



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:52 pm BST

PDB ID : 6UNZ
Title : Crystal structure of cytosolic fumarate hydratase from Leishmania major
Authors : Feliciano, P.R.; Drennan, C.L.
Deposited on : 2019-10-14
Resolution : 3.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

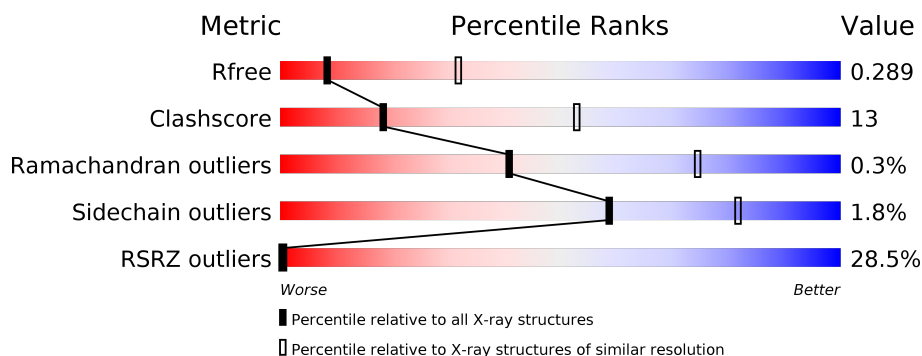
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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.



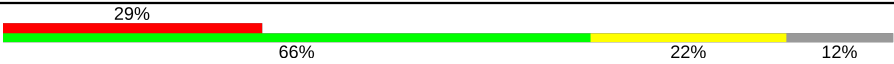

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	604	<div> <div>22%</div> <div>68%</div> <div>20%</div> <div>11%</div> </div>
1	B	604	<div> <div>20%</div> <div>67%</div> <div>21%</div> <div>12%</div> </div>
1	C	604	<div> <div>29%</div> <div>62%</div> <div>25%</div> <div>12%</div> </div>
1	D	604	<div> <div>28%</div> <div>66%</div> <div>21%</div> <div>12%</div> </div>
1	E	604	<div> <div>29%</div> <div>66%</div> <div>21%</div> <div>12%</div> </div>
1	F	604	<div> <div>20%</div> <div>64%</div> <div>24%</div> <div>12%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	604	
1	H	604	

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
2	SF4	B	601	-	-	X	-
2	SF4	C	601	-	-	X	-
2	SF4	F	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31246 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 fumarate hydratase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			3933	2469	688	758	18			
1	B	534	Total	C	N	O	S	0	0	0
			3933	2480	681	755	17			
1	C	532	Total	C	N	O	S	0	0	0
			3822	2387	678	737	20			
1	D	530	Total	C	N	O	S	0	0	0
			3874	2440	677	738	19			
1	E	531	Total	C	N	O	S	0	0	0
			3863	2429	677	736	21			
1	F	531	Total	C	N	O	S	0	1	0
			3981	2512	690	759	20			
1	G	532	Total	C	N	O	S	0	0	0
			3873	2430	684	742	17			
1	H	531	Total	C	N	O	S	0	0	0
			3888	2448	673	749	18			

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	expression tag	UNP E9AE57
A	-34	GLY	-	expression tag	UNP E9AE57
A	-33	SER	-	expression tag	UNP E9AE57
A	-32	SER	-	expression tag	UNP E9AE57
A	-31	HIS	-	expression tag	UNP E9AE57
A	-30	HIS	-	expression tag	UNP E9AE57
A	-29	HIS	-	expression tag	UNP E9AE57
A	-28	HIS	-	expression tag	UNP E9AE57
A	-27	HIS	-	expression tag	UNP E9AE57
A	-26	HIS	-	expression tag	UNP E9AE57
A	-25	SER	-	expression tag	UNP E9AE57
A	-24	SER	-	expression tag	UNP E9AE57
A	-23	GLY	-	expression tag	UNP E9AE57

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	LEU	-	expression tag	UNP E9AE57
A	-21	VAL	-	expression tag	UNP E9AE57
A	-20	PRO	-	expression tag	UNP E9AE57
A	-19	ARG	-	expression tag	UNP E9AE57
A	-18	GLY	-	expression tag	UNP E9AE57
A	-17	SER	-	expression tag	UNP E9AE57
A	-16	HIS	-	expression tag	UNP E9AE57
A	-15	MET	-	expression tag	UNP E9AE57
A	-14	ALA	-	expression tag	UNP E9AE57
A	-13	SER	-	expression tag	UNP E9AE57
A	-12	MET	-	expression tag	UNP E9AE57
A	-11	THR	-	expression tag	UNP E9AE57
A	-10	GLY	-	expression tag	UNP E9AE57
A	-9	GLY	-	expression tag	UNP E9AE57
A	-8	GLN	-	expression tag	UNP E9AE57
A	-7	GLN	-	expression tag	UNP E9AE57
A	-6	MET	-	expression tag	UNP E9AE57
A	-5	GLY	-	expression tag	UNP E9AE57
A	-4	ARG	-	expression tag	UNP E9AE57
A	-3	GLY	-	expression tag	UNP E9AE57
A	-2	SER	-	expression tag	UNP E9AE57
A	-1	GLU	-	expression tag	UNP E9AE57
A	0	PHE	-	expression tag	UNP E9AE57
B	-35	MET	-	expression tag	UNP E9AE57
B	-34	GLY	-	expression tag	UNP E9AE57
B	-33	SER	-	expression tag	UNP E9AE57
B	-32	SER	-	expression tag	UNP E9AE57
B	-31	HIS	-	expression tag	UNP E9AE57
B	-30	HIS	-	expression tag	UNP E9AE57
B	-29	HIS	-	expression tag	UNP E9AE57
B	-28	HIS	-	expression tag	UNP E9AE57
B	-27	HIS	-	expression tag	UNP E9AE57
B	-26	HIS	-	expression tag	UNP E9AE57
B	-25	SER	-	expression tag	UNP E9AE57
B	-24	SER	-	expression tag	UNP E9AE57
B	-23	GLY	-	expression tag	UNP E9AE57
B	-22	LEU	-	expression tag	UNP E9AE57
B	-21	VAL	-	expression tag	UNP E9AE57
B	-20	PRO	-	expression tag	UNP E9AE57
B	-19	ARG	-	expression tag	UNP E9AE57
B	-18	GLY	-	expression tag	UNP E9AE57
B	-17	SER	-	expression tag	UNP E9AE57

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP E9AE57
B	-15	MET	-	expression tag	UNP E9AE57
B	-14	ALA	-	expression tag	UNP E9AE57
B	-13	SER	-	expression tag	UNP E9AE57
B	-12	MET	-	expression tag	UNP E9AE57
B	-11	THR	-	expression tag	UNP E9AE57
B	-10	GLY	-	expression tag	UNP E9AE57
B	-9	GLY	-	expression tag	UNP E9AE57
B	-8	GLN	-	expression tag	UNP E9AE57
B	-7	GLN	-	expression tag	UNP E9AE57
B	-6	MET	-	expression tag	UNP E9AE57
B	-5	GLY	-	expression tag	UNP E9AE57
B	-4	ARG	-	expression tag	UNP E9AE57
B	-3	GLY	-	expression tag	UNP E9AE57
B	-2	SER	-	expression tag	UNP E9AE57
B	-1	GLU	-	expression tag	UNP E9AE57
B	0	PHE	-	expression tag	UNP E9AE57
C	-35	MET	-	expression tag	UNP E9AE57
C	-34	GLY	-	expression tag	UNP E9AE57
C	-33	SER	-	expression tag	UNP E9AE57
C	-32	SER	-	expression tag	UNP E9AE57
C	-31	HIS	-	expression tag	UNP E9AE57
C	-30	HIS	-	expression tag	UNP E9AE57
C	-29	HIS	-	expression tag	UNP E9AE57
C	-28	HIS	-	expression tag	UNP E9AE57
C	-27	HIS	-	expression tag	UNP E9AE57
C	-26	HIS	-	expression tag	UNP E9AE57
C	-25	SER	-	expression tag	UNP E9AE57
C	-24	SER	-	expression tag	UNP E9AE57
C	-23	GLY	-	expression tag	UNP E9AE57
C	-22	LEU	-	expression tag	UNP E9AE57
C	-21	VAL	-	expression tag	UNP E9AE57
C	-20	PRO	-	expression tag	UNP E9AE57
C	-19	ARG	-	expression tag	UNP E9AE57
C	-18	GLY	-	expression tag	UNP E9AE57
C	-17	SER	-	expression tag	UNP E9AE57
C	-16	HIS	-	expression tag	UNP E9AE57
C	-15	MET	-	expression tag	UNP E9AE57
C	-14	ALA	-	expression tag	UNP E9AE57
C	-13	SER	-	expression tag	UNP E9AE57
C	-12	MET	-	expression tag	UNP E9AE57
C	-11	THR	-	expression tag	UNP E9AE57

