	D	115	3% 83% 17% •
1	G	115	4% 79% 19% ••
1	J	115	5% 79% 19% •
1	M	115	7% 82% 17% ••
1	P	115	11% 81% 17% •

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Mol	Chain	Length	Quality of chain
1	S	115	13% 79% 20%
1	V	115	55% 34% 28% 38%
2	B	112	4% 70% 8% 21%
2	E	112	6% 71% 8% 21%
2	H	112	27% 62% 16% 21%
2	K	112	33% 55% 22% 21%
2	N	112	35% 56% 21% 21%
2	Q	112	9% 70% 9% 21%
2	T	112	48% 47% 25% 5% 22%
3	C	114	3% 86% 8% 6%
3	F	114	4% 90% 6%
3	I	114	2% 91% 7%
3	L	114	3% 90% 6%
3	O	114	2% 87% 7% 6%
3	R	114	3% 87% 7% 6%
3	U	114	4% 86% 8% 6%
3	W	114	71% 54% 31% 14%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	M	201	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18993 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 Ferredoxin-thioredoxin reductase catalytic chain, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	113	889	551	153	174	11	0	0	0
1	D	114	898	557	155	175	11	0	0	0
1	G	114	898	557	155	175	11	0	0	0
1	J	113	889	551	153	174	11	0	0	0
1	M	114	898	557	155	175	11	0	0	0
1	P	113	889	551	153	174	11	0	0	0
1	S	114	898	557	155	175	11	0	0	0
1	V	71	546	344	87	111	4	0	0	0

- Molecule 2 is a protein called Ferredoxin-thioredoxin reductase variable chain, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	88	722	473	119	128	2	0	0	0
2	E	89	731	478	120	131	2	0	0	0
2	H	88	722	473	119	128	2	0	0	0
2	K	88	722	473	119	128	2	0	0	0
2	N	88	722	473	119	128	2	0	0	0
2	Q	88	722	473	119	128	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	T	87	713	468	118	125	2	0	0	0

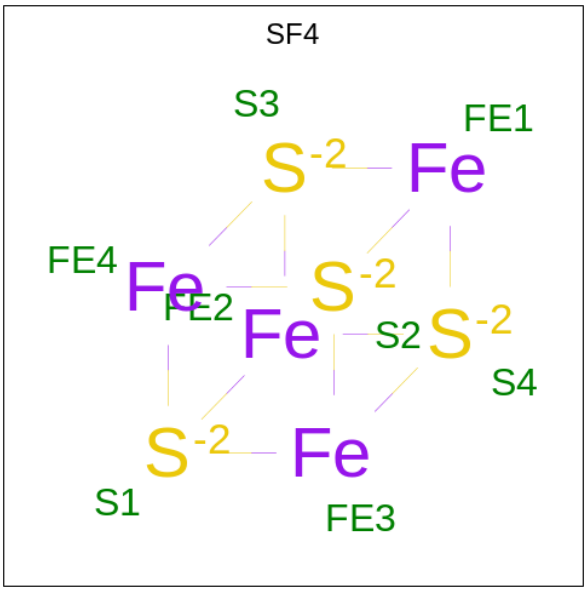
- Molecule 3 is a protein called Thioredoxin M2, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	107	827	535	131	158	3	0	0	0
3	F	107	827	535	131	158	3	0	0	0
3	I	106	820	531	130	156	3	0	0	0
3	L	107	827	535	131	158	3	0	0	0
3	O	107	827	535	131	158	3	0	0	0
3	R	107	827	535	131	158	3	0	0	0
3	U	107	827	535	131	158	3	0	0	0
3	W	98	756	493	117	143	3	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	41	SER	CYS	engineered mutation	UNP Q9SEU8
F	41	SER	CYS	engineered mutation	UNP Q9SEU8
I	41	SER	CYS	engineered mutation	UNP Q9SEU8
L	41	SER	CYS	engineered mutation	UNP Q9SEU8
O	41	SER	CYS	engineered mutation	UNP Q9SEU8
R	41	SER	CYS	engineered mutation	UNP Q9SEU8
U	41	SER	CYS	engineered mutation	UNP Q9SEU8
W	41	SER	CYS	engineered mutation	UNP Q9SEU8

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	A	1	8	4	4	0	0
4	D	1	8	4	4	0	0
4	G	1	8	4	4	0	0
4	J	1	8	4	4	0	0
4	M	1	8	4	4	0	0
4	P	1	8	4	4	0	0
4	S	1	8	4	4	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	A	1	1	1	0	0
5	C	1	1	1	0	0
5	D	1	1	1	0	0
5	E	1	1	1	0	0
5	G	1	1	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	1	Total Na 1 1	0	0
5	L	1	Total Na 1 1	0	0
5	M	1	Total Na 1 1	0	0
5	O	1	Total Na 1 1	0	0
5	P	1	Total Na 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	36	Total O 36 36	0	0
6	B	16	Total O 16 16	0	0
6	C	60	Total O 60 60	0	0
6	D	30	Total O 30 30	0	0
6	E	21	Total O 21 21	0	0
6	F	43	Total O 43 43	0	0
6	G	25	Total O 25 25	0	0
6	H	11	Total O 11 11	0	0
6	I	47	Total O 47 47	0	0
6	J	26	Total O 26 26	0	0
6	K	7	Total O 7 7	0	0
6	L	47	Total O 47 47	0	0
6	M	16	Total O 16 16	0	0
6	N	1	Total O 1 1	0	0

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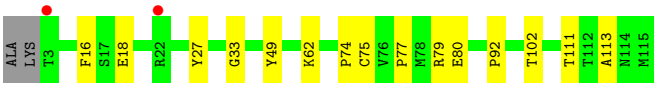
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	O	51	Total O 51 51	0	0
6	P	16	Total O 16 16	0	0
6	Q	7	Total O 7 7	0	0
6	R	19	Total O 19 19	0	0
6	S	11	Total O 11 11	0	0
6	T	2	Total O 2 2	0	0
6	U	32	Total O 32 32	0	0
6	V	6	Total O 6 6	0	0

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.

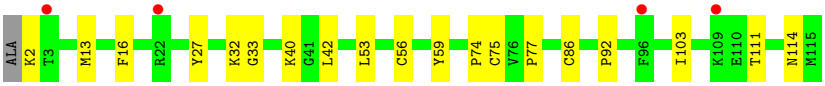
• Molecule 1: Ferredoxin-thioredoxin reductase catalytic chain, chloroplastic

Chain A:



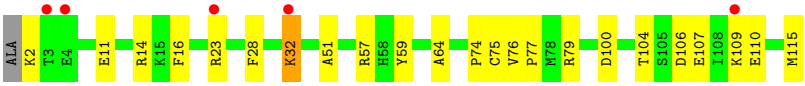
• Molecule 1: Ferredoxin-thioredoxin reductase catalytic chain, chloroplastic

Chain D:



• Molecule 1: Ferredoxin-thioredoxin reductase catalytic chain, chloroplastic

Chain G:



• Molecule 1: Ferredoxin-thioredoxin reductase catalytic chain, chloroplastic

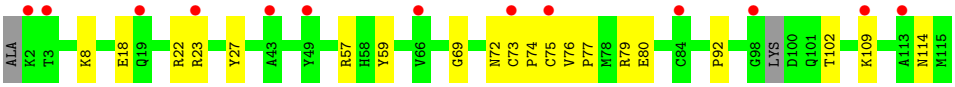
Chain J:

• Molecule 1: Ferredoxin-thioredoxin reductase catalytic chain, chloroplastic

Chain M:

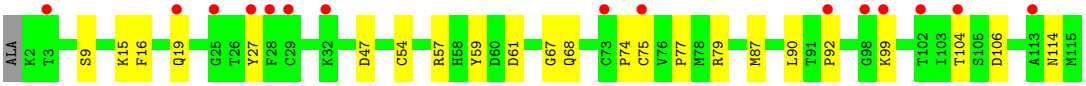
• Molecule 1: Ferredoxin-thioredoxin reductase catalytic chain, chloroplastic

Chain P:



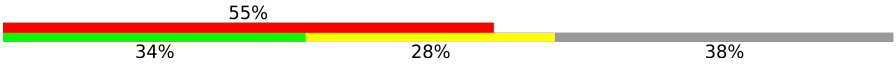
• Molecule 1: Ferredoxin-thioredoxin reductase catalytic chain, chloroplastic

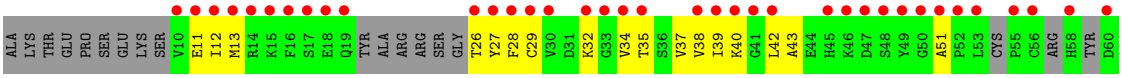
Chain S:

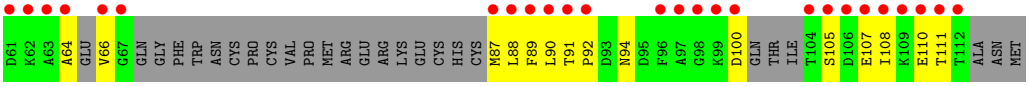


• Molecule 1: Ferredoxin-thioredoxin reductase catalytic chain, chloroplastic

Chain V:

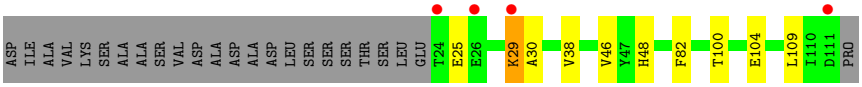






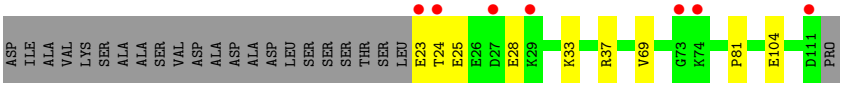
• Molecule 2: Ferredoxin-thioredoxin reductase variable chain, chloroplastic

Chain B:



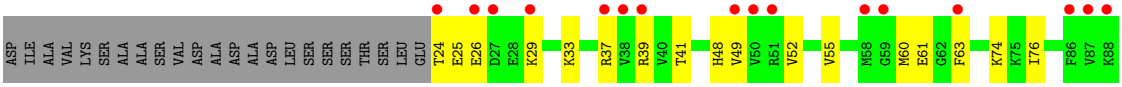
• Molecule 2: Ferredoxin-thioredoxin reductase variable chain, chloroplastic

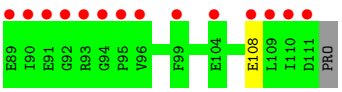
Chain E:



• Molecule 2: Ferredoxin-thioredoxin reductase variable chain, chloroplastic

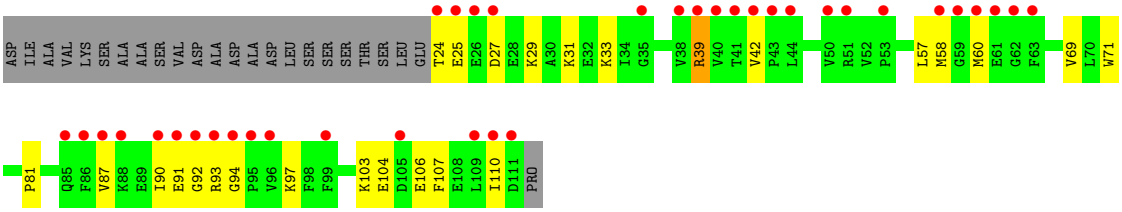
Chain H:





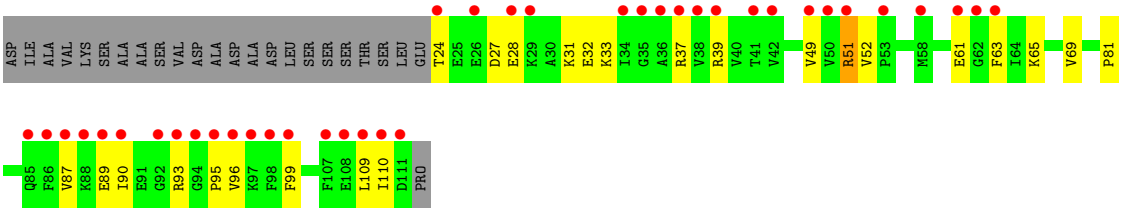
• Molecule 2: Ferredoxin-thioredoxin reductase variable chain, chloroplastic

Chain K:



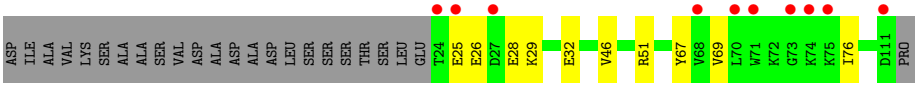
• Molecule 2: Ferredoxin-thioredoxin reductase variable chain, chloroplastic

Chain N:



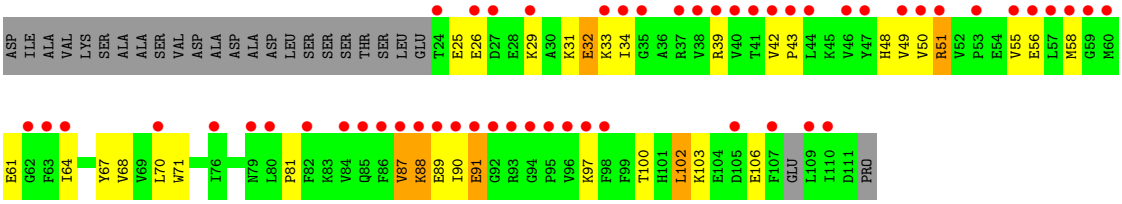
• Molecule 2: Ferredoxin-thioredoxin reductase variable chain, chloroplastic

Chain Q:



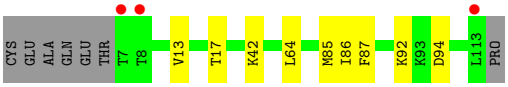
• Molecule 2: Ferredoxin-thioredoxin reductase variable chain, chloroplastic

Chain T:



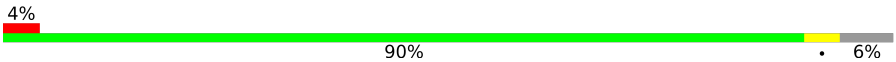
• Molecule 3: Thioredoxin M2, chloroplastic

Chain C:



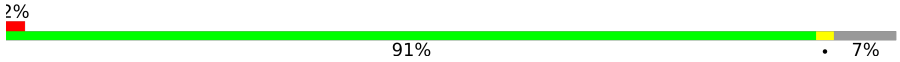
• Molecule 3: Thioredoxin M2, chloroplastic

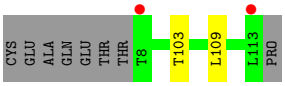
Chain F:



• Molecule 3: Thioredoxin M2, chloroplastic

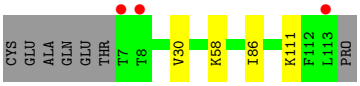
Chain I:





• Molecule 3: Thioredoxin M2, chloroplastic

Chain L:

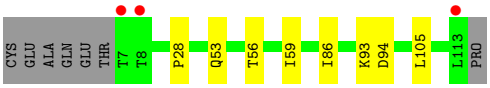


• Molecule 3: Thioredoxin M2, chloroplastic

Chain O:

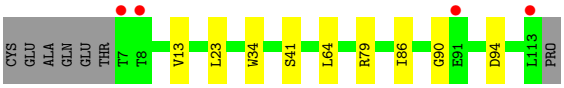
• Molecule 3: Thioredoxin M2, chloroplastic

Chain R:



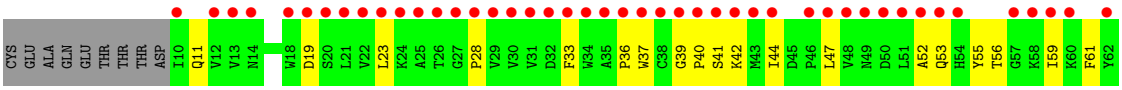
• Molecule 3: Thioredoxin M2, chloroplastic

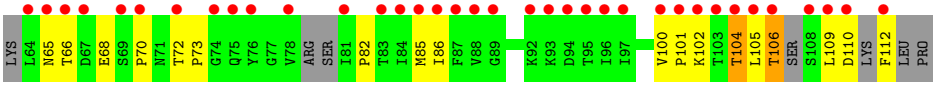
Chain U:



• Molecule 3: Thioredoxin M2, chloroplastic

Chain W:




LYS
L64
N65
T66
D67
E68
S69
P70
N71
T72
P73
G74
Q75
Y76
G77
V78
ARG
SER
I81
P82
T83
I84
M85
I86
F87
V88
G89
K92
K93
D94
T95
I96
I97
V100
P101
K102
T103
T104
L105
T106
SER
S108
L109
D110
LYS
F112
LEU
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	174.26Å 137.21Å 192.46Å 90.00° 90.21° 90.00°	Depositor
Resolution (Å)	43.57 – 2.40 43.57 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (43.57-2.40) 99.2 (43.57-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.209 , 0.245 0.210 , 0.245	Depositor DCC
R_{free} test set	8770 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	52.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18993	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: SF4, NA

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	0.21	0/908	0.38	0/1223
1	D	0.17	0/917	0.41	0/1234
1	G	0.27	0/917	0.66	3/1234 (0.2%)
1	J	0.36	1/908 (0.1%)	0.71	8/1223 (0.7%)
1	M	0.28	0/917	0.58	1/1234 (0.1%)
1	P	0.28	0/907	0.63	3/1220 (0.2%)
1	S	0.16	0/917	0.41	0/1234
1	V	0.30	0/549	0.62	0/728
2	B	0.21	0/737	0.60	2/989 (0.2%)
2	E	0.13	0/746	0.41	0/1001
2	H	0.23	0/737	0.57	0/989
2	K	0.29	0/737	0.73	1/989 (0.1%)
2	N	0.36	0/737	0.79	1/989 (0.1%)
2	Q	0.27	0/737	0.59	2/989 (0.2%)
2	T	0.49	0/727	1.13	14/974 (1.4%)
3	C	0.13	0/848	0.32	0/1159
3	F	0.12	0/848	0.33	0/1159
3	I	0.13	0/841	0.32	0/1149
3	L	0.11	0/848	0.32	0/1159
3	O	0.16	0/848	0.33	0/1159
3	R	0.12	0/848	0.30	0/1159
3	U	0.16	0/848	0.34	0/1159
3	W	0.43	0/773	0.79	2/1053 (0.2%)
All	All	0.25	1/18800 (0.0%)	0.56	37/25406 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	K	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	32	LYS	CG-CD	-7.63	1.29	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	32	LYS	CD-CE-NZ	11.35	148.21	111.90
2	B	29	LYS	CB-CG-CD	9.11	132.25	111.30
2	T	25	GLU	CA-C-N	8.48	131.98	120.44
2	T	25	GLU	C-N-CA	8.48	131.98	120.44
1	P	109	LYS	CG-CD-CE	8.21	130.19	111.30
2	T	102	LEU	CA-C-N	8.19	134.21	122.09
2	T	102	LEU	C-N-CA	8.19	134.21	122.09
1	M	23	ARG	CB-CG-CD	7.87	129.39	111.30
2	N	51	ARG	CB-CG-CD	-7.67	93.66	111.30
1	J	7	GLU	CA-CB-CG	-7.42	99.25	114.10
1	P	109	LYS	CB-CG-CD	7.33	128.15	111.30
1	J	32	LYS	CA-CB-CG	-7.24	99.62	114.10
2	T	51	ARG	CG-CD-NE	-6.83	96.97	112.00
1	G	32	LYS	CB-CG-CD	6.74	126.79	111.30
1	J	32	LYS	CD-CE-NZ	-6.73	90.38	111.90
3	W	106	THR	OG1-CB-CG2	6.65	122.61	109.30
1	P	23	ARG	CB-CG-CD	-6.60	96.13	111.30
2	Q	51	ARG	CA-CB-CG	-5.88	102.33	114.10
2	T	91	GLU	CA-CB-CG	5.58	125.27	114.10
2	T	87	VAL	CA-C-N	-5.58	113.69	122.73
2	T	87	VAL	C-N-CA	-5.58	113.69	122.73
2	B	29	LYS	CA-CB-CG	-5.57	102.97	114.10
2	T	32	GLU	CB-CA-C	-5.53	101.61	110.79
2	T	26	GLU	CA-C-N	5.37	128.48	120.31
2	T	26	GLU	C-N-CA	5.37	128.48	120.31
1	J	7	GLU	N-CA-CB	-5.35	101.68	110.40
3	W	104	THR	OG1-CB-CG2	-5.34	98.61	109.30
2	K	91	GLU	CB-CG-CD	-5.29	103.60	112.60
2	T	32	GLU	CA-CB-CG	5.28	124.65	114.10
1	G	23	ARG	CB-CG-CD	5.20	123.27	111.30
1	J	3	THR	CA-C-N	5.18	138.90	121.27
1	J	3	THR	C-N-CA	5.18	138.90	121.27
2	T	26	GLU	CB-CA-C	-5.15	102.77	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	88	LYS	CB-CG-CD	5.08	122.99	111.30
2	Q	26	GLU	CB-CG-CD	-5.01	104.09	112.60
1	J	31	ASP	CA-C-N	-5.00	113.32	122.38
1	J	31	ASP	C-N-CA	-5.00	113.32	122.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	39	ARG	Sidechain

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	889	0	845	11	0
1	D	898	0	860	12	0
1	G	898	0	860	19	0
1	J	889	0	847	12	0
1	M	898	0	860	15	1
1	P	889	0	848	13	0
1	S	898	0	861	19	0
1	V	546	0	522	40	0
2	B	722	0	748	10	0
2	E	731	0	754	6	0
2	H	722	0	748	13	0
2	K	722	0	748	24	0
2	N	722	0	748	19	0
2	Q	722	0	748	6	0
2	T	713	0	741	32	0
3	C	827	0	832	6	0
3	F	827	0	832	2	0
3	I	820	0	825	1	0
3	L	827	0	832	3	0
3	O	827	0	832	6	0
3	R	827	0	832	5	0
3	U	827	0	832	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	W	756	0	750	33	1
4	A	8	0	0	0	0
4	D	8	0	0	0	0
4	G	8	0	0	0	0
4	J	8	0	0	0	0
4	M	8	0	0	2	0
4	P	8	0	0	1	0
4	S	8	0	0	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
6	A	36	0	0	2	0
6	B	16	0	0	0	0
6	C	60	0	0	1	0
6	D	30	0	0	2	0
6	E	21	0	0	0	0
6	F	43	0	0	0	0
6	G	25	0	0	1	0
6	H	11	0	0	0	0
6	I	47	0	0	0	0
6	J	26	0	0	0	0
6	K	7	0	0	0	0
6	L	47	0	0	1	0
6	M	16	0	0	0	0
6	N	1	0	0	0	0
6	O	51	0	0	1	0
6	P	16	0	0	0	0
6	Q	7	0	0	0	0
6	R	19	0	0	1	0
6	S	11	0	0	0	0
6	T	2	0	0	0	0
6	U	32	0	0	0	0
6	V	6	0	0	0	0
All	All	18993	0	18305	294	1

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 8.