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	GLY	-	expression tag	UNP E9AE57
C	-9	GLY	-	expression tag	UNP E9AE57
C	-8	GLN	-	expression tag	UNP E9AE57
C	-7	GLN	-	expression tag	UNP E9AE57
C	-6	MET	-	expression tag	UNP E9AE57
C	-5	GLY	-	expression tag	UNP E9AE57
C	-4	ARG	-	expression tag	UNP E9AE57
C	-3	GLY	-	expression tag	UNP E9AE57
C	-2	SER	-	expression tag	UNP E9AE57
C	-1	GLU	-	expression tag	UNP E9AE57
C	0	PHE	-	expression tag	UNP E9AE57
D	-35	MET	-	expression tag	UNP E9AE57
D	-34	GLY	-	expression tag	UNP E9AE57
D	-33	SER	-	expression tag	UNP E9AE57
D	-32	SER	-	expression tag	UNP E9AE57
D	-31	HIS	-	expression tag	UNP E9AE57
D	-30	HIS	-	expression tag	UNP E9AE57
D	-29	HIS	-	expression tag	UNP E9AE57
D	-28	HIS	-	expression tag	UNP E9AE57
D	-27	HIS	-	expression tag	UNP E9AE57
D	-26	HIS	-	expression tag	UNP E9AE57
D	-25	SER	-	expression tag	UNP E9AE57
D	-24	SER	-	expression tag	UNP E9AE57
D	-23	GLY	-	expression tag	UNP E9AE57
D	-22	LEU	-	expression tag	UNP E9AE57
D	-21	VAL	-	expression tag	UNP E9AE57
D	-20	PRO	-	expression tag	UNP E9AE57
D	-19	ARG	-	expression tag	UNP E9AE57
D	-18	GLY	-	expression tag	UNP E9AE57
D	-17	SER	-	expression tag	UNP E9AE57
D	-16	HIS	-	expression tag	UNP E9AE57
D	-15	MET	-	expression tag	UNP E9AE57
D	-14	ALA	-	expression tag	UNP E9AE57
D	-13	SER	-	expression tag	UNP E9AE57
D	-12	MET	-	expression tag	UNP E9AE57
D	-11	THR	-	expression tag	UNP E9AE57
D	-10	GLY	-	expression tag	UNP E9AE57
D	-9	GLY	-	expression tag	UNP E9AE57
D	-8	GLN	-	expression tag	UNP E9AE57
D	-7	GLN	-	expression tag	UNP E9AE57
D	-6	MET	-	expression tag	UNP E9AE57
D	-5	GLY	-	expression tag	UNP E9AE57

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	ARG	-	expression tag	UNP E9AE57
D	-3	GLY	-	expression tag	UNP E9AE57
D	-2	SER	-	expression tag	UNP E9AE57
D	-1	GLU	-	expression tag	UNP E9AE57
D	0	PHE	-	expression tag	UNP E9AE57
E	-35	MET	-	expression tag	UNP E9AE57
E	-34	GLY	-	expression tag	UNP E9AE57
E	-33	SER	-	expression tag	UNP E9AE57
E	-32	SER	-	expression tag	UNP E9AE57
E	-31	HIS	-	expression tag	UNP E9AE57
E	-30	HIS	-	expression tag	UNP E9AE57
E	-29	HIS	-	expression tag	UNP E9AE57
E	-28	HIS	-	expression tag	UNP E9AE57
E	-27	HIS	-	expression tag	UNP E9AE57
E	-26	HIS	-	expression tag	UNP E9AE57
E	-25	SER	-	expression tag	UNP E9AE57
E	-24	SER	-	expression tag	UNP E9AE57
E	-23	GLY	-	expression tag	UNP E9AE57
E	-22	LEU	-	expression tag	UNP E9AE57
E	-21	VAL	-	expression tag	UNP E9AE57
E	-20	PRO	-	expression tag	UNP E9AE57
E	-19	ARG	-	expression tag	UNP E9AE57
E	-18	GLY	-	expression tag	UNP E9AE57
E	-17	SER	-	expression tag	UNP E9AE57
E	-16	HIS	-	expression tag	UNP E9AE57
E	-15	MET	-	expression tag	UNP E9AE57
E	-14	ALA	-	expression tag	UNP E9AE57
E	-13	SER	-	expression tag	UNP E9AE57
E	-12	MET	-	expression tag	UNP E9AE57
E	-11	THR	-	expression tag	UNP E9AE57
E	-10	GLY	-	expression tag	UNP E9AE57
E	-9	GLY	-	expression tag	UNP E9AE57
E	-8	GLN	-	expression tag	UNP E9AE57
E	-7	GLN	-	expression tag	UNP E9AE57
E	-6	MET	-	expression tag	UNP E9AE57
E	-5	GLY	-	expression tag	UNP E9AE57
E	-4	ARG	-	expression tag	UNP E9AE57
E	-3	GLY	-	expression tag	UNP E9AE57
E	-2	SER	-	expression tag	UNP E9AE57
E	-1	GLU	-	expression tag	UNP E9AE57
E	0	PHE	-	expression tag	UNP E9AE57
F	-35	MET	-	expression tag	UNP E9AE57

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-34	GLY	-	expression tag	UNP E9AE57
F	-33	SER	-	expression tag	UNP E9AE57
F	-32	SER	-	expression tag	UNP E9AE57
F	-31	HIS	-	expression tag	UNP E9AE57
F	-30	HIS	-	expression tag	UNP E9AE57
F	-29	HIS	-	expression tag	UNP E9AE57
F	-28	HIS	-	expression tag	UNP E9AE57
F	-27	HIS	-	expression tag	UNP E9AE57
F	-26	HIS	-	expression tag	UNP E9AE57
F	-25	SER	-	expression tag	UNP E9AE57
F	-24	SER	-	expression tag	UNP E9AE57
F	-23	GLY	-	expression tag	UNP E9AE57
F	-22	LEU	-	expression tag	UNP E9AE57
F	-21	VAL	-	expression tag	UNP E9AE57
F	-20	PRO	-	expression tag	UNP E9AE57
F	-19	ARG	-	expression tag	UNP E9AE57
F	-18	GLY	-	expression tag	UNP E9AE57
F	-17	SER	-	expression tag	UNP E9AE57
F	-16	HIS	-	expression tag	UNP E9AE57
F	-15	MET	-	expression tag	UNP E9AE57
F	-14	ALA	-	expression tag	UNP E9AE57
F	-13	SER	-	expression tag	UNP E9AE57
F	-12	MET	-	expression tag	UNP E9AE57
F	-11	THR	-	expression tag	UNP E9AE57
F	-10	GLY	-	expression tag	UNP E9AE57
F	-9	GLY	-	expression tag	UNP E9AE57
F	-8	GLN	-	expression tag	UNP E9AE57
F	-7	GLN	-	expression tag	UNP E9AE57
F	-6	MET	-	expression tag	UNP E9AE57
F	-5	GLY	-	expression tag	UNP E9AE57
F	-4	ARG	-	expression tag	UNP E9AE57
F	-3	GLY	-	expression tag	UNP E9AE57
F	-2	SER	-	expression tag	UNP E9AE57
F	-1	GLU	-	expression tag	UNP E9AE57
F	0	PHE	-	expression tag	UNP E9AE57
G	-35	MET	-	expression tag	UNP E9AE57
G	-34	GLY	-	expression tag	UNP E9AE57
G	-33	SER	-	expression tag	UNP E9AE57
G	-32	SER	-	expression tag	UNP E9AE57
G	-31	HIS	-	expression tag	UNP E9AE57
G	-30	HIS	-	expression tag	UNP E9AE57
G	-29	HIS	-	expression tag	UNP E9AE57

Continued on next page...

Continued from previous page...