All (294) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:88:LYS:NZ	2:T:90:ILE:HD13	1.54	1.21
2:K:93:ARG:HD3	2:K:94:GLY:H	0.98	1.06
1:V:35:THR:HA	1:V:88:LEU:HD22	1.45	0.97
2:T:88:LYS:HZ1	2:T:90:ILE:HD13	1.13	0.94
2:K:93:ARG:HD3	2:K:94:GLY:N	1.82	0.93
2:K:24:THR:HG22	2:K:25:GLU:H	1.32	0.93
2:K:93:ARG:CD	2:K:94:GLY:H	1.84	0.89
1:V:13:MET:HE2	1:V:42:LEU:HB3	1.56	0.88
2:T:88:LYS:HZ2	2:T:90:ILE:HD13	1.39	0.87
2:T:29:LYS:HG2	2:T:33:LYS:HZ3	1.42	0.83
1:V:32:LYS:HE3	1:V:107:GLU:OE2	1.78	0.83
1:V:35:THR:HA	1:V:88:LEU:CD2	2.11	0.80
2:T:50:VAL:HG12	2:T:51:ARG:HG3	1.64	0.79
1:V:32:LYS:HA	1:V:35:THR:HB	1.63	0.79
1:J:104:THR:HG23	1:J:107:GLU:H	1.49	0.76
3:W:40:PRO:HB2	3:W:82:PRO:HD3	1.67	0.76
1:S:104:THR:HG22	1:S:106:ASP:H	1.49	0.76
3:W:44:ILE:HD11	3:W:100:VAL:H	1.53	0.74
1:G:28:PHE:HB2	1:G:32:LYS:HZ1	1.53	0.73
1:V:32:LYS:CE	1:V:107:GLU:OE2	2.36	0.73
1:M:15:LYS:O	1:M:19:GLN:HB2	1.89	0.72
3:C:85:MET:HE3	3:C:92:LYS:HG3	1.71	0.72
1:G:32:LYS:HZ2	1:G:100:ASP:HB2	1.55	0.71
2:K:33:LYS:NZ	2:K:104:GLU:OE1	2.24	0.71
3:R:86:ILE:HD12	3:R:94:ASP:HB3	1.73	0.70
3:W:47:LEU:HD11	3:W:102:LYS:HB2	1.72	0.70
1:D:33:GLY:HA2	1:D:111:THR:HG21	1.75	0.69
3:W:100:VAL:HG13	3:W:104:THR:HG21	1.74	0.69
3:F:86:ILE:HD12	3:F:94:ASP:HB3	1.76	0.68
2:K:42:VAL:C	2:K:58:MET:CE	2.67	0.67
1:M:23:ARG:HG2	1:M:23:ARG:HH21	1.59	0.67
2:N:39:ARG:NH1	2:N:61:GLU:OE1	2.27	0.67
2:N:49:VAL:HG23	2:N:52:VAL:HB	1.76	0.67
2:K:24:THR:HG22	2:K:25:GLU:N	2.04	0.67
1:V:26:THR:HG23	1:V:89:PHE:HB2	1.76	0.67
3:L:30:VAL:HG22	3:L:86:ILE:HD12	1.78	0.66
3:W:28:PRO:HB2	3:W:59:ILE:HG23	1.77	0.66
1:V:11:GLU:HB2	1:V:13:MET:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:86:ILE:HD12	3:U:94:ASP:HB3	1.78	0.65
1:A:33:GLY:HA2	1:A:111:THR:HG21	1.79	0.64
1:D:32:LYS:HE2	1:D:103:ILE:HD12	1.80	0.64
3:C:86:ILE:HD12	3:C:94:ASP:HB3	1.79	0.64
2:K:90:ILE:HG12	2:K:92:GLY:H	1.62	0.64
2:B:48:HIS:CE1	2:B:100:THR:HG22	2.33	0.64
2:B:29:LYS:HG3	2:B:30:ALA:N	2.01	0.63
1:V:38:VAL:HG23	1:V:88:LEU:HD11	1.80	0.63
1:A:18:GLU:HG2	1:A:102:THR:HA	1.81	0.62
2:T:29:LYS:HG2	2:T:33:LYS:NZ	2.14	0.62
3:W:36:PRO:HD3	3:W:65:ASN:HD21	1.65	0.61
1:V:64:ALA:O	1:V:66:VAL:N	2.33	0.61
3:W:66:THR:O	3:W:70:PRO:HA	1.99	0.61
2:E:33:LYS:NZ	2:E:104:GLU:OE1	2.31	0.61
1:S:16:PHE:HZ	1:S:74:PRO:HD3	1.65	0.61
1:V:29:CYS:SG	1:V:35:THR:OG1	2.48	0.61
1:G:28:PHE:HB2	1:G:32:LYS:NZ	2.15	0.61
3:O:86:ILE:HD12	3:O:94:ASP:HB3	1.83	0.60
1:P:18:GLU:HG2	1:P:102:THR:HA	1.83	0.60
1:S:15:LYS:O	1:S:19:GLN:HB2	2.01	0.60
2:K:87:VAL:HG12	2:K:97:LYS:HG2	1.85	0.59
3:W:100:VAL:CG1	3:W:104:THR:CG2	2.80	0.59
1:D:2:LYS:NZ	6:D:302:HOH:O	2.35	0.58
3:I:103:THR:HG21	1:S:61:ASP:HB2	1.85	0.58
3:W:39:GLY:HA2	1:V:37:VAL:HG11	1.84	0.58
1:J:24:SER:O	1:J:82:LYS:NZ	2.27	0.58
2:N:49:VAL:CG2	2:N:52:VAL:HB	2.33	0.58
2:T:88:LYS:HE3	2:T:89:GLU:O	2.04	0.58
1:J:11:GLU:HG3	1:J:15:LYS:HE3	1.85	0.58
3:W:19:ASP:HA	3:W:23:LEU:HD12	1.85	0.58
3:W:33:PHE:HE2	3:W:85:MET:HG3	1.68	0.58
1:A:27:TYR:HE1	1:A:92:PRO:HG3	1.69	0.57
1:P:27:TYR:HE1	1:P:92:PRO:HG3	1.69	0.57
1:G:2:LYS:NZ	1:G:115:MET:O	2.38	0.57
3:W:41:SER:OG	3:W:82:PRO:HB3	2.04	0.57
1:V:107:GLU:O	1:V:111:THR:HG23	2.05	0.56
1:M:23:ARG:HG2	1:M:23:ARG:NH2	2.19	0.56
1:V:26:THR:OG1	1:V:27:TYR:N	2.37	0.56
3:W:33:PHE:CE2	3:W:85:MET:HG3	2.40	0.56
2:T:43:PRO:HA	2:T:58:MET:HB2	1.88	0.56
3:W:37:TRP:O	1:V:38:VAL:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:NH1	6:A:303:HOH:O	2.39	0.56
1:V:32:LYS:NZ	1:V:35:THR:O	2.38	0.56
1:A:113:ALA:O	6:A:301:HOH:O	2.18	0.55
1:A:27:TYR:CE1	1:A:92:PRO:HG3	2.42	0.55
1:D:33:GLY:HA2	1:D:111:THR:CG2	2.37	0.55
1:M:27:TYR:HE1	1:M:92:PRO:HG3	1.71	0.55
3:W:100:VAL:CG1	3:W:104:THR:HG21	2.35	0.55
1:V:38:VAL:HG23	1:V:88:LEU:CD1	2.37	0.55
2:T:88:LYS:HZ1	2:T:90:ILE:CD1	2.03	0.55
3:W:47:LEU:HD21	3:W:102:LYS:HA	1.89	0.55
3:W:44:ILE:HG23	3:W:47:LEU:HB3	1.88	0.54
2:K:42:VAL:C	2:K:58:MET:HE1	2.31	0.54
1:P:69:GLY:HA2	1:P:72:ASN:ND2	2.23	0.54
2:T:48:HIS:CE1	2:T:100:THR:HG22	2.42	0.54
1:V:35:THR:HG23	1:V:88:LEU:HD22	1.90	0.53
1:D:40:LYS:NZ	6:D:304:HOH:O	2.39	0.53
2:B:29:LYS:CG	2:B:30:ALA:N	2.67	0.53
2:N:28:GLU:OE1	2:N:31:LYS:HE2	2.09	0.53
2:N:28:GLU:O	2:N:32:GLU:HG3	2.09	0.53
2:N:65:LYS:HD3	2:N:99:PHE:HE1	1.74	0.53
2:Q:25:GLU:OE1	2:Q:25:GLU:N	2.34	0.53
2:H:24:THR:HG23	2:H:26:GLU:H	1.73	0.53
1:M:54:CYS:HB2	4:M:201:SF4:S1	2.48	0.53
1:P:22:ARG:HG2	1:P:22:ARG:HH21	1.74	0.53
2:T:39:ARG:HB3	2:T:61:GLU:HG2	1.91	0.53
1:G:106:ASP:O	1:G:110:GLU:HG3	2.08	0.52
1:P:27:TYR:CE1	1:P:92:PRO:HG3	2.45	0.52
1:J:27:TYR:HE1	1:J:92:PRO:HG3	1.75	0.52
2:T:49:VAL:HG21	2:T:55:VAL:HG23	1.91	0.52
2:T:87:VAL:HG12	2:T:97:LYS:HB3	1.90	0.52
2:K:39:ARG:HH11	2:K:110:ILE:HD13	1.75	0.52
1:S:27:TYR:HE1	1:S:92:PRO:HG3	1.74	0.52
2:B:82:PHE:CE2	2:B:104:GLU:HG3	2.45	0.52
3:W:101:PRO:O	3:W:104:THR:HG22	2.10	0.52
1:A:33:GLY:HA2	1:A:111:THR:CG2	2.40	0.52
1:V:27:TYR:HB3	1:V:100:ASP:C	2.35	0.52
2:Q:67:TYR:CE2	2:Q:69:VAL:HB	2.45	0.51
1:S:74:PRO:O	1:S:79:ARG:HD2	2.10	0.51
2:T:49:VAL:HG21	2:T:55:VAL:CG2	2.41	0.51
1:V:107:GLU:HG3	1:V:108:ILE:HG13	1.92	0.51
1:J:18:GLU:HG2	1:J:102:THR:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:33:LYS:HD3	2:N:109:LEU:HD11	1.92	0.51
2:N:65:LYS:HD3	2:N:99:PHE:CE1	2.46	0.51
3:W:55:TYR:OH	3:W:110:ASP:OD1	2.20	0.51
1:V:12:ILE:HG22	1:V:12:ILE:O	2.11	0.51
2:K:25:GLU:OE1	3:O:58:LYS:NZ	2.44	0.51
1:V:35:THR:O	1:V:35:THR:HG22	2.11	0.51
2:T:67:TYR:CD2	2:T:70:LEU:HD12	2.46	0.50
3:W:106:THR:O	3:W:110:ASP:N	2.39	0.50
1:M:27:TYR:CE1	1:M:92:PRO:HG3	2.46	0.50
1:V:38:VAL:O	1:V:42:LEU:N	2.31	0.50
2:N:69:VAL:HG23	2:N:81:PRO:HB3	1.92	0.50
1:M:104:THR:OG1	1:M:107:GLU:HG3	2.12	0.50
2:N:51:ARG:HH22	2:N:93:ARG:HG2	1.76	0.50
1:S:16:PHE:CZ	1:S:74:PRO:HD3	2.47	0.50
1:V:13:MET:HG3	1:V:39:ILE:O	2.12	0.50
1:V:51:ALA:HB3	1:V:66:VAL:HG12	1.93	0.50
2:B:82:PHE:HE2	2:B:104:GLU:HG3	1.77	0.50
1:S:57:ARG:HB2	1:S:59:TYR:CZ	2.47	0.50
3:W:33:PHE:HD1	3:W:66:THR:HG22	1.76	0.50
2:K:24:THR:CG2	2:K:25:GLU:H	2.16	0.49
1:P:74:PRO:O	1:P:79:ARG:HD2	2.11	0.49
1:S:68:GLN:NE2	2:T:68:VAL:HB	2.27	0.49
2:H:37:ARG:NH2	2:H:63:PHE:HB3	2.27	0.49
2:T:67:TYR:HD2	2:T:70:LEU:HD12	1.77	0.49
3:U:13:VAL:HG13	3:U:64:LEU:HD12	1.93	0.49
2:B:29:LYS:HZ1	2:B:104:GLU:CD	2.21	0.49
1:G:16:PHE:HZ	1:G:74:PRO:HD3	1.77	0.49
3:U:23:LEU:HA	3:U:90:GLY:HA2	1.93	0.49
1:D:56:CYS:HB2	1:D:86:CYS:SG	2.53	0.49
2:E:23:GLU:HG2	2:E:25:GLU:H	1.78	0.48
1:G:64:ALA:HB2	2:H:74:LYS:HD3	1.95	0.48
1:V:87:MET:O	1:V:87:MET:HG2	2.12	0.48
1:G:75:CYS:SG	1:G:77:PRO:HD2	2.54	0.48
2:K:25:GLU:H	2:K:25:GLU:CD	2.22	0.48
1:P:75:CYS:SG	1:P:77:PRO:HD2	2.54	0.48
1:S:9:SER:OG	1:S:47:ASP:OD1	2.23	0.48
1:P:8:LYS:HB3	1:P:8:LYS:HE3	1.59	0.48
1:P:22:ARG:HG2	1:P:22:ARG:NH2	2.27	0.47
1:J:27:TYR:CE1	1:J:92:PRO:HG3	2.49	0.47
1:V:32:LYS:O	1:V:32:LYS:HG2	2.14	0.47
3:C:85:MET:HE2	3:C:87:PHE:CZ	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:87:MET:HA	1:S:90:LEU:HD21	1.95	0.47
2:K:69:VAL:HG23	2:K:81:PRO:HB3	1.96	0.47
1:M:49:TYR:CZ	1:M:62:LYS:HD2	2.48	0.47
3:R:93:LYS:NZ	6:R:202:HOH:O	2.46	0.47
3:C:42:LYS:NZ	6:C:304:HOH:O	2.47	0.47
2:T:33:LYS:HB3	2:T:64:ILE:HD12	1.96	0.47
1:A:49:TYR:CE2	1:A:62:LYS:HE2	2.49	0.47
2:E:37:ARG:HD2	1:G:51:ALA:HB2	1.96	0.47
1:G:104:THR:OG1	1:G:107:GLU:HG3	2.15	0.47
1:J:19:GLN:HE22	1:J:23:ARG:NH1	2.13	0.47
1:G:32:LYS:NZ	1:G:100:ASP:HB2	2.26	0.47
1:S:99:LYS:HD2	1:S:99:LYS:HA	1.56	0.47
3:W:100:VAL:HG13	3:W:101:PRO:HD2	1.96	0.47
2:T:31:LYS:HE2	2:T:31:LYS:HB2	1.77	0.47
1:G:32:LYS:NZ	6:G:301:HOH:O	2.49	0.46
1:V:39:ILE:O	1:V:43:ALA:N	2.47	0.46
2:B:38:VAL:HG12	2:B:109:LEU:HD23	1.97	0.46
1:V:107:GLU:O	1:V:110:GLU:HB3	2.16	0.46
2:H:41:THR:CG2	2:H:108:GLU:HB2	2.46	0.46
1:V:34:VAL:O	1:V:37:VAL:HG12	2.15	0.46
1:M:99:LYS:HA	1:M:99:LYS:HD2	1.73	0.46
2:N:37:ARG:HA	2:N:63:PHE:HA	1.96	0.46
1:V:87:MET:HG2	1:V:90:LEU:HD11	1.96	0.46
3:W:65:ASN:HB3	3:W:68:GLU:HB3	1.98	0.46
1:V:91:THR:HB	1:V:92:PRO:HD2	1.98	0.46
2:T:48:HIS:HE1	2:T:100:THR:HG22	1.81	0.46
2:N:93:ARG:HH12	2:N:96:VAL:HA	1.81	0.46
3:L:111:LYS:NZ	6:L:307:HOH:O	2.49	0.45
2:H:39:ARG:HB2	2:H:61:GLU:HG2	1.98	0.45
1:G:57:ARG:HB2	1:G:59:TYR:CZ	2.51	0.45
2:H:49:VAL:HG11	2:H:55:VAL:HG21	1.97	0.45
2:T:88:LYS:HZ2	2:T:90:ILE:CD1	2.22	0.45
2:B:25:GLU:H	2:B:25:GLU:CD	2.25	0.45
1:V:108:ILE:O	1:V:111:THR:OG1	2.26	0.45
3:R:53:GLN:O	3:R:56:THR:OG1	2.34	0.45
3:O:18:TRP:CE3	3:O:72:THR:HG21	2.52	0.45
3:W:52:ALA:HA	3:W:61:PHE:CE1	2.52	0.45
2:H:60:MET:HE2	2:H:60:MET:HB3	1.76	0.45
1:J:75:CYS:SG	1:J:77:PRO:HD2	2.57	0.45
1:S:54:CYS:HB2	4:S:201:SF4:S1	2.56	0.45
2:E:24:THR:O	2:E:28:GLU:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:80:GLU:O	2:Q:46:VAL:HA	2.17	0.45
1:G:79:ARG:O	2:H:48:HIS:HB3	2.17	0.44
1:A:75:CYS:SG	1:A:77:PRO:HD2	2.56	0.44
1:D:75:CYS:SG	1:D:77:PRO:HD2	2.58	0.44
1:P:57:ARG:HB2	1:P:59:TYR:CZ	2.52	0.44
1:S:104:THR:HG22	1:S:106:ASP:N	2.24	0.44
3:U:34:TRP:HB2	3:U:41:SER:OG	2.17	0.44
1:V:28:PHE:HB3	1:V:35:THR:HG21	2.00	0.44
1:G:11:GLU:OE1	1:G:14:ARG:NH2	2.38	0.44
3:W:39:GLY:CA	1:V:37:VAL:HG11	2.47	0.44
1:M:75:CYS:SG	1:M:77:PRO:HD2	2.58	0.44
2:T:39:ARG:CB	2:T:61:GLU:HG2	2.46	0.44
2:H:25:GLU:OE1	3:L:58:LYS:NZ	2.50	0.44
1:J:109:LYS:HB2	1:J:109:LYS:HE3	1.61	0.44
2:K:24:THR:CG2	2:K:25:GLU:N	2.77	0.44
1:P:73:CYS:HB2	4:P:201:SF4:S1	2.58	0.44
1:M:76:VAL:HB	1:M:77:PRO:HD3	2.00	0.44
2:Q:76:ILE:HD13	2:Q:76:ILE:HA	1.86	0.44
3:W:47:LEU:HD11	3:W:102:LYS:HD2	1.99	0.44
2:T:29:LYS:HA	2:T:32:GLU:CG	2.47	0.44
2:T:102:LEU:HD22	2:T:106:GLU:HG3	2.00	0.44
1:S:75:CYS:SG	1:S:77:PRO:HD2	2.58	0.43
1:J:67:GLY:HA3	2:K:71:TRP:CH2	2.52	0.43
1:G:16:PHE:CZ	1:G:74:PRO:HD3	2.52	0.43
2:K:103:LYS:HG3	2:K:106:GLU:HG3	2.00	0.43
1:V:39:ILE:HG13	1:V:40:LYS:H	1.83	0.43
2:Q:28:GLU:O	2:Q:32:GLU:HG3	2.18	0.43
3:W:42:LYS:HB3	3:W:42:LYS:HE3	1.85	0.43
1:G:64:ALA:C	2:H:76:ILE:HD11	2.43	0.43
3:O:79:ARG:HD3	3:O:79:ARG:HA	1.85	0.43
1:V:90:LEU:HD22	1:V:94:ASN:ND2	2.33	0.43
1:A:80:GLU:O	2:B:46:VAL:HA	2.19	0.43
3:O:109:LEU:HD23	3:O:109:LEU:HA	1.83	0.43
1:S:27:TYR:CE1	1:S:92:PRO:HG3	2.53	0.43
3:W:86:ILE:HG21	3:W:112:PHE:CZ	2.54	0.43
2:N:24:THR:HB	2:N:27:ASP:HB2	1.99	0.43
2:K:57:LEU:HA	2:K:60:MET:HE3	2.01	0.43
1:M:73:CYS:HB2	4:M:201:SF4:S1	2.59	0.43
2:T:34:ILE:O	2:T:34:ILE:HG13	2.18	0.43
2:T:67:TYR:CE1	2:T:81:PRO:HB2	2.54	0.43
1:M:16:PHE:CZ	1:M:74:PRO:HD3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:37:ARG:HH11	2:N:110:ILE:CD1	2.32	0.43
1:A:16:PHE:CZ	1:A:74:PRO:HD3	2.54	0.42
3:C:13:VAL:HG13	3:C:64:LEU:HD12	2.00	0.42
1:M:2:LYS:HE3	1:M:2:LYS:HB3	1.78	0.42
2:T:103:LYS:HB3	2:T:106:GLU:CD	2.44	0.42
2:N:37:ARG:HE	2:N:37:ARG:HB2	1.61	0.42
2:H:49:VAL:HG13	2:H:52:VAL:HB	2.02	0.42
2:N:89:GLU:OE2	2:N:95:PRO:HG3	2.20	0.42
1:V:32:LYS:HG2	1:V:35:THR:C	2.44	0.42
1:V:35:THR:CA	1:V:88:LEU:HD22	2.31	0.42
3:C:17:THR:HG21	1:D:111:THR:HG23	2.02	0.42
2:H:29:LYS:HD3	2:H:33:LYS:HE3	2.02	0.42
1:P:76:VAL:HB	1:P:77:PRO:HD3	2.01	0.42
3:W:53:GLN:HA	3:W:56:THR:HG23	2.01	0.42
2:N:87:VAL:HA	2:N:96:VAL:O	2.19	0.42
3:O:7:THR:N	6:O:305:HOH:O	2.52	0.42
2:T:56:GLU:CD	2:T:58:MET:H	2.27	0.42
2:H:76:ILE:HD13	2:H:76:ILE:HA	1.76	0.41
1:D:13:MET:HE2	1:D:42:LEU:HB3	2.02	0.41
1:J:104:THR:HG22	1:J:107:GLU:OE2	2.19	0.41
2:Q:29:LYS:HE2	2:Q:29:LYS:HB2	1.91	0.41
3:R:28:PRO:HG2	3:R:59:ILE:HG12	2.03	0.41
1:V:105:SER:HA	1:V:107:GLU:HG2	2.03	0.41
2:N:90:ILE:HD12	2:N:90:ILE:HA	1.80	0.41
1:S:57:ARG:NH1	3:U:79:ARG:HB3	2.35	0.41
1:D:53:LEU:HD22	1:D:59:TYR:CZ	2.55	0.41
1:M:74:PRO:O	1:M:79:ARG:HD2	2.20	0.41
2:N:28:GLU:OE1	2:N:28:GLU:HA	2.20	0.41
1:S:67:GLY:HA3	2:T:71:TRP:CH2	2.56	0.41
3:W:105:LEU:O	3:W:109:LEU:HG	2.19	0.41
2:B:29:LYS:NZ	2:B:104:GLU:OE2	2.52	0.41
1:J:57:ARG:HB2	1:J:59:TYR:CZ	2.55	0.41
2:K:29:LYS:O	2:K:33:LYS:HG3	2.20	0.41
2:K:39:ARG:O	2:K:107:PHE:HA	2.21	0.41
2:K:93:ARG:CD	2:K:94:GLY:N	2.61	0.41
3:F:13:VAL:HG13	3:F:64:LEU:HD12	2.02	0.41
2:T:42:VAL:HA	2:T:58:MET:HE3	2.03	0.41
2:E:24:THR:HG22	2:E:28:GLU:HG2	2.02	0.40
1:G:109:LYS:HA	1:G:109:LYS:HD3	1.72	0.40
1:S:79:ARG:O	2:T:48:HIS:HB3	2.21	0.40
3:W:52:ALA:HA	3:W:61:PHE:CD1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:72:THR:N	3:W:73:PRO:HD2	2.36	0.40
1:D:27:TYR:CE1	1:D:92:PRO:HG3	2.56	0.40
1:G:76:VAL:HB	1:G:77:PRO:HD3	2.04	0.40
2:K:27:ASP:O	2:K:31:LYS:HB2	2.20	0.40
2:K:42:VAL:CA	2:K:58:MET:HE1	2.51	0.40
1:D:16:PHE:CZ	1:D:74:PRO:HD3	2.56	0.40
3:R:105:LEU:HD12	3:R:105:LEU:HA	1.92	0.40
2:E:69:VAL:HG23	2:E:81:PRO:HB3	2.03	0.40
2:T:49:VAL:H	2:T:49:VAL:HG22	1.58	0.40
3:W:86:ILE:HG21	3:W:112:PHE:CE2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:46:LYS:O	3:W:11:GLN:NE2[2_555]	2.18	0.02