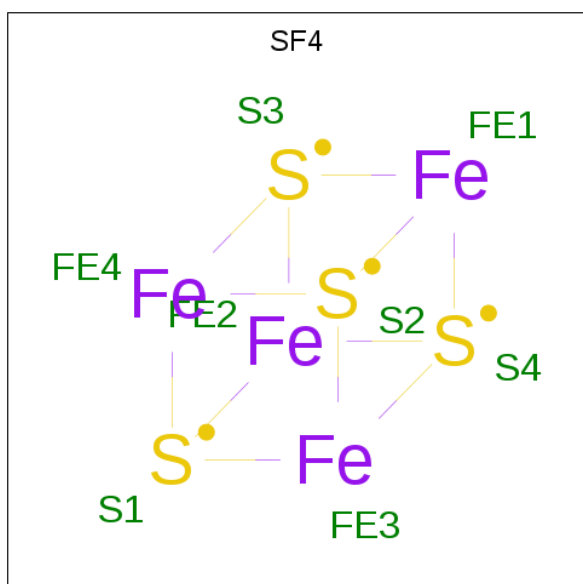
Chain	Residue	Modelled	Actual	Comment	Reference
G	-28	HIS	-	expression tag	UNP E9AE57
G	-27	HIS	-	expression tag	UNP E9AE57
G	-26	HIS	-	expression tag	UNP E9AE57
G	-25	SER	-	expression tag	UNP E9AE57
G	-24	SER	-	expression tag	UNP E9AE57
G	-23	GLY	-	expression tag	UNP E9AE57
G	-22	LEU	-	expression tag	UNP E9AE57
G	-21	VAL	-	expression tag	UNP E9AE57
G	-20	PRO	-	expression tag	UNP E9AE57
G	-19	ARG	-	expression tag	UNP E9AE57
G	-18	GLY	-	expression tag	UNP E9AE57
G	-17	SER	-	expression tag	UNP E9AE57
G	-16	HIS	-	expression tag	UNP E9AE57
G	-15	MET	-	expression tag	UNP E9AE57
G	-14	ALA	-	expression tag	UNP E9AE57
G	-13	SER	-	expression tag	UNP E9AE57
G	-12	MET	-	expression tag	UNP E9AE57
G	-11	THR	-	expression tag	UNP E9AE57
G	-10	GLY	-	expression tag	UNP E9AE57
G	-9	GLY	-	expression tag	UNP E9AE57
G	-8	GLN	-	expression tag	UNP E9AE57
G	-7	GLN	-	expression tag	UNP E9AE57
G	-6	MET	-	expression tag	UNP E9AE57
G	-5	GLY	-	expression tag	UNP E9AE57
G	-4	ARG	-	expression tag	UNP E9AE57
G	-3	GLY	-	expression tag	UNP E9AE57
G	-2	SER	-	expression tag	UNP E9AE57
G	-1	GLU	-	expression tag	UNP E9AE57
G	0	PHE	-	expression tag	UNP E9AE57
H	-35	MET	-	expression tag	UNP E9AE57
H	-34	GLY	-	expression tag	UNP E9AE57
H	-33	SER	-	expression tag	UNP E9AE57
H	-32	SER	-	expression tag	UNP E9AE57
H	-31	HIS	-	expression tag	UNP E9AE57
H	-30	HIS	-	expression tag	UNP E9AE57
H	-29	HIS	-	expression tag	UNP E9AE57
H	-28	HIS	-	expression tag	UNP E9AE57
H	-27	HIS	-	expression tag	UNP E9AE57
H	-26	HIS	-	expression tag	UNP E9AE57
H	-25	SER	-	expression tag	UNP E9AE57
H	-24	SER	-	expression tag	UNP E9AE57
H	-23	GLY	-	expression tag	UNP E9AE57

Continued on next page...

Continued from previous page...

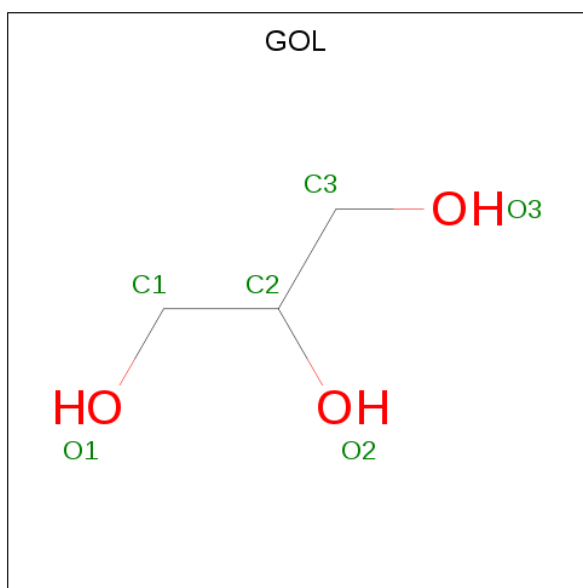
Chain	Residue	Modelled	Actual	Comment	Reference
H	-22	LEU	-	expression tag	UNP E9AE57
H	-21	VAL	-	expression tag	UNP E9AE57
H	-20	PRO	-	expression tag	UNP E9AE57
H	-19	ARG	-	expression tag	UNP E9AE57
H	-18	GLY	-	expression tag	UNP E9AE57
H	-17	SER	-	expression tag	UNP E9AE57
H	-16	HIS	-	expression tag	UNP E9AE57
H	-15	MET	-	expression tag	UNP E9AE57
H	-14	ALA	-	expression tag	UNP E9AE57
H	-13	SER	-	expression tag	UNP E9AE57
H	-12	MET	-	expression tag	UNP E9AE57
H	-11	THR	-	expression tag	UNP E9AE57
H	-10	GLY	-	expression tag	UNP E9AE57
H	-9	GLY	-	expression tag	UNP E9AE57
H	-8	GLN	-	expression tag	UNP E9AE57
H	-7	GLN	-	expression tag	UNP E9AE57
H	-6	MET	-	expression tag	UNP E9AE57
H	-5	GLY	-	expression tag	UNP E9AE57
H	-4	ARG	-	expression tag	UNP E9AE57
H	-3	GLY	-	expression tag	UNP E9AE57
H	-2	SER	-	expression tag	UNP E9AE57
H	-1	GLU	-	expression tag	UNP E9AE57
H	0	PHE	-	expression tag	UNP E9AE57

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	E	1	Total	Fe	S	0	0
			8	4	4		
2	F	1	Total	Fe	S	0	0
			8	4	4		
2	G	1	Total	Fe	S	0	0
			8	4	4		
2	H	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		

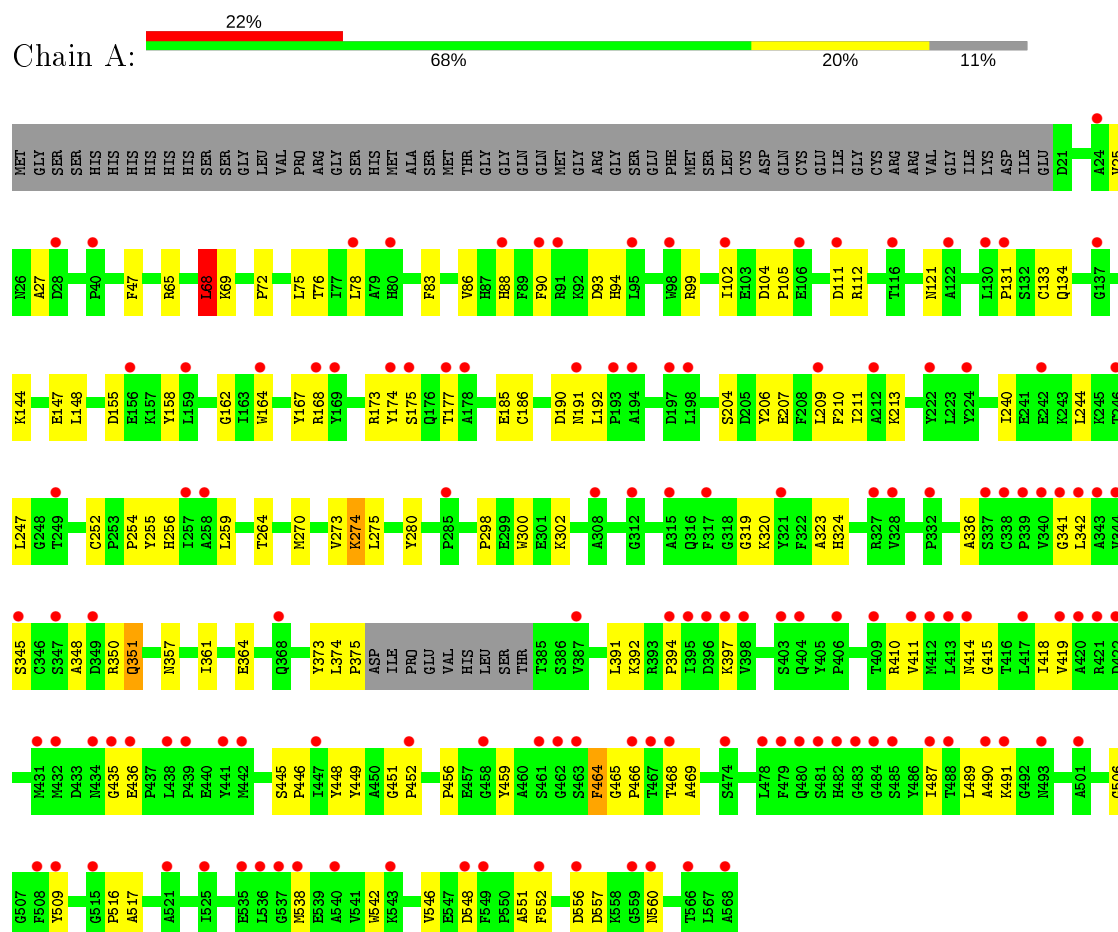
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	O 1	0	0
4	D	1	Total 1	O 1	0	0
4	F	1	Total 1	O 1	0	0