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	111/115 (96%)	110 (99%)	1 (1%)	0	100	100
1	D	112/115 (97%)	110 (98%)	1 (1%)	1 (1%)	14	22
1	G	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	J	111/115 (96%)	110 (99%)	1 (1%)	0	100	100
1	M	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	P	109/115 (95%)	107 (98%)	1 (1%)	1 (1%)	14	22
1	S	112/115 (97%)	111 (99%)	0	1 (1%)	14	22
1	V	56/115 (49%)	54 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	86/112 (77%)	84 (98%)	2 (2%)	0	100	100
2	E	87/112 (78%)	86 (99%)	1 (1%)	0	100	100
2	H	86/112 (77%)	85 (99%)	1 (1%)	0	100	100
2	K	86/112 (77%)	86 (100%)	0	0	100	100
2	N	86/112 (77%)	86 (100%)	0	0	100	100
2	Q	86/112 (77%)	84 (98%)	2 (2%)	0	100	100
2	T	83/112 (74%)	82 (99%)	0	1 (1%)	10	16
3	C	105/114 (92%)	104 (99%)	1 (1%)	0	100	100
3	F	105/114 (92%)	104 (99%)	1 (1%)	0	100	100
3	I	104/114 (91%)	103 (99%)	1 (1%)	0	100	100
3	L	105/114 (92%)	104 (99%)	1 (1%)	0	100	100
3	O	105/114 (92%)	104 (99%)	1 (1%)	0	100	100
3	R	105/114 (92%)	103 (98%)	2 (2%)	0	100	100
3	U	105/114 (92%)	104 (99%)	1 (1%)	0	100	100
3	W	89/114 (78%)	89 (100%)	0	0	100	100
All	All	2258/2616 (86%)	2230 (99%)	24 (1%)	4 (0%)	43	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	114	ASN
2	T	91	GLU
1	D	114	ASN
1	S	114	ASN

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	99/100 (99%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	100/100 (100%)	100 (100%)	0	100	100
1	G	100/100 (100%)	100 (100%)	0	100	100
1	J	99/100 (99%)	99 (100%)	0	100	100
1	M	100/100 (100%)	100 (100%)	0	100	100
1	P	99/100 (99%)	99 (100%)	0	100	100
1	S	100/100 (100%)	100 (100%)	0	100	100
1	V	61/100 (61%)	61 (100%)	0	100	100
2	B	79/98 (81%)	79 (100%)	0	100	100
2	E	80/98 (82%)	80 (100%)	0	100	100
2	H	79/98 (81%)	79 (100%)	0	100	100
2	K	79/98 (81%)	79 (100%)	0	100	100
2	N	79/98 (81%)	79 (100%)	0	100	100
2	Q	79/98 (81%)	79 (100%)	0	100	100
2	T	78/98 (80%)	78 (100%)	0	100	100
3	C	95/101 (94%)	95 (100%)	0	100	100
3	F	95/101 (94%)	95 (100%)	0	100	100
3	I	94/101 (93%)	93 (99%)	1 (1%)	65	82
3	L	95/101 (94%)	95 (100%)	0	100	100
3	O	95/101 (94%)	95 (100%)	0	100	100
3	R	95/101 (94%)	95 (100%)	0	100	100
3	U	95/101 (94%)	95 (100%)	0	100	100
3	W	86/101 (85%)	86 (100%)	0	100	100
All	All	2061/2294 (90%)	2060 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	109	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	85	HIS

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Mol	Chain	Res	Type
3	F	54	HIS
1	G	58	HIS
3	I	14	ASN
3	I	54	HIS
1	J	85	HIS
3	O	54	HIS
1	P	58	HIS
1	P	114	ASN
3	R	49	ASN
3	U	14	ASN
3	U	54	HIS
3	U	75	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 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	SF4	P	201	1	0,12,12	-	-	-		
4	SF4	A	201	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SF4	G	201	1	0,12,12	-	-	-		
4	SF4	S	201	1	0,12,12	-	-	-		
4	SF4	J	201	1	0,12,12	-	-	-		
4	SF4	D	201	1	0,12,12	-	-	-		
4	SF4	M	201	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	SF4	P	201	1	-	-	0/6/5/5
4	SF4	A	201	1	-	-	0/6/5/5
4	SF4	G	201	1	-	-	0/6/5/5
4	SF4	S	201	1	-	-	0/6/5/5
4	SF4	J	201	1	-	-	0/6/5/5
4	SF4	D	201	1	-	-	0/6/5/5
4	SF4	M	201	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

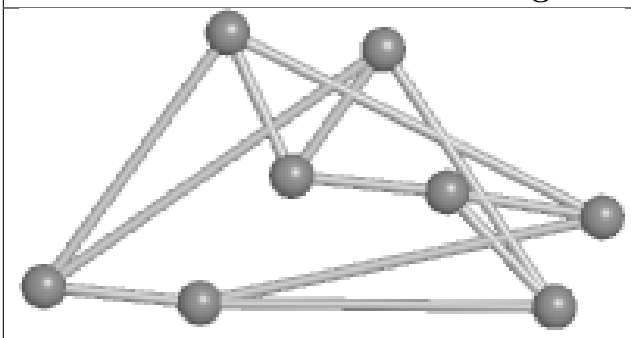
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	201	SF4	1	0
4	S	201	SF4	1	0
4	M	201	SF4	2	0

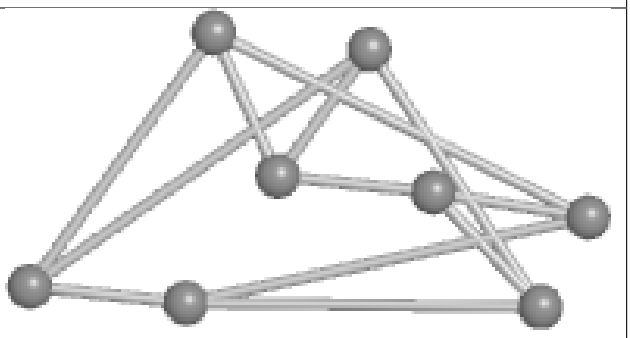
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