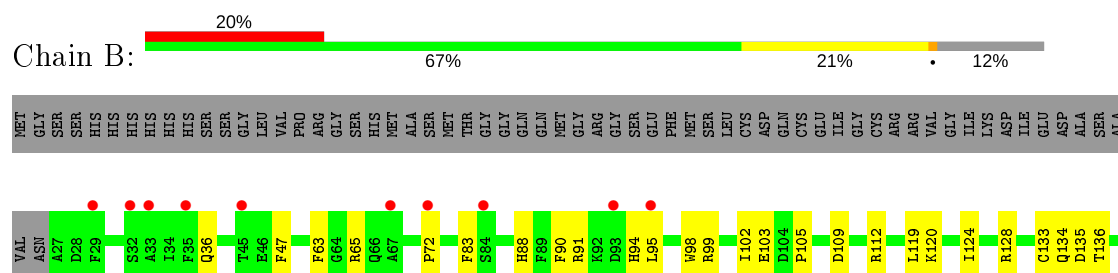
3 Residue-property plots

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

- Molecule 1: fumarate hydratase 2



- Molecule 1: fumarate hydratase 2



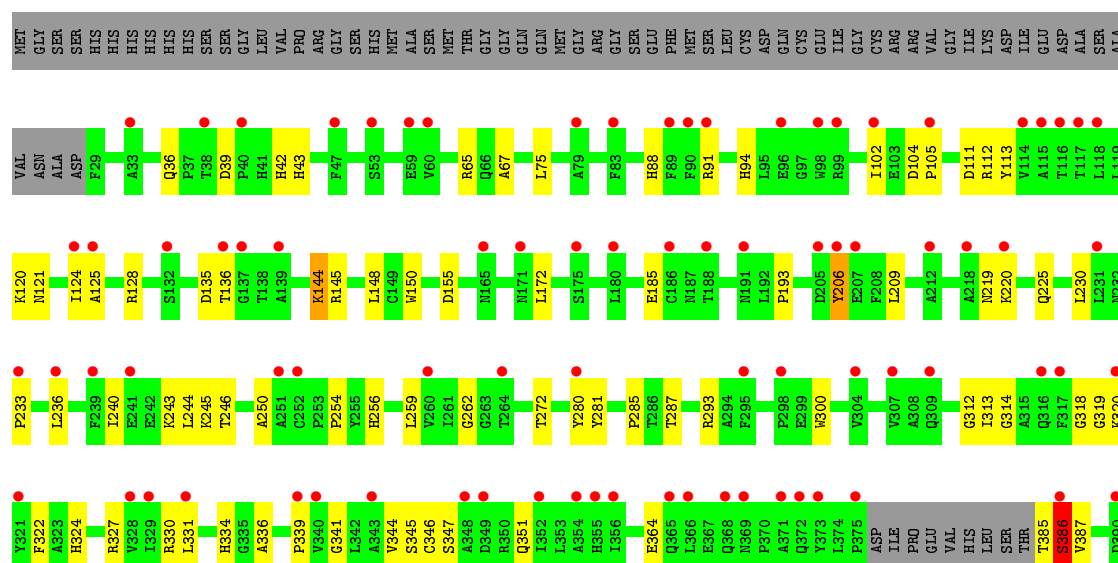


Chain D: 

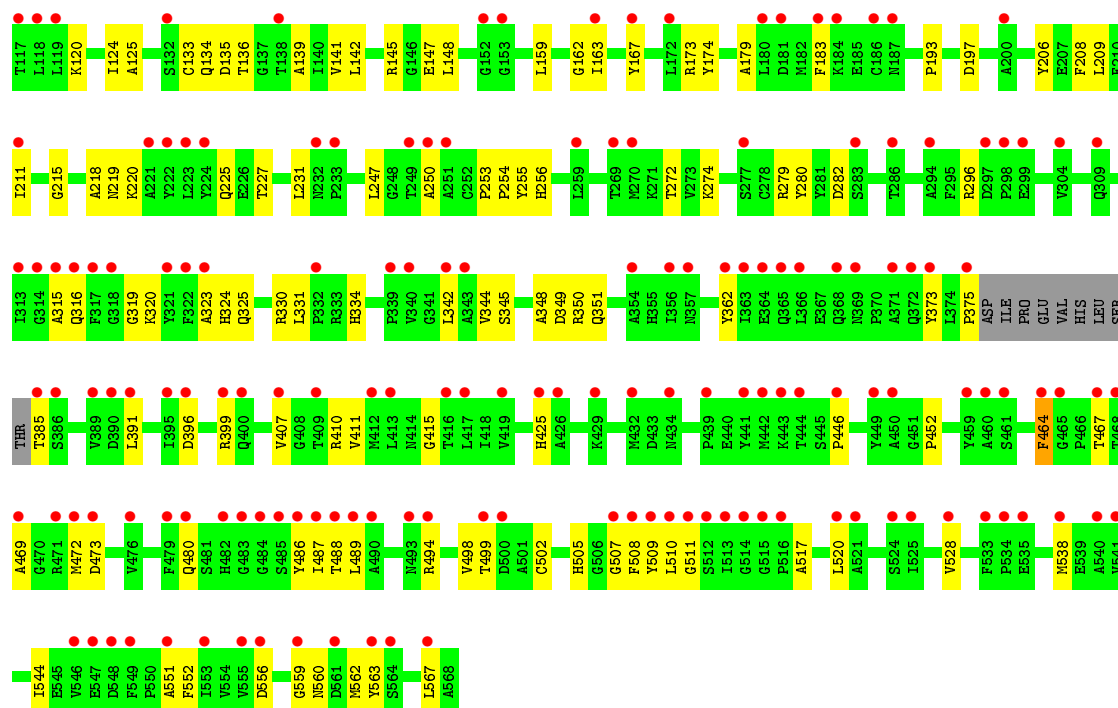


• Molecule 1: fumarate hydratase 2

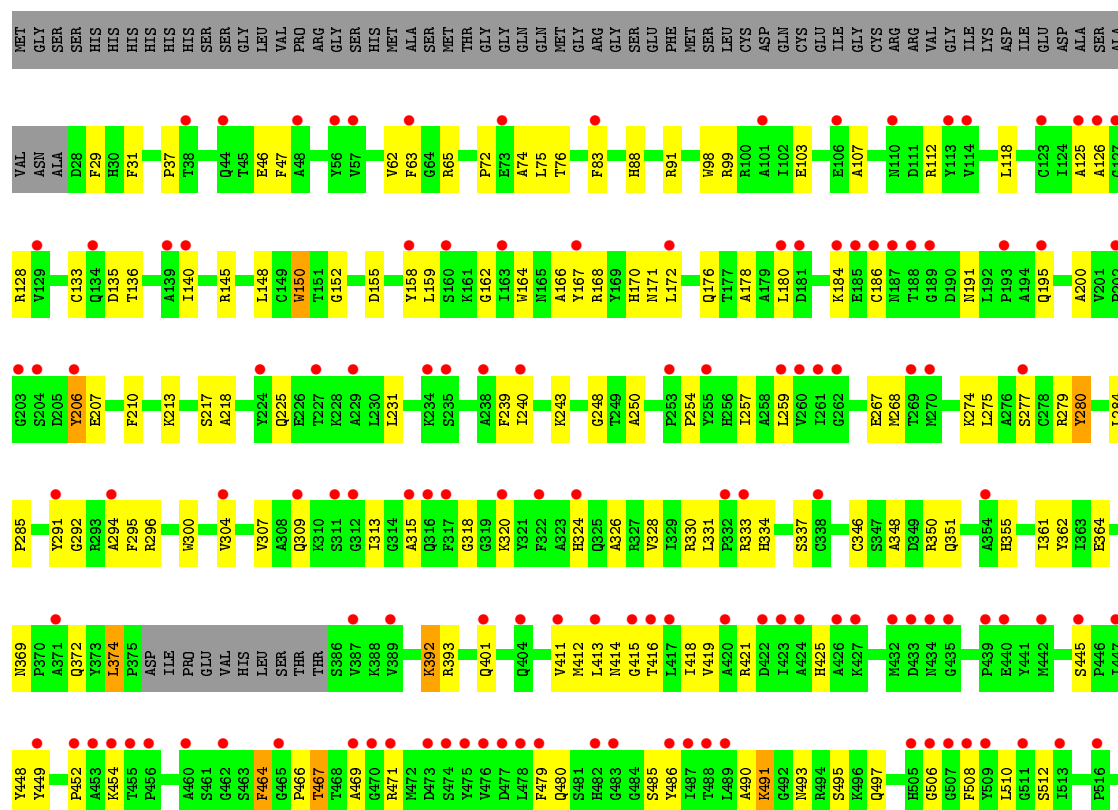
Chain E: 

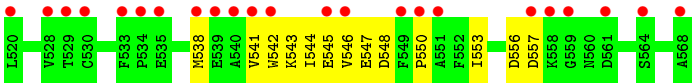






• Molecule 1: fumarate hydratase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	159.09Å 66.07Å 238.09Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	49.71 – 3.19 49.71 – 3.19	Depositor EDS
% Data completeness (in resolution range)	90.2 (49.71-3.19) 90.2 (49.71-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	714.55 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.245 , 0.289 0.246 , 0.289	Depositor DCC
R_{free} test set	3752 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.398 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
Outliers	0 of 75107 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	31246	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.36	0/4024	0.67	1/5476 (0.0%)
1	B	0.39	0/4029	0.69	0/5489
1	C	0.34	0/3911	0.64	0/5329
1	D	0.35	0/3966	0.62	0/5399
1	E	0.36	0/3952	0.63	0/5380
1	F	0.36	0/4076	0.62	0/5542
1	G	0.36	0/3965	0.65	0/5401
1	H	0.38	1/3984 (0.0%)	0.65	0/5432
All	All	0.36	1/31907 (0.0%)	0.65	1/43448 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	150	TRP	CB-CG	-5.38	1.40	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	LEU	CA-CB-CG	5.32	127.53	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3933	0	3563	90	0
1	B	3933	0	3571	97	0
1	C	3822	0	3400	123	0
1	D	3874	0	3531	91	0
1	E	3863	0	3537	102	0
1	F	3981	0	3721	115	0
1	G	3873	0	3489	107	0
1	H	3888	0	3506	124	0
2	A	8	0	0	1	0
2	B	8	0	0	2	0
2	C	8	0	0	5	0
2	D	8	0	0	0	0
2	E	8	0	0	1	0
2	F	8	0	0	3	0
2	G	8	0	0	0	0
2	H	8	0	0	0	0
3	B	6	0	8	2	0
3	E	6	0	8	1	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
All	All	31246	0	28334	792	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (792) 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:G:494:ARG:HD2	1:G:509:TYR:CD1	2.00	0.96
1:B:421:ARG:HH11	1:B:451:GLY:HA3	1.32	0.95
1:G:494:ARG:HD2	1:G:509:TYR:CE1	2.07	0.89
1:E:399:ARG:HD2	1:E:506:GLY:O	1.73	0.89
1:C:134:GLN:NE2	2:C:601:SF4:S4	2.48	0.87
1:F:72:PRO:HB2	1:F:158:TYR:HD2	1.42	0.85
1:D:102:ILE:HA	1:D:112:ARG:HG2	1.58	0.83
1:F:217:SER:HB3	1:F:346:CYS:HB3	1.61	0.83
1:B:65:ARG:HE	1:B:148:LEU:HD11	1.42	0.82
1:C:473:ASP:HA	1:C:494:ARG:HH21	1.45	0.81
1:B:136:THR:HG21	1:B:172:LEU:HB3	1.61	0.80
1:H:72:PRO:HB2	1:H:158:TYR:HD2	1.46	0.80
1:F:532:ALA:HB3	1:F:541:VAL:HB	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:418:ILE:HG12	1:F:445:SER:HB2	1.65	0.77
1:B:506:GLY:HA2	1:B:557:ASP:HB2	1.66	0.77
1:A:336:ALA:HB2	3:B:602:GOL:H31	1.67	0.76
1:E:399:ARG:CD	1:E:506:GLY:O	2.33	0.76
1:C:245:LYS:HD2	1:C:567:LEU:HA	1.68	0.76
1:E:136:THR:HG21	1:E:172:LEU:HB3	1.67	0.75
1:A:104:ASP:O	1:A:112:ARG:NH2	2.20	0.75
1:G:219:ASN:HD21	1:H:337:SER:HA	1.51	0.75
1:G:93:ASP:OD2	1:G:279:ARG:NE	2.20	0.75
1:C:140:ILE:HA	1:C:195:GLN:HB3	1.69	0.74
1:H:88:HIS:ND1	1:H:125:ALA:O	2.19	0.74
1:H:275:LEU:HD22	1:H:280:TYR:HD2	1.53	0.74
1:B:148:LEU:HB2	1:B:204:SER:HB3	1.70	0.74
1:A:72:PRO:HB2	1:A:158:TYR:HD2	1.53	0.74
1:B:102:ILE:O	1:B:112:ARG:NH2	2.22	0.73
1:D:358:LYS:H	1:D:358:LYS:HD3	1.52	0.73
1:B:393:ARG:NH2	1:B:401:GLN:OE1	2.21	0.72
1:F:109:ASP:OD1	1:F:112:ARG:NH1	2.22	0.72
1:A:469:ALA:HB2	1:A:490:ALA:HB3	1.71	0.72
1:G:282:ASP:O	1:G:296:ARG:NH1	2.23	0.72
1:A:336:ALA:O	1:B:219:ASN:ND2	2.23	0.72
1:F:143:GLY:O	1:F:199:LEU:N	2.20	0.72
1:H:72:PRO:HB2	1:H:158:TYR:CD2	2.24	0.72
1:D:138:THR:N	1:D:213:LYS:O	2.20	0.71
1:D:49:LYS:NZ	1:D:359:SER:O	2.22	0.71
1:E:102:ILE:O	1:E:112:ARG:NH1	2.24	0.71
1:C:47:PHE:HA	1:C:364:GLU:HA	1.72	0.70
1:F:62:VAL:HG11	1:F:150:TRP:HH2	1.55	0.70
1:D:399:ARG:NH2	1:D:506:GLY:O	2.23	0.70
1:D:330:ARG:NH1	1:D:331:LEU:O	2.23	0.70
1:B:213:LYS:NZ	1:B:344:VAL:O	2.25	0.70
1:B:489:LEU:HA	1:B:510:LEU:O	1.92	0.69
1:D:473:ASP:OD1	1:D:494:ARG:NH2	2.26	0.69
1:G:494:ARG:HH11	1:G:509:TYR:HD1	1.40	0.69
1:B:99:ARG:HG3	1:B:375:PRO:HG3	1.74	0.69
1:H:425:HIS:HD2	1:H:479:PHE:HE2	1.41	0.69
1:D:136:THR:HG21	1:D:172:LEU:HB3	1.74	0.69
1:E:395:ILE:O	1:E:397:LYS:N	2.21	0.69
1:B:173:ARG:NH2	3:B:602:GOL:O3	2.26	0.69
1:F:72:PRO:HB2	1:F:158:TYR:CD2	2.28	0.69
1:H:330:ARG:NH1	1:H:331:LEU:O	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:LEU:N	1:D:203:GLY:O	2.24	0.68
1:A:435:GLY:O	1:A:436:GLU:HG3	1.93	0.68
1:H:107:ALA:O	1:H:112:ARG:NH2	2.27	0.68
1:D:422:ASP:OD2	1:D:471:ARG:NH1	2.26	0.68
1:F:467:THR:OG1	1:F:471:ARG:NH1	2.27	0.68
1:C:48:ALA:N	1:C:363:ILE:O	2.18	0.67
1:E:65:ARG:HH22	1:F:152:GLY:HA2	1.60	0.67
1:A:252:CYS:SG	1:A:491:LYS:NZ	2.63	0.67
1:C:164:TRP:HB2	1:C:192:LEU:HD11	1.77	0.66
1:G:134:GLN:OE1	1:G:173:ARG:NH1	2.29	0.66
1:G:135:ASP:OD1	1:H:334:HIS:NE2	2.27	0.66
1:B:428:ILE:HG12	1:B:439:PRO:HG2	1.77	0.66
1:A:134:GLN:NE2	2:A:601:SF4:S1	2.68	0.66