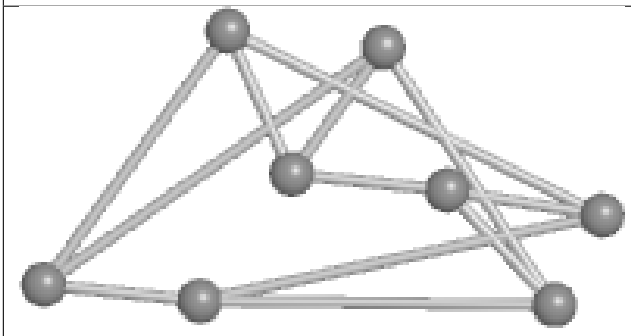
Ligand SF4 P 201



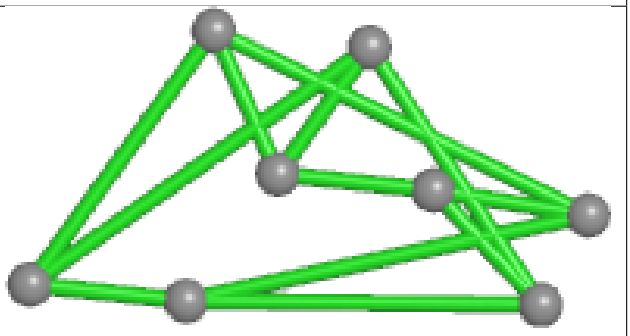
Bond lengths



Bond angles

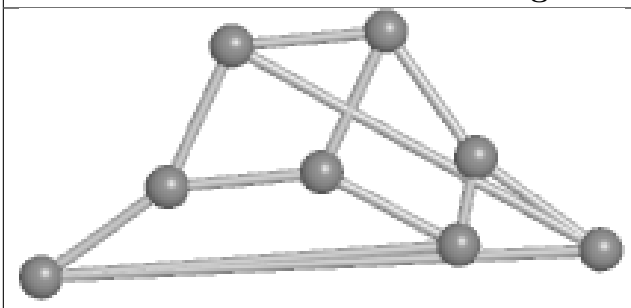


Torsions

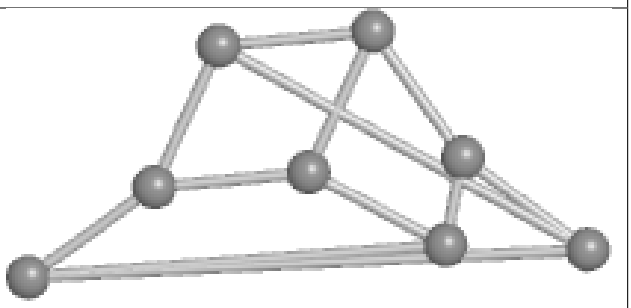


Rings

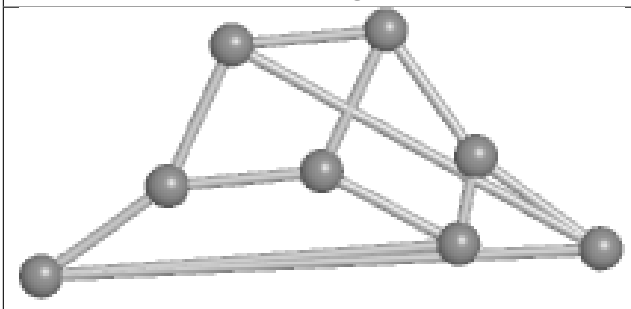
Ligand SF4 A 201



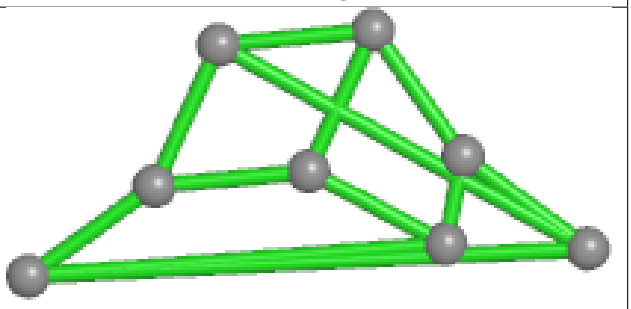
Bond lengths



Bond angles

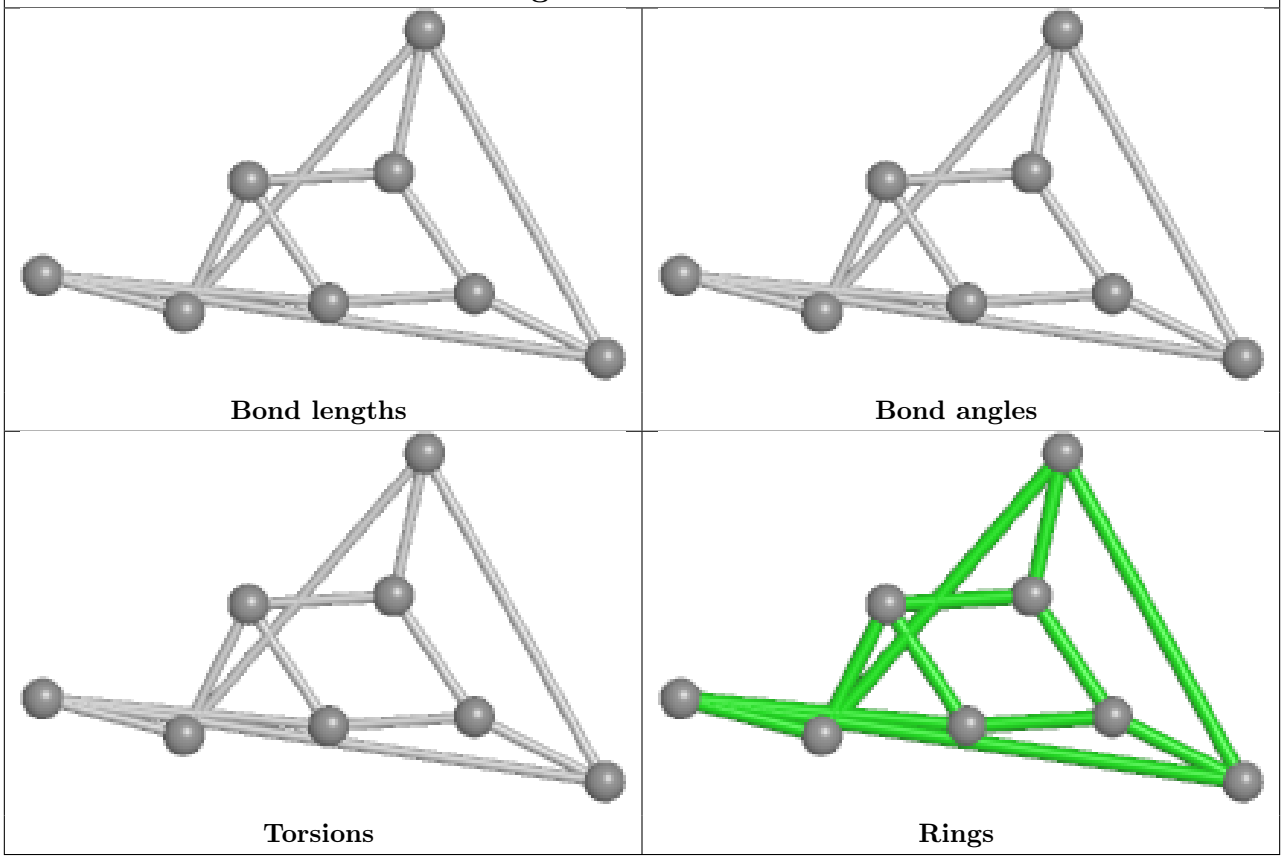


Torsions

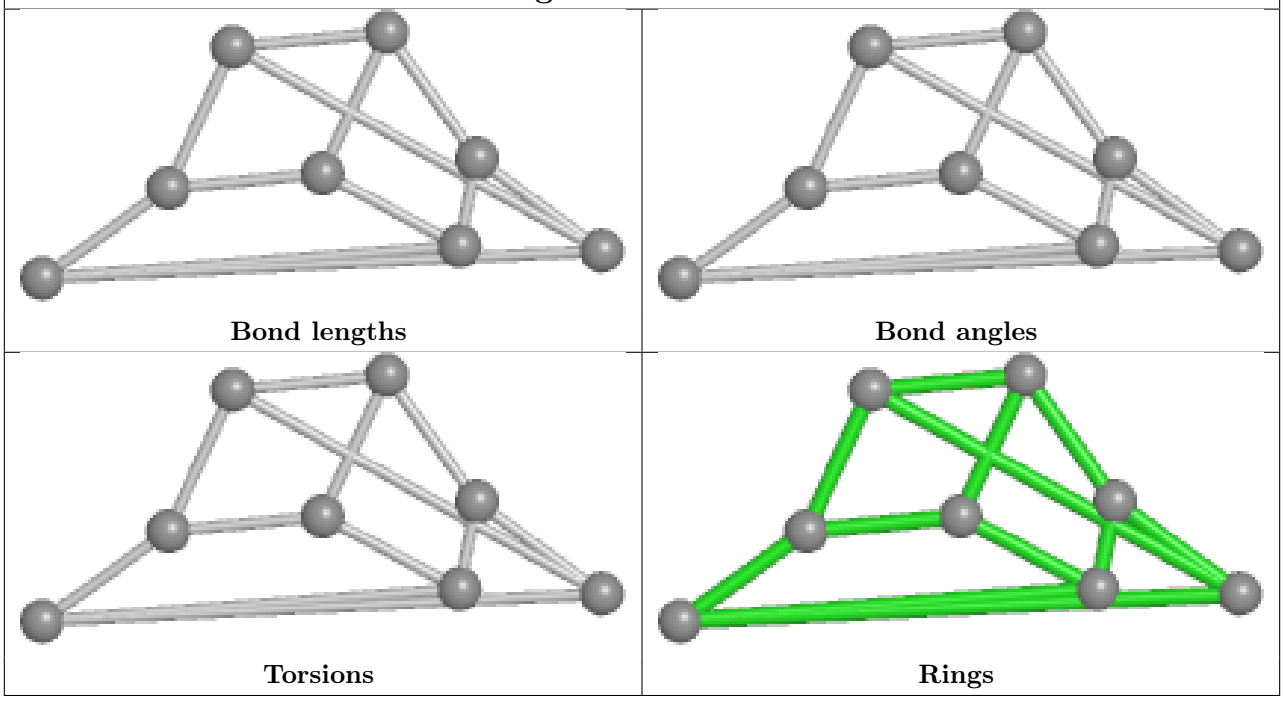


Rings

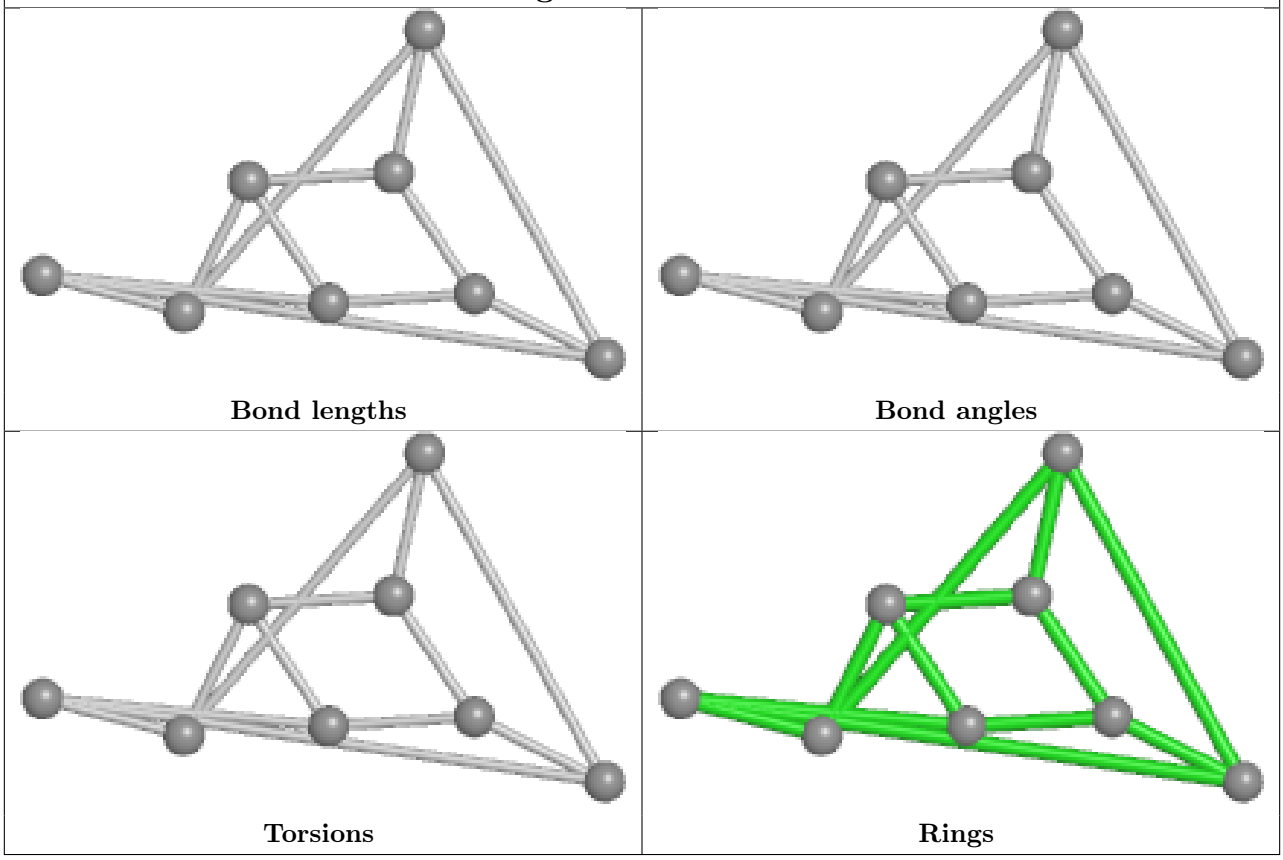
Ligand SF4 G 201



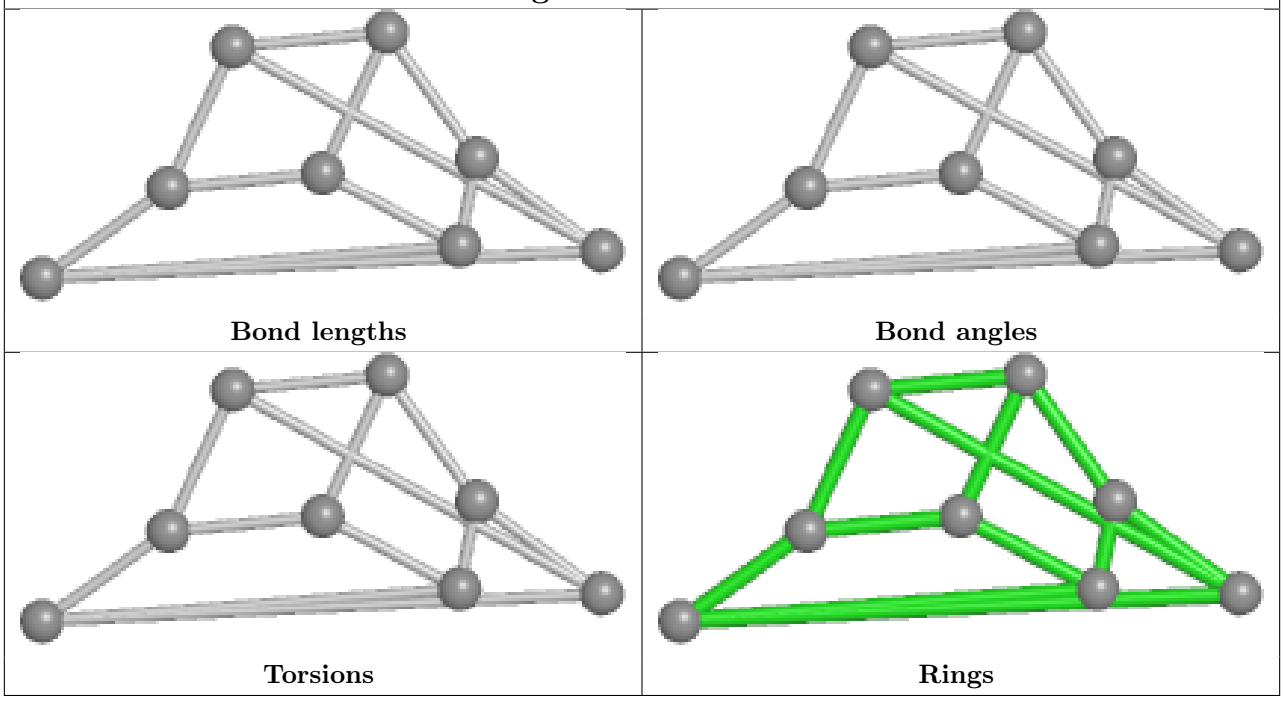
Ligand SF4 S 201

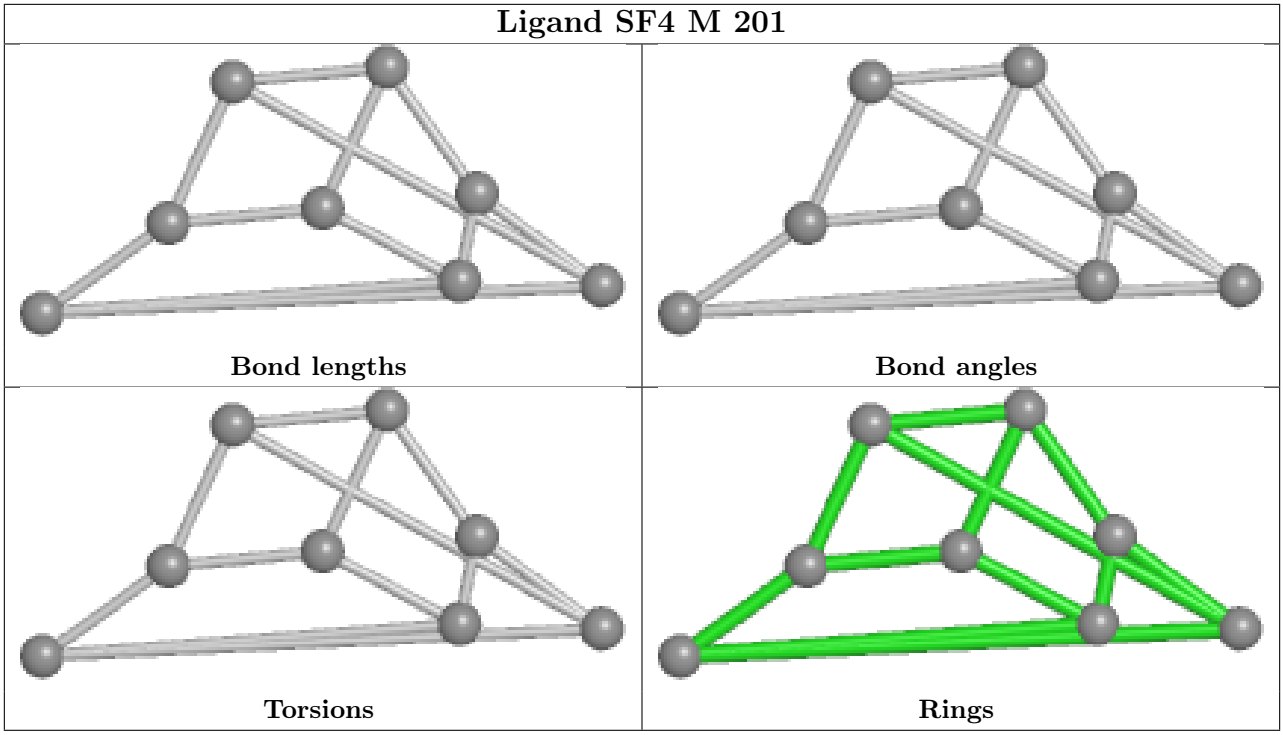


Ligand SF4 J 201



Ligand SF4 D 201





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	113/115 (98%)	0.42	2 (1%)	67	63	37, 52, 74, 101	0
1	D	114/115 (99%)	0.37	4 (3%)	47	43	37, 52, 73, 104	0
1	G	114/115 (99%)	0.50	5 (4%)	39	34	37, 54, 80, 110	0
1	J	113/115 (98%)	0.52	6 (5%)	32	28	41, 53, 76, 102	0
1	M	114/115 (99%)	0.73	8 (7%)	22	19	44, 57, 85, 104	0
1	P	113/115 (98%)	1.02	13 (11%)	9	7	49, 62, 87, 109	0
1	S	114/115 (99%)	0.90	15 (13%)	7	5	46, 63, 87, 102	0
1	V	71/115 (61%)	3.92	63 (88%)	0	0	95, 131, 146, 167	0
2	B	88/112 (78%)	0.63	4 (4%)	38	34	41, 57, 88, 106	0
2	E	89/112 (79%)	0.64	7 (7%)	18	15	43, 60, 104, 122	0
2	H	88/112 (78%)	1.63	30 (34%)	1	1	50, 82, 137, 158	0
2	K	88/112 (78%)	1.78	37 (42%)	0	0	50, 82, 133, 146	0
2	N	88/112 (78%)	1.89	39 (44%)	0	0	53, 91, 131, 148	0
2	Q	88/112 (78%)	1.04	10 (11%)	10	7	54, 69, 112, 141	0
2	T	87/112 (77%)	2.40	54 (62%)	0	0	65, 110, 140, 151	0
3	C	107/114 (93%)	0.09	3 (2%)	55	51	35, 45, 65, 122	0
3	F	107/114 (93%)	0.25	4 (3%)	45	41	36, 47, 67, 119	0
3	I	106/114 (92%)	0.11	2 (1%)	66	62	38, 48, 63, 94	0
3	L	107/114 (93%)	0.16	3 (2%)	55	51	39, 48, 60, 122	0
3	O	107/114 (93%)	0.09	2 (1%)	66	62	36, 46, 60, 113	0
3	R	107/114 (93%)	0.52	3 (2%)	55	51	42, 53, 73, 134	0
3	U	107/114 (93%)	0.48	4 (3%)	45	41	41, 53, 74, 123	0
3	W	98/114 (85%)	3.16	81 (82%)	0	0	90, 122, 149, 162	0
All	All	2328/2616 (88%)	0.93	399 (17%)	4	3	35, 58, 129, 167	0

All (399) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	55	PRO	11.4
1	V	56	CYS	9.0
1	V	27	TYR	8.2
1	V	90	LEU	7.7
3	R	7	THR	6.8
1	V	53	LEU	6.4
3	W	64	LEU	6.3
2	T	34	ILE	6.2
3	L	7	THR	6.2
2	T	109	LEU	6.2
3	W	43	MET	6.0
1	V	51	ALA	5.9
1	V	88	LEU	5.9
1	V	87	MET	5.9
1	V	30	VAL	5.8
3	O	7	THR	5.8
2	T	110	ILE	5.7
3	W	38	CYS	5.7
1	V	39	ILE	5.7
3	W	105	LEU	5.6
2	H	90	ILE	5.6
1	V	16	PHE	5.6
3	W	78	VAL	5.5
3	W	112	PHE	5.4
1	V	92	PRO	5.4
2	N	36	ALA	5.4
2	T	90	ILE	5.3
2	H	95	PRO	5.3
1	V	12	ILE	5.2
1	A	3	THR	5.2
1	V	15	LYS	5.2
1	V	26	THR	5.2
3	W	92	LYS	5.1
1	V	96	PHE	5.1
1	V	91	THR	5.0
3	W	36	PRO	4.9
2	N	90	ILE	4.9
3	U	7	THR	4.9
2	K	39	ARG	4.9
1	V	99	LYS	4.9
3	W	13	VAL	4.9
1	J	3	THR	4.9

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Mol	Chain	Res	Type	RSRZ
3	W	70	PRO	4.8
3	W	48	VAL	4.8
3	R	113	LEU	4.8
2	T	94	GLY	4.8
3	W	100	VAL	4.8
3	U	113	LEU	4.8
2	K	90	ILE	4.7
2	H	24	THR	4.7
3	W	37	TRP	4.7
1	V	28	PHE	4.7
3	W	104	THR	4.6
3	W	76	TYR	4.6
1	P	3	THR	4.6
2	E	73	GLY	4.5
2	K	59	GLY	4.5
1	V	35	THR	4.5
3	F	113	LEU	4.5
1	V	67	GLY	4.5
2	K	96	VAL	4.5
1	V	10	VAL	4.4
3	W	108	SER	4.4
1	V	100	ASP	4.4
2	T	24	THR	4.4
3	W	46	PRO	4.4
1	V	63	ALA	4.4
2	N	94	GLY	4.4
2	T	87	VAL	4.4
1	V	34	VAL	4.3
3	F	7	THR	4.3
2	N	35	GLY	4.3
3	W	40	PRO	4.3
2	T	44	LEU	4.3
3	W	96	ILE	4.3
2	N	63	PHE	4.2
2	K	60	MET	4.2
3	W	62	TYR	4.2
3	W	34	TRP	4.2
3	W	44	ILE	4.2
3	W	54	HIS	4.2
1	V	112	THR	4.1
2	K	110	ILE	4.1
2	T	60	MET	4.1

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Mol	Chain	Res	Type	RSRZ
3	W	88	VAL	4.1
2	N	24	THR	4.1
2	T	107	PHE	4.1
3	L	8	THR	4.1
1	V	40	LYS	4.1
2	H	96	VAL	4.1
1	V	89	PHE	4.0
1	V	66	VAL	4.0
1	V	52	PRO	4.0
1	S	3	THR	4.0
2	B	24	THR	4.0
3	W	39	GLY	4.0
2	K	87	VAL	3.9
2	Q	111	ASP	3.9
1	V	108	ILE	3.9
2	N	110	ILE	3.9
1	V	19	GLN	3.9
3	C	113	LEU	3.9
1	V	32	LYS	3.9
2	H	63	PHE	3.9
1	V	13	MET	3.9
3	W	47	LEU	3.9
3	W	109	LEU	3.9
1	V	14	ARG	3.9
2	E	24	THR	3.9
3	W	110	ASP	3.8
2	Q	24	THR	3.8
3	R	8	THR	3.8
1	M	96	PHE	3.8
2	T	63	PHE	3.8
1	D	3	THR	3.8
3	W	106	THR	3.8
1	A	22	ARG	3.8
1	V	49	TYR	3.7
1	P	2	LYS	3.7
3	W	85	MET	3.7
1	V	17	SER	3.7
3	W	29	VAL	3.7
3	U	8	THR	3.7
1	G	4	GLU	3.7
3	W	101	PRO	3.7
1	V	58	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
2	H	94	GLY	3.6
1	V	38	VAL	3.6
3	W	103	THR	3.6
3	W	97	ILE	3.6
2	H	58	MET	3.6
3	W	51	LEU	3.6
3	W	26	THR	3.6
2	T	64	ILE	3.6
2	H	50	VAL	3.6
2	T	55	VAL	3.6