1:A:72:PRO:HB2	1:A:158:TYR:CD2	2.30	0.66
1:E:421:ARG:HG3	1:E:539:GLU:HG2	1.77	0.66
1:A:167:TYR:HB3	1:A:174:TYR:HE1	1.59	0.65
1:B:253:PRO:HG3	1:B:255:TYR:CZ	2.31	0.65
1:E:135:ASP:OD1	1:F:334:HIS:NE2	2.27	0.65
1:F:134:GLN:NE2	2:F:601:SF4:S2	2.68	0.65
1:E:287:THR:OG1	1:E:293:ARG:NH2	2.30	0.65
1:A:133:CYS:HB3	1:A:350:ARG:HH22	1.62	0.65
1:G:88:HIS:ND1	1:G:125:ALA:O	2.30	0.64
1:G:247:LEU:HD11	1:G:342:LEU:HD21	1.77	0.64
1:H:178:ALA:N	1:H:186:CYS:O	2.28	0.64
1:H:217:SER:HB3	1:H:346:CYS:HB3	1.79	0.64
1:F:97:GLY:HA3	1:F:324:HIS:HD2	1.63	0.64
1:A:175:SER:N	1:A:191:ASN:OD1	2.24	0.64
1:D:407:VAL:HB	1:D:562:MET:HB3	1.79	0.64
1:A:336:ALA:HB3	1:B:215:GLY:HA3	1.80	0.64
1:E:494:ARG:HD3	1:E:498:VAL:HG11	1.80	0.64
1:C:425:HIS:HB3	1:C:475:TYR:CD1	2.33	0.64
1:D:147:GLU:N	1:D:201:VAL:O	2.31	0.64
1:A:102:ILE:HA	1:A:112:ARG:HG2	1.80	0.64
1:C:270:MET:HA	1:C:273:VAL:HG12	1.79	0.64
1:G:111:ASP:OD2	1:G:320:LYS:N	2.21	0.63
1:D:213:LYS:NZ	1:D:344:VAL:O	2.31	0.63
1:F:333:ARG:NH1	1:F:337:SER:O	2.29	0.63
1:A:254:PRO:HB2	1:A:324:HIS:CD2	2.33	0.63
1:A:65:ARG:NH1	1:A:147:GLU:OE2	2.32	0.63
1:C:330:ARG:NH1	1:C:331:LEU:O	2.31	0.63
1:F:142:LEU:HD11	1:F:199:LEU:HD11	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:511:GLY:N	1:G:552:PHE:O	2.31	0.63
1:H:277:SER:O	1:H:279:ARG:NH1	2.31	0.63
1:C:111:ASP:HA	1:C:315:ALA:HB3	1.81	0.62
1:D:75:LEU:HB2	1:D:158:TYR:HB3	1.82	0.62
1:F:413:LEU:O	1:F:548:ASP:N	2.32	0.62
1:G:469:ALA:CB	1:G:509:TYR:CE1	2.81	0.62
1:A:394:PRO:HD2	1:A:397:LYS:HD2	1.81	0.62
1:C:287:THR:OG1	1:C:293:ARG:NH2	2.31	0.62
1:B:386:SER:OG	1:B:410:ARG:NH2	2.32	0.62
1:B:529:THR:O	1:B:543:LYS:N	2.22	0.62
1:E:422:ASP:OD2	1:E:471:ARG:NH1	2.31	0.62
1:E:150:TRP:HB3	1:F:65:ARG:HH12	1.64	0.62
1:G:486:TYR:O	1:G:508:PHE:N	2.32	0.62
1:A:164:TRP:HB2	1:A:192:LEU:HD11	1.81	0.62
1:F:473:ASP:OD1	1:F:494:ARG:NE	2.31	0.62
1:F:449:TYR:HB2	1:F:490:ALA:HB2	1.81	0.61
1:H:418:ILE:HG12	1:H:445:SER:HB2	1.81	0.61
1:G:256:HIS:O	1:G:344:VAL:HA	1.99	0.61
1:H:480:GLN:NE2	1:H:485:SER:O	2.32	0.61
1:A:144:LYS:HE3	1:A:207:GLU:HB2	1.82	0.61
1:H:171:ASN:HA	1:H:454:LYS:HB2	1.80	0.61
1:A:456:PRO:HB2	1:A:459:TYR:CD2	2.35	0.61
1:E:385:THR:O	1:E:387:VAL:N	2.33	0.61
1:F:245:LYS:HZ1	1:F:568:ALA:N	1.99	0.61
1:D:411:VAL:N	1:D:551:ALA:O	2.28	0.61
1:E:488:THR:OG1	1:E:494:ARG:NH1	2.34	0.61
1:A:174:TYR:HD1	1:A:191:ASN:HB2	1.65	0.60
1:A:391:LEU:N	1:A:414:ASN:O	2.22	0.60
1:C:74:ALA:HB1	1:C:361:ILE:HD11	1.83	0.60
1:E:422:ASP:HB3	1:F:228:LYS:HB3	1.81	0.60
1:F:173:ARG:HD2	1:F:538:MET:HB3	1.83	0.60
1:D:490:ALA:O	1:D:512:SER:N	2.34	0.60
1:G:399:ARG:HD2	1:G:486:TYR:HB3	1.83	0.60
1:G:274:LYS:NZ	1:H:267:GLU:OE2	2.34	0.60
1:D:282:ASP:O	1:D:296:ARG:NH1	2.27	0.60
1:H:415:GLY:N	1:H:546:VAL:O	2.28	0.60
1:C:425:HIS:HB3	1:C:475:TYR:CE1	2.37	0.60
1:C:193:PRO:HB2	1:D:34:ILE:HD11	1.83	0.60
1:G:114:VAL:HG21	1:G:315:ALA:O	2.01	0.60
1:H:254:PRO:HG3	1:H:315:ALA:HB1	1.82	0.60
1:D:137:GLY:HA2	1:D:214:GLY:HA2	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:257:ILE:O	1:H:326:ALA:HA	2.02	0.59
1:C:87:HIS:O	1:C:132:SER:N	2.26	0.59
1:F:148:LEU:HB2	1:F:204:SER:HB3	1.84	0.59
1:H:449:TYR:HB3	1:H:467:THR:HG22	1.84	0.59
1:H:176:GLN:HG2	1:H:191:ASN:HA	1.85	0.59
1:D:419:VAL:HB	1:D:542:TRP:HB2	1.83	0.59
1:F:100:ARG:HG2	1:F:321:TYR:OH	2.03	0.59
1:G:396:ASP:HA	1:G:399:ARG:HD3	1.83	0.59
1:F:134:GLN:HB3	1:F:465:GLY:H	1.67	0.59
1:C:72:PRO:HB2	1:C:158:TYR:HD2	1.68	0.59
1:C:136:THR:HG21	1:C:172:LEU:HB3	1.85	0.59
1:D:91:ARG:HD2	1:D:279:ARG:HH21	1.68	0.58
1:G:256:HIS:CD2	1:G:345:SER:HB3	2.38	0.58
1:H:416:THR:HG21	1:H:543:LYS:HE2	1.84	0.58
1:E:135:ASP:HB2	3:E:602:GOL:H2	1.84	0.58
1:F:254:PRO:HB2	1:F:324:HIS:CE1	2.38	0.58
1:B:483:GLY:HA2	1:B:486:TYR:OH	2.03	0.58
1:E:336:ALA:O	1:F:219:ASN:ND2	2.28	0.58
1:H:506:GLY:HA2	1:H:557:ASP:HB2	1.86	0.58
1:E:220:LYS:HE2	1:E:250:ALA:HB3	1.85	0.58
1:C:248:GLY:HA3	1:C:493:ASN:HD21	1.68	0.58
1:E:104:ASP:O	1:E:112:ARG:NH2	2.36	0.57
1:E:393:ARG:NH2	1:E:401:GLN:OE1	2.37	0.57
1:C:388:LYS:HA	1:C:412:MET:HB2	1.85	0.57
1:A:452:PRO:HB3	1:A:464:PHE:CD2	2.40	0.57
1:G:488:THR:O	1:G:510:LEU:N	2.31	0.57
1:B:438:LEU:HD21	1:B:482:HIS:O	2.05	0.57
1:E:245:LYS:NZ	1:E:568:ALA:HB2	2.20	0.57
1:G:254:PRO:HB2	1:G:324:HIS:CE1	2.40	0.57
1:D:253:PRO:HD2	1:D:316:GLN:HG2	1.85	0.57
1:E:67:ALA:HA	1:E:148:LEU:HB3	1.87	0.57
1:F:490:ALA:O	1:F:512:SER:N	2.37	0.57
1:G:480:GLN:NE2	1:G:507:GLY:HA3	2.19	0.57
1:D:506:GLY:HA2	1:D:557:ASP:HB2	1.85	0.56
1:C:449:TYR:HB2	1:C:490:ALA:HB2	1.88	0.56
1:F:135[B]:ASP:O	1:F:350:ARG:NH1	2.34	0.56
1:B:358:LYS:H	1:B:358:LYS:HD3	1.70	0.56
1:C:119:LEU:HB3	1:C:374:LEU:HD22	1.87	0.56
1:F:87:HIS:HE1	1:F:136:THR:HB	1.71	0.56
1:G:134:GLN:HB3	1:G:517:ALA:HB1	1.86	0.56
1:H:88:HIS:CE1	1:H:128:ARG:HA	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:TYR:O	1:B:454:LYS:NZ	2.31	0.56
1:C:452:PRO:HB3	1:C:464:PHE:CG	2.39	0.56
1:F:135[A]:ASP:O	1:F:350:ARG:NH1	2.34	0.56
1:G:111:ASP:OD1	1:G:319:GLY:HA3	2.06	0.56
1:G:145:ARG:CZ	1:H:200:ALA:HB1	2.35	0.56
1:H:83:PHE:HE1	1:H:210:PHE:HB3	1.69	0.56
1:E:185:GLU:OE2	1:F:330:ARG:NH2	2.39	0.56
1:C:251:ALA:HA	2:C:601:SF4:S1	2.45	0.56
1:F:155:ASP:OD1	1:F:155:ASP:N	2.38	0.56
1:H:369:ASN:O	1:H:372:GLN:HG2	2.06	0.56
1:B:253:PRO:HD2	1:B:316:GLN:HG2	1.86	0.56
1:D:49:LYS:NZ	1:D:54:GLU:OE1	2.37	0.56
1:D:503:LYS:HD2	1:D:559:GLY:HA3	1.88	0.56
1:E:120:LYS:O	1:E:124:ILE:HG12	2.06	0.56
1:G:385:THR:O	1:G:410:ARG:NH1	2.39	0.56
1:G:399:ARG:HD2	1:G:486:TYR:CB	2.36	0.56
1:A:213:LYS:HE3	1:A:274:LYS:HD2	1.87	0.55
1:B:144:LYS:HE3	1:B:207:GLU:HB2	1.87	0.55
1:A:490:ALA:H	1:A:509:TYR:HE1	1.54	0.55
1:B:120:LYS:O	1:B:124:ILE:HG12	2.06	0.55
1:C:147:GLU:HA	1:D:145:ARG:NH2	2.21	0.55
1:D:54:GLU:HB3	1:D:359:SER:O	2.06	0.55
1:B:413:LEU:HB2	1:B:549:PHE:HB3	1.88	0.55
1:C:178:ALA:N	1:C:186:CYS:O	2.37	0.55
1:A:134:GLN:HB3	1:A:465:GLY:H	1.72	0.55
1:C:213:LYS:HE2	1:C:274:LYS:HE2	1.88	0.55
1:E:397:LYS:O	1:E:401:GLN:HG3	2.06	0.55
1:G:142:LEU:O	1:G:208:PHE:HA	2.06	0.55
1:B:314:GLY:O	1:B:322:PHE:HD1	1.89	0.55
1:C:134:GLN:HB3	1:C:465:GLY:H	1.71	0.55
1:C:97:GLY:HA3	1:C:324:HIS:ND1	2.21	0.55
1:D:528:VAL:HG22	1:D:544:ILE:HG22	1.87	0.55
1:B:428:ILE:HG12	1:B:439:PRO:CG	2.37	0.55
1:F:177:THR:HG22	1:F:185:GLU:HB3	1.89	0.55
1:C:453:ALA:N	1:C:463:SER:O	2.33	0.55
1:G:33:ALA:O	1:G:36:GLN:NE2	2.28	0.55
1:D:62:VAL:HG22	1:D:63:PHE:CD2	2.43	0.55
1:C:135:ASP:O	1:C:350:ARG:NH2	2.36	0.54
1:E:475:TYR:HB3	1:E:479:PHE:CE2	2.43	0.54
1:G:253:PRO:HG3	1:G:255:TYR:CZ	2.41	0.54
1:A:411:VAL:N	1:A:551:ALA:O	2.31	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:SER:HB3	1:C:346:CYS:HB3	1.89	0.54
1:C:521:ALA:HA	1:C:525:ILE:HB	1.90	0.54
1:E:272:THR:HG23	1:E:281:TYR:HE2	1.72	0.54
1:H:508:PHE:HD1	1:H:556:ASP:HA	1.72	0.54
1:H:62:VAL:HG22	1:H:63:PHE:CD2	2.43	0.54
1:B:252:CYS:HB2	2:B:601:SF4:S2	2.48	0.54
1:D:120:LYS:O	1:D:124:ILE:HG12	2.07	0.54
1:C:149:CYS:SG	1:C:206:TYR:HB2	2.47	0.54
1:E:65:ARG:NH2	1:F:152:GLY:HA2	2.23	0.54
1:E:391:LEU:HD22	1:E:446:PRO:HG2	1.90	0.54
1:H:155:ASP:N	1:H:155:ASP:OD1	2.40	0.54
1:H:213:LYS:HE2	1:H:274:LYS:HE2	1.90	0.54
1:H:254:PRO:HB2	1:H:324:HIS:NE2	2.23	0.54
1:D:53:SER:OG	1:D:361:ILE:N	2.32	0.54
1:H:495:SER:OG	1:H:497:GLN:HG2	2.07	0.54
1:D:49:LYS:HB2	1:D:362:TYR:CE2	2.42	0.54
1:E:254:PRO:HB2	1:E:324:HIS:CD2	2.43	0.54
1:H:469:ALA:HB2	1:H:490:ALA:HB3	1.89	0.53
1:C:178:ALA:HB3	1:C:186:CYS:SG	2.48	0.53
1:E:225:GLN:HG3	1:F:222:TYR:HE1	1.73	0.53
1:B:135:ASP:O	1:B:350:ARG:NH1	2.41	0.53
1:G:104:ASP:O	1:G:112:ARG:NH2	2.41	0.53
1:A:556:ASP:OD2	1:A:560:ASN:ND2	2.37	0.53
1:C:135:ASP:HA	1:C:173:ARG:CZ	2.38	0.53
1:D:452:PRO:HB3	1:D:464:PHE:CE2	2.44	0.53
1:F:412:MET:HE3	1:F:548:ASP:HB3	1.91	0.53
1:A:83:PHE:CE1	1:A:210:PHE:HB3	2.43	0.53
1:D:36:GLN:O	1:D:285:PRO:HD3	2.08	0.53
1:D:469:ALA:O	1:D:494:ARG:NH2	2.42	0.53
1:E:287:THR:O	1:E:293:ARG:NE	2.37	0.53
1:E:111:ASP:OD2	1:E:320:LYS:N	2.42	0.53
1:A:174:TYR:HA	1:A:191:ASN:HB2	1.90	0.53
1:C:171:ASN:HB3	1:C:454:LYS:O	2.09	0.53
1:E:314:GLY:HA3	1:E:318:GLY:C	2.29	0.53
1:B:72:PRO:HB2	1:B:158:TYR:CG	2.44	0.53
1:D:217:SER:HB3	1:D:346:CYS:HB3	1.90	0.53
1:G:147:GLU:OE2	1:H:152:GLY:N	2.35	0.53
1:D:253:PRO:O	1:D:316:GLN:NE2	2.34	0.52
1:G:469:ALA:HB2	1:G:509:TYR:CE1	2.44	0.52
1:D:237:ARG:O	1:D:241:GLU:HG3	2.09	0.52
1:E:121:ASN:ND2	1:E:516:PRO:HA	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:480:GLN:NE2	1:F:507:GLY:HA3	2.25	0.52
1:F:62:VAL:HG22	1:F:63:PHE:CD2	2.45	0.52
1:D:101:ALA:HA	1:D:321:TYR:CZ	2.43	0.52
1:E:449:TYR:HB3	1:E:467:THR:HG22	1.91	0.52
1:H:145:ARG:HB2	1:H:206:TYR:CZ	2.43	0.52
1:H:416:THR:OG1	1:H:545:GLU:OE1	2.22	0.52
1:B:418:ILE:O	1:B:448:TYR:N	2.28	0.52
1:C:141:VAL:N	1:C:195:GLN:O	2.29	0.52
1:D:222:TYR:HE2	1:D:247:LEU:HD23	1.75	0.52
1:D:285:PRO:O	1:D:296:ARG:N	2.39	0.52
1:H:413:LEU:O	1:H:548:ASP:N	2.43	0.52
1:C:253:PRO:HD2	1:C:316:GLN:HG2	1.92	0.52
1:C:134:GLN:HG3	1:C:465:GLY:O	2.10	0.52
1:C:452:PRO:HD2	1:C:538:MET:HB2	1.91	0.52
1:H:83:PHE:CE1	1:H:210:PHE:HB3	2.45	0.52
1:A:186:CYS:SG	1:B:290:LYS:HA	2.49	0.52
1:C:452:PRO:HB3	1:C:464:PHE:CD2	2.44	0.52
1:D:469:ALA:HB2	1:D:490:ALA:HB3	1.92	0.52
1:A:105:PRO:HA	1:A:112:ARG:HH22	1.75	0.51
1:C:264:THR:O	1:D:138:THR:HG21	2.10	0.51
1:G:93:ASP:OD2	1:G:325:GLN:NE2	2.41	0.51
1:H:393:ARG:NH1	1:H:401:GLN:HB2	2.26	0.51
1:B:210:PHE:HB2	1:B:352:ILE:HG22	1.93	0.51
1:B:464:PHE:H	1:B:517:ALA:HB1	1.75	0.51
1:B:90:PHE:CD2	1:B:94:HIS:CD2	2.98	0.51
1:H:295:PHE:CE1	1:H:330:ARG:HB3	2.45	0.51
1:C:387:VAL:O	1:C:412:MET:N	2.29	0.51
1:C:347:SER:HB2	2:C:601:SF4:S3	2.49	0.51
1:B:91:ARG:HD2	1:B:279:ARG:HH21	1.76	0.51
1:C:150:TRP:HB3	1:D:65:ARG:HH12	1.75	0.51
1:G:469:ALA:CB	1:G:509:TYR:HE1	2.24	0.51
1:B:135:ASP:O	1:B:350:ARG:NH2	2.44	0.51
1:C:240:ILE:HG22	1:C:307:VAL:HG11	1.92	0.51
1:B:109:ASP:OD2	1:F:531:LEU:HA	2.10	0.51
1:F:419:VAL:O	1:F:541:VAL:HA	2.09	0.51
1:B:464:PHE:N	1:B:517:ALA:HB1	2.25	0.51
1:E:193:PRO:HD3	1:F:291:TYR:O	2.10	0.51
1:F:78:LEU:C	1:F:80:HIS:H	2.14	0.51
1:H:145:ARG:NH1	1:H:155:ASP:OD2	2.42	0.51
1:G:90:PHE:CD2	1:G:94:HIS:HD2	2.29	0.51
1:G:167:TYR:HB3	1:G:174:TYR:HE1	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:136:THR:HB	1:H:167:TYR:HE2	1.76	0.51
1:H:411:VAL:O	1:H:550:PRO:HA	2.11	0.51
1:A:88:HIS:CE1	1:A:131:PRO:HA	2.46	0.50
1:F:101:ALA:HA	1:F:321:TYR:CE2	2.46	0.50
1:E:336:ALA:O	1:F:471:ARG:NH2	2.43	0.50
1:H:74:ALA:HB1	1:H:361:ILE:HD11	1.93	0.50
1:H:419:VAL:O	1:H:541:VAL:HA	2.11	0.50
1:A:255:TYR:H	1:A:323:ALA:HA	1.76	0.50
1:C:171:ASN:O	1:C:453:ALA:HB1	2.10	0.50
1:E:414:ASN:OD1	1:E:548:ASP:N	2.32	0.50
1:A:264:THR:OG1	1:B:195:GLN:HB2	2.11	0.50
1:F:253:PRO:HG2	1:F:316:GLN:HG2	1.92	0.50
1:H:275:LEU:HD22	1:H:280:TYR:CD2	2.39	0.50
1:H:285:PRO:O	1:H:296:ARG:N	2.42	0.50
1:A:466:PRO:O	1:A:491:LYS:HE2	2.12	0.50
1:B:393:ARG:NH2	1:B:398:VAL:HA	2.27	0.50
1:A:155:ASP:OD1	1:A:155:ASP:N	2.44	0.50
1:B:213:LYS:HE2	1:B:274:LYS:HE2	1.92	0.50
1:B:275:LEU:HB3	1:B:280:TYR:HB3	1.93	0.50
1:C:300:TRP:O	1:C:304:VAL:HG23	2.12	0.50
1:E:330:ARG:NH1	1:E:331:LEU:O	2.43	0.50
1:F:257:ILE:O	1:F:326:ALA:HA	2.11	0.50
1:G:135:ASP:O	1:G:350:ARG:NH1	2.40	0.50
1:A:133:CYS:HB3	1:A:350:ARG:NH2	2.26	0.50
1:C:121:ASN:OD1	1:C:519:ILE:N	2.31	0.50
1:E:113:TYR:HE2	1:E:552:PHE:HZ	1.60	0.50
1:E:386:SER:HA	1:E:412:MET:HG3	1.94	0.50
1:F:134:GLN:OE1	1:F:517:ALA:HB2	2.12	0.50
1:C:107:ALA:HB3	1:C:112:ARG:HE	1.76	0.50
1:D:466:PRO:HG2	1:D:491:LYS:HG2	1.94	0.50
1:E:256:HIS:HB2	1:E:345:SER:HB3	1.92	0.50
1:E:395:ILE:C	1:E:397:LYS:H	2.13	0.50
1:F:240:ILE:O	1:F:244:LEU:HG	2.12	0.50
1:F:411:VAL:O	1:F:550:PRO:HA	2.12	0.50
1:G:79:ALA:HB3	1:G:162:GLY:HA3	1.94	0.50
1:H:414:ASN:HA	1:H:547:GLU:HA	1.92	0.50
1:B:88:HIS:CD2	1:B:128:ARG:HA	2.47	0.50
1:A:419:VAL:HG11	1:A:464:PHE:HZ	1.77	0.49
1:A:419:VAL:HB	1:A:542:TRP:HB2	1.94	0.49
1:A:68:LEU:HD11	1:A:357:ASN:C	2.32	0.49
1:C:178:ALA:HB2	1:C:188:THR:HG22	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:386:SER:O	1:F:386:SER:OG	2.30	0.49
1:G:563:TYR:HB3	1:G:567:LEU:HD12	1.93	0.49
1:F:300:TRP:O	1:F:304:VAL:HG23	2.11	0.49
1:H:448:TYR:HE1	1:H:466:PRO:HB3	1.77	0.49
1:A:211:ILE:HG22	1:A:213:LYS:HG2	1.94	0.49
1:C:520:LEU:O	1:C:525:ILE:N	2.40	0.49
1:D:563:TYR:HB3	1:D:567:LEU:HD12	1.94	0.49
1:E:121:ASN:OD1	1:E:518:ALA:HB3	2.12	0.49
1:F:80:HIS:HE1	1:F:170:HIS:CE1	2.31	0.49
1:G:141:VAL:HG11	1:G:159:LEU:HD13	1.94	0.49
1:B:99:ARG:O	1:B:103:GLU:HG3	2.12	0.49
1:C:466:PRO:HG2	1:C:491:LYS:HG2	1.93	0.49
1:H:449:TYR:O	1:H:467:THR:N	2.43	0.49
1:A:69:LYS:HD2	1:B:63:PHE:CE2	2.47	0.49
1:C:352:ILE:HG23	1:C:364:GLU:HB3	1.94	0.49
1:C:419:VAL:HA	1:C:448:TYR:O	2.13	0.49
1:H:412:MET:HB3	1:H:548:ASP:HA	1.94	0.49
1:A:164:TRP:O	1:A:168:ARG:N	2.35	0.49
1:C:48:ALA:O	1:C:363:ILE:HG22	2.13	0.49
1:D:87:HIS:HA	1:D:350:ARG:HD2	1.94	0.49
1:D:443:LYS:HG2	1:D:483:GLY:O	2.13	0.49
1:A:247:LEU:HD11	1:A:342:LEU:HD21	1.94	0.49
1:A:456:PRO:HB2	1:A:459:TYR:HD2	1.74	0.49
1:B:295:PHE:CZ	1:B:330:ARG:HB3	2.48	0.49
1:C:101:ALA:O	1:C:112:ARG:HG2	2.13	0.49
1:C:491:LYS:HE2	2:C:601:SF4:S4	2.52	0.49
1:E:243:LYS:O	1:E:246:THR:OG1	2.18	0.49
1:E:399:ARG:HD3	1:E:506:GLY:O	2.12	0.49
1:E:65:ARG:HH12	1:F:152:GLY:HA2	1.78	0.49
1:A:148:LEU:HB2	1:A:204:SER:HB3	1.95	0.48
1:E:39:ASP:OD2	1:E:42:HIS:HA	2.13	0.48
1:G:469:ALA:HB2	1:G:509:TYR:HE1	1.77	0.48
1:B:554:VAL:O	1:B:562:MET:N	2.32	0.48
1:G:480:GLN:NE2	1:G:502:CYS:SG	2.80	0.48
1:H:140:ILE:HG12	1:H:195:GLN:HB3	1.95	0.48
1:H:167:TYR:HA	1:H:172:LEU:HD12	1.94	0.48
1:H:240:ILE:HG22	1:H:307:VAL:HG11	1.95	0.48
1:B:358:LYS:H	1:B:358:LYS:CD	2.26	0.48
1:D:104:ASP:O	1:D:112:ARG:NH2	2.45	0.48
1:G:47:PHE:HB3	1:G:362:TYR:HB3	1.94	0.48
1:G:499:THR:HG22	1:G:559:GLY:HA2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:407:VAL:HB	1:G:562:MET:HB3	1.95	0.48
1:H:466:PRO:HG2	1:H:491:LYS:HG2	1.94	0.48
1:B:119:LEU:HD13	1:B:374:LEU:HD13	1.95	0.48
1:G:142:LEU:HD12	1:G:197:ASP:HB3	1.95	0.48
1:A:164:TRP:HB2	1:A:192:LEU:CD1	2.44	0.48
1:C:138:THR:OG1	1:D:334:HIS:HB2	2.13	0.48
1:A:415:GLY:N	1:A:546:VAL:O	2.34	0.48
1:C:389:VAL:N	1:C:412:MET:O	2.34	0.48
1:E:105:PRO:HA	1:E:112:ARG:HH22	1.77	0.48
1:E:209:LEU