3	W	30	VAL	3.6
3	W	53	GLN	3.5
1	V	42	LEU	3.5
2	N	53	PRO	3.5
1	V	109	LYS	3.5
1	P	98	GLY	3.5
2	H	92	GLY	3.5
3	W	86	ILE	3.5
3	W	28	PRO	3.4
3	W	18	TRP	3.4
2	B	111	ASP	3.4
2	K	85	GLN	3.4
2	K	111	ASP	3.4
3	W	14	ASN	3.4
3	W	67	ASP	3.4
3	W	93	LYS	3.4
2	K	95	PRO	3.4
1	G	3	THR	3.4
1	V	107	GLU	3.4
1	J	96	PHE	3.4
1	V	111	THR	3.4
3	W	81	ILE	3.3
3	W	33	PHE	3.3
1	G	32	LYS	3.3
2	K	42	VAL	3.3
2	N	85	GLN	3.3
2	T	92	GLY	3.3
2	T	53	PRO	3.3
2	N	37	ARG	3.3
2	K	25	GLU	3.3
2	T	50	VAL	3.3
1	V	60	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
3	W	42	LYS	3.2
2	T	43	PRO	3.2
2	N	107	PHE	3.2
2	N	87	VAL	3.2
3	I	113	LEU	3.2
2	N	41	THR	3.2
1	V	33	GLY	3.2
2	E	111	ASP	3.2
2	H	49	VAL	3.2
2	T	35	GLY	3.1
2	K	50	VAL	3.1
2	N	111	ASP	3.1
2	K	41	THR	3.1
3	I	8	THR	3.1
3	W	66	THR	3.1
1	D	22	ARG	3.1
3	W	24	LYS	3.1
3	W	84	ILE	3.1
1	G	109	LYS	3.1
2	H	110	ILE	3.0
3	W	31	VAL	3.0
3	F	8	THR	3.0
1	V	97	ALA	3.0
2	N	108	GLU	3.0
2	Q	25	GLU	3.0
2	T	39	ARG	3.0
2	Q	74	LYS	3.0
3	W	32	ASP	3.0
1	V	110	GLU	3.0
2	H	91	GLU	3.0
3	W	23	LEU	2.9
2	H	87	VAL	2.9
3	O	8	THR	2.9
3	W	41	SER	2.9
2	E	27	ASP	2.9
1	V	45	HIS	2.9
2	N	109	LEU	2.9
3	W	22	VAL	2.9
3	W	58	LYS	2.9
2	K	24	THR	2.9
1	V	50	GLY	2.9
2	N	62	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	N	95	PRO	2.9
2	N	50	VAL	2.9
2	Q	68	VAL	2.9
2	N	97	LYS	2.8
2	T	96	VAL	2.8
2	K	40	VAL	2.8
1	V	104	THR	2.8
2	N	51	ARG	2.8
1	P	19	GLN	2.8
2	T	95	PRO	2.8
2	T	89	GLU	2.8
2	T	33	LYS	2.8
1	M	23	ARG	2.8
3	W	72	THR	2.8
1	S	27	TYR	2.8
2	K	44	LEU	2.8
2	T	70	LEU	2.8
2	H	93	ARG	2.8
2	N	42	VAL	2.8
2	N	96	VAL	2.8
1	V	62	LYS	2.7
2	H	109	LEU	2.7
3	L	113	LEU	2.7
1	M	19	GLN	2.7
2	T	93	ARG	2.7
2	K	86	PHE	2.7
3	W	12	VAL	2.7
2	E	23	GLU	2.7
2	K	61	GLU	2.7
2	H	104	GLU	2.7
2	K	88	LYS	2.7
2	Q	71	TRP	2.7
2	N	98	PHE	2.6
2	N	38	VAL	2.6
3	W	50	ASP	2.6
1	P	73	CYS	2.6
1	P	84	CYS	2.6
2	E	74	LYS	2.6
2	K	99	PHE	2.6
2	T	27	ASP	2.6
1	S	102	THR	2.6
2	T	46	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	8	THR	2.6
2	K	109	LEU	2.6
2	T	98	PHE	2.6
1	M	3	THR	2.6
2	K	94	GLY	2.6
2	N	49	VAL	2.6
2	T	40	VAL	2.6
3	W	83	THR	2.6
2	T	76	ILE	2.6
3	W	69	SER	2.6
2	K	105	ASP	2.6
3	W	94	ASP	2.6
1	S	104	THR	2.6
2	Q	73	GLY	2.6
1	V	48	SER	2.6
3	W	10	ILE	2.6
1	S	73	CYS	2.5
2	T	38	VAL	2.5
2	K	93	ARG	2.5
1	V	29	CYS	2.5
2	K	92	GLY	2.5
2	T	86	PHE	2.5
3	W	35	ALA	2.5
3	W	74	GLY	2.5
1	V	11	GLU	2.5
2	K	63	PHE	2.5
2	H	51	ARG	2.5
3	W	25	ALA	2.5
1	P	23	ARG	2.4
2	N	93	ARG	2.4
2	H	99	PHE	2.4
2	B	29	LYS	2.4
1	V	98	GLY	2.4
3	W	27	GLY	2.4
1	D	96	PHE	2.4
2	K	38	VAL	2.4
1	M	8	LYS	2.4
1	V	106	ASP	2.4
2	K	51	ARG	2.4
2	N	99	PHE	2.4
2	T	29	LYS	2.4
2	T	42	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	T	82	PHE	2.4
3	W	102	LYS	2.4
2	Q	27	ASP	2.4
3	W	65	ASN	2.4
1	S	99	LYS	2.4
1	V	105	SER	2.4
1	P	66	VAL	2.4
3	W	87	PHE	2.4
2	H	108	GLU	2.4
2	N	89	GLU	2.4
1	V	61	ASP	2.3
2	N	92	GLY	2.3
3	C	7	THR	2.3
1	S	75	CYS	2.3
2	H	38	VAL	2.3
2	T	49	VAL	2.3
2	H	37	ARG	2.3
2	T	91	GLU	2.3
2	K	35	GLY	2.3
2	T	41	THR	2.3
1	M	24	SER	2.3
1	M	7	GLU	2.3
1	S	19	GLN	2.3
3	U	91	GLU	2.3
1	S	29	CYS	2.3
2	T	80	LEU	2.3
1	J	99	LYS	2.3
2	H	29	LYS	2.3
3	W	49	ASN	2.3
2	T	47	TYR	2.3
2	K	58	MET	2.3
2	T	58	MET	2.3
3	W	95	THR	2.3
2	N	39	ARG	2.3
2	H	26	GLU	2.3
2	N	28	GLU	2.3
1	D	109	LYS	2.3
2	H	88	LYS	2.3
2	N	29	LYS	2.3
2	H	27	ASP	2.3
2	K	27	ASP	2.3
2	K	43	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	59	GLY	2.3
1	P	49	TYR	2.3
1	P	113	ALA	2.3
2	K	53	PRO	2.2
1	S	113	ALA	2.2
1	V	64	ALA	2.2
2	N	26	GLU	2.2
2	T	85	GLN	2.2
3	W	52	ALA	2.2
1	G	23	ARG	2.2
3	W	19	ASP	2.2
3	W	57	GLY	2.2
1	J	7	GLU	2.2
1	V	18	GLU	2.2
2	K	91	GLU	2.2
2	T	56	GLU	2.2
2	E	29	LYS	2.2
2	T	37	ARG	2.2
2	T	57	LEU	2.2
2	T	84	VAL	2.2
2	B	26	GLU	2.2
2	K	26	GLU	2.2
2	N	61	GLU	2.2
2	N	88	LYS	2.2
2	T	88	LYS	2.2
1	V	41	GLY	2.2
3	W	75	GLN	2.2
2	H	39	ARG	2.1
2	T	51	ARG	2.1
2	T	79	ASN	2.1
1	M	18	GLU	2.1
1	S	28	PHE	2.1
1	S	32	LYS	2.1
2	K	62	GLY	2.1
1	P	75	CYS	2.1
1	P	43	ALA	2.1
3	W	20	SER	2.1
2	N	58	MET	2.1
1	P	109	LYS	2.1
1	V	46	LYS	2.1
1	J	44	GLU	2.1
2	Q	70	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	W	59	ILE	2.1
2	T	59	GLY	2.1
2	Q	75	LYS	2.1
2	H	111	ASP	2.1
1	S	25	GLY	2.1
1	S	98	GLY	2.1
2	H	86	PHE	2.1
2	N	86	PHE	2.1
2	T	62	GLY	2.1
3	W	89	GLY	2.1
2	T	97	LYS	2.0
3	W	60	LYS	2.0
1	J	4	GLU	2.0
2	H	89	GLU	2.0
2	T	105	ASP	2.0
2	N	34	ILE	2.0
1	S	92	PRO	2.0
2	T	26	GLU	2.0
3	F	38	CYS	2.0
1	V	47	ASP	2.0
3	W	21	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NA	G	202	1/1	0.93	0.18	56,56,56,56	0
5	NA	J	202	1/1	0.94	0.20	52,52,52,52	0

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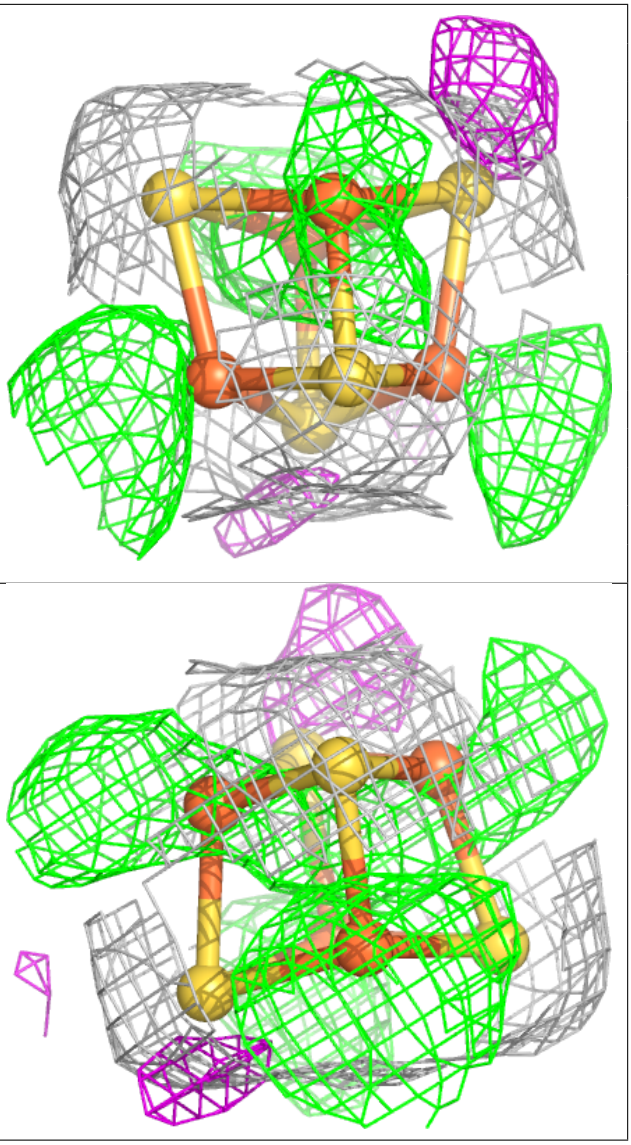
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NA	M	202	1/1	0.94	0.26	61,61,61,61	0
5	NA	P	202	1/1	0.94	0.28	60,60,60,60	0
5	NA	D	202	1/1	0.95	0.21	51,51,51,51	0
5	NA	O	201	1/1	0.95	0.10	53,53,53,53	0
5	NA	E	201	1/1	0.95	0.20	58,58,58,58	0
5	NA	A	202	1/1	0.97	0.15	52,52,52,52	0
5	NA	C	201	1/1	0.97	0.23	57,57,57,57	0
5	NA	L	201	1/1	0.97	0.30	52,52,52,52	0
4	SF4	J	201	8/8	0.98	0.06	38,43,47,47	0
4	SF4	M	201	8/8	0.98	0.07	40,48,49,49	0
4	SF4	P	201	8/8	0.98	0.06	43,48,52,54	0
4	SF4	S	201	8/8	0.98	0.06	46,49,54,54	0
4	SF4	A	201	8/8	0.98	0.06	36,39,41,44	0
4	SF4	D	201	8/8	0.98	0.06	36,38,41,44	0
4	SF4	G	201	8/8	0.98	0.05	36,42,44,47	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.

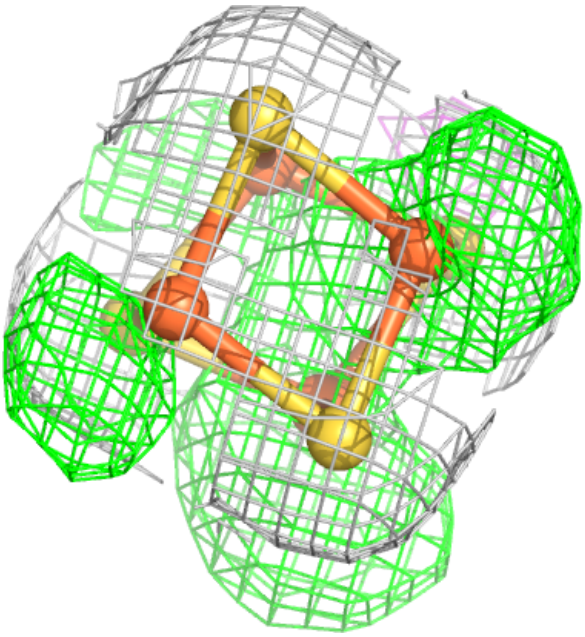
Electron density around SF4 J 201:

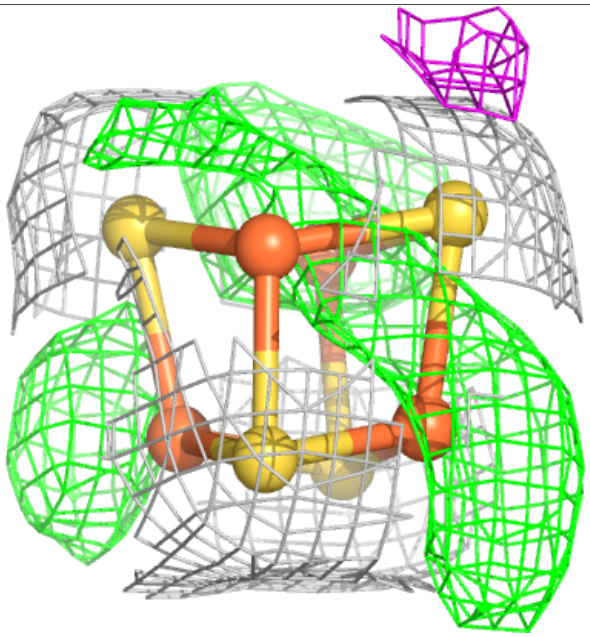
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

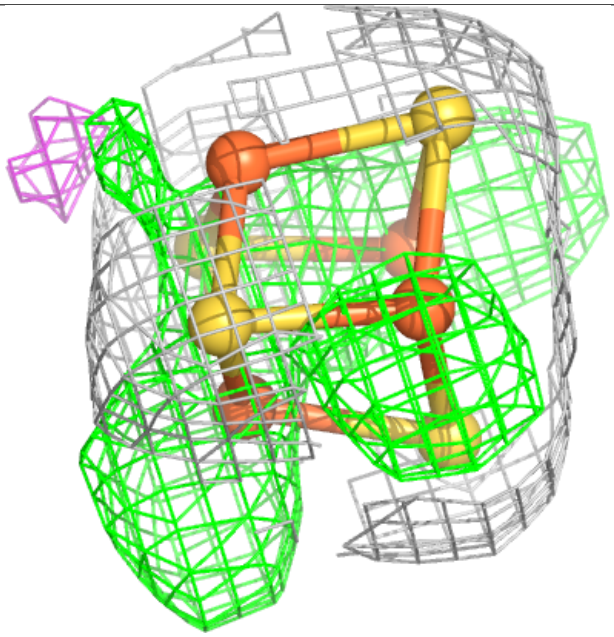


Electron density around SF4 M 201:

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

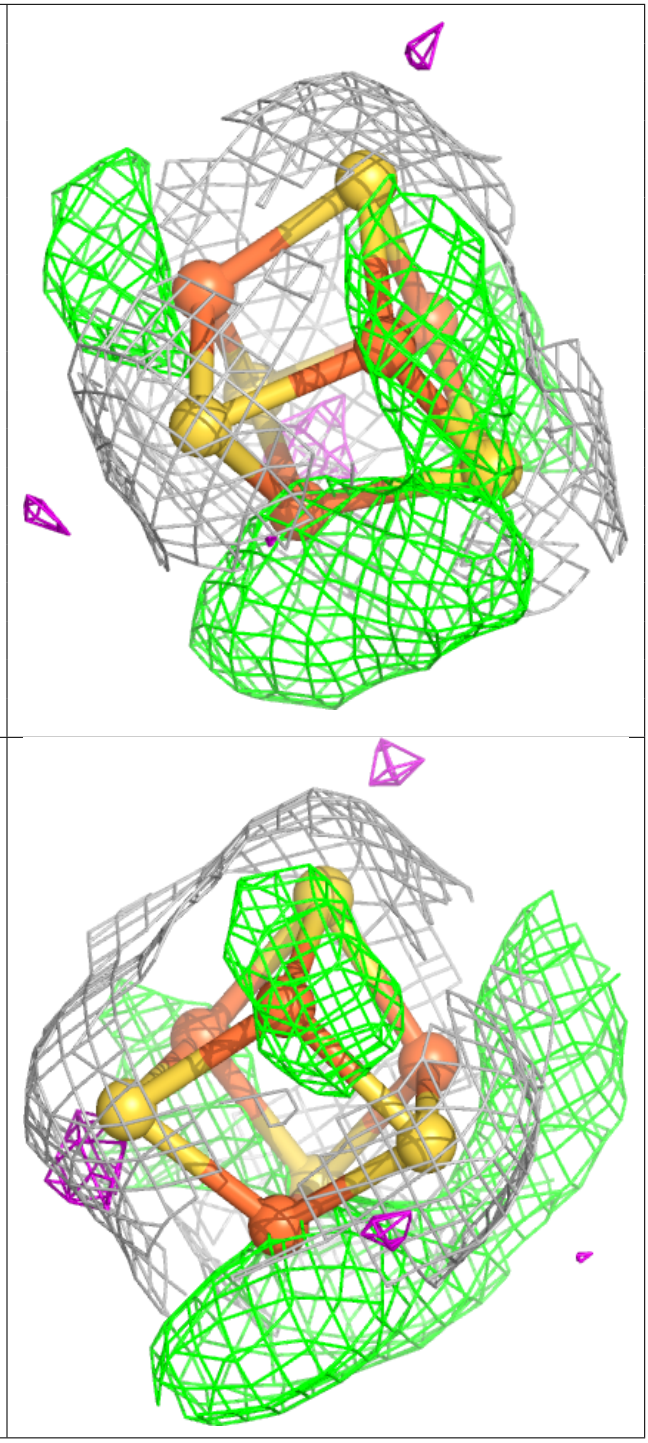






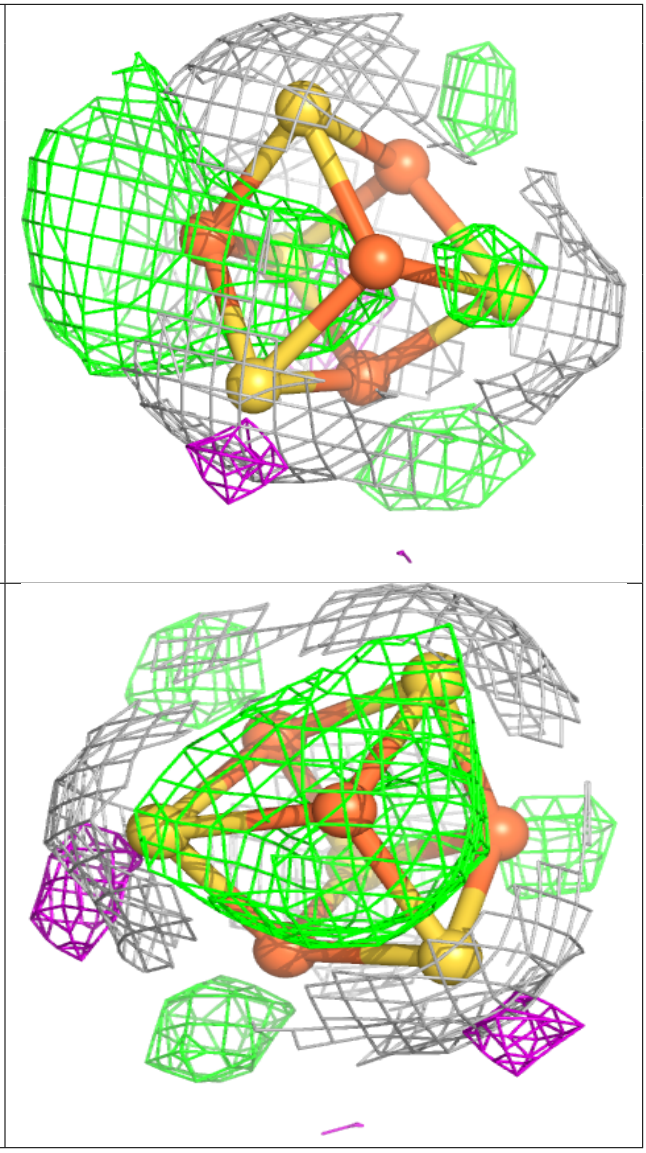
Electron density around SF4 P 201:

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



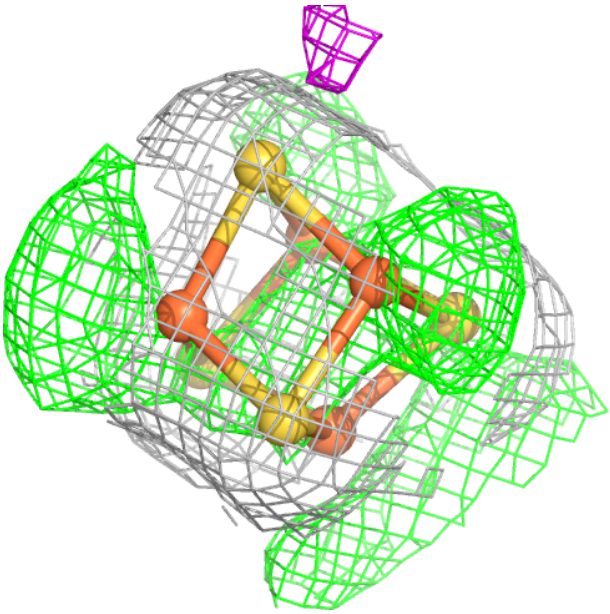
Electron density around SF4 S 201:

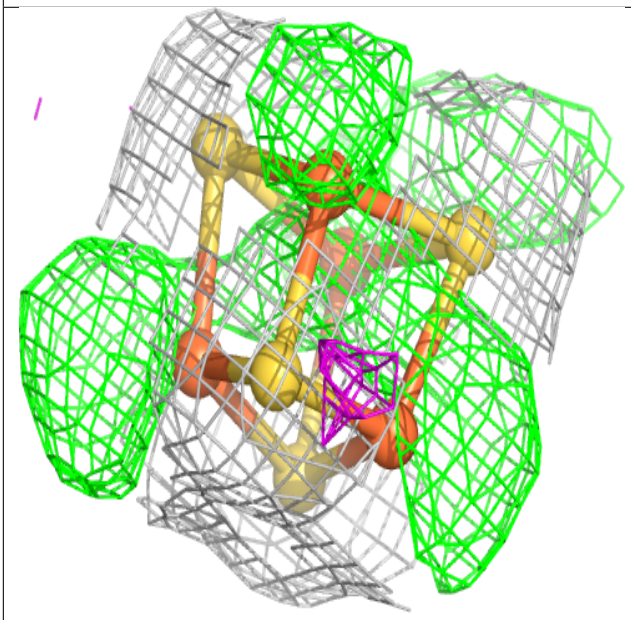
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

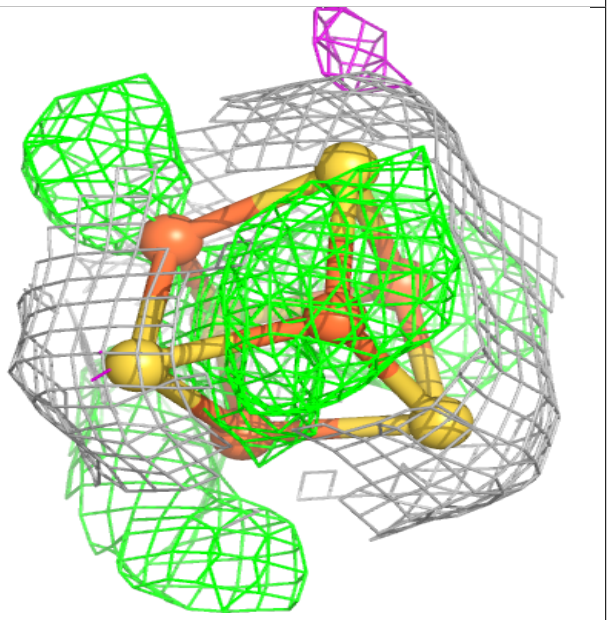


Electron density around SF4 A 201:

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

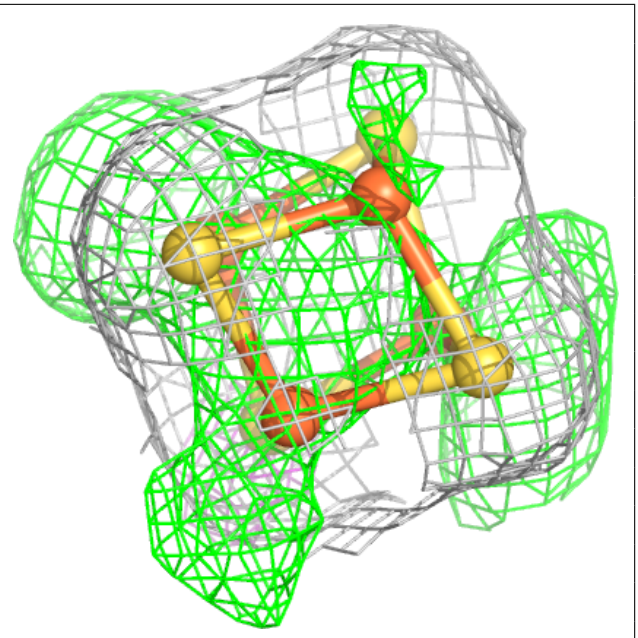


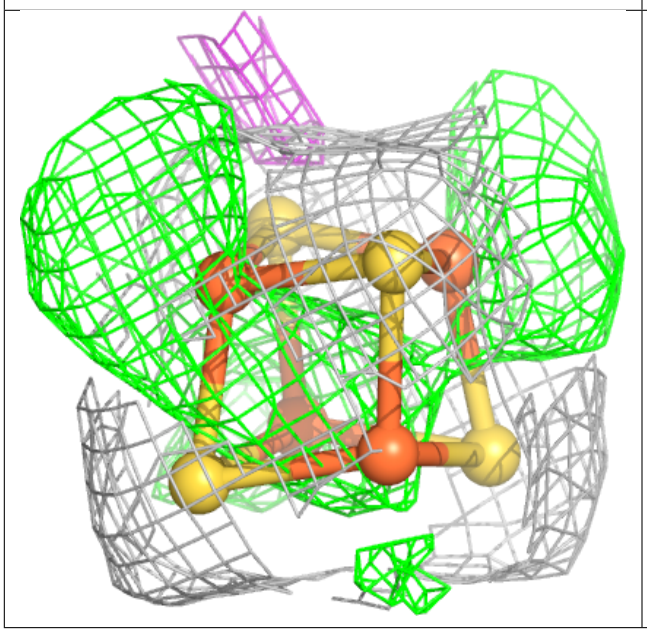


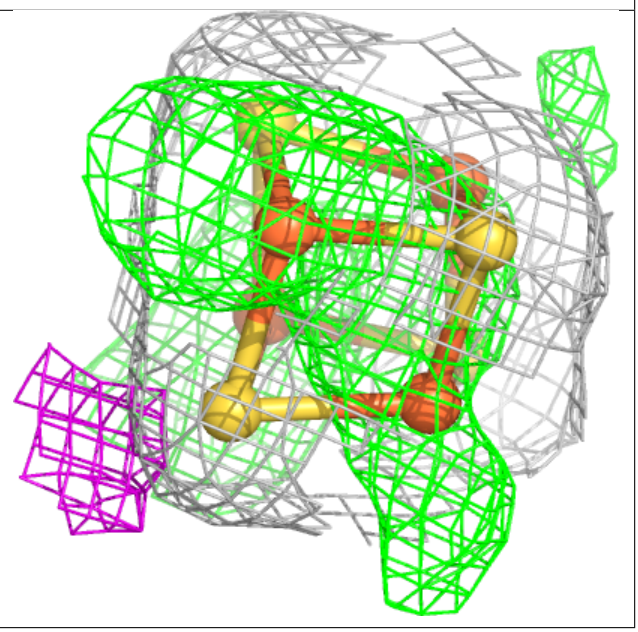


Electron density around SF4 D 201:

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

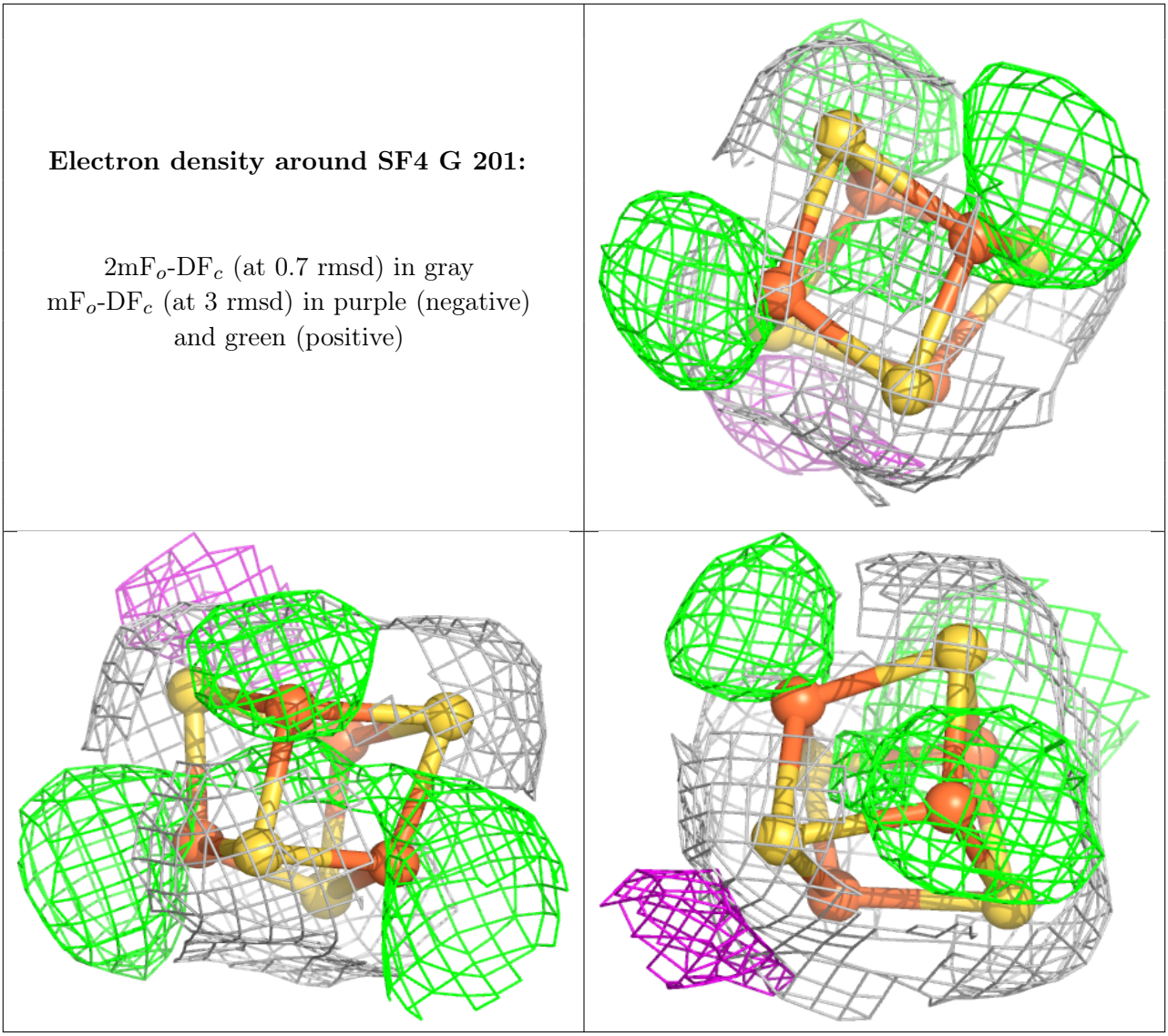






Electron density around SF4 G 201:

$2mF_o$-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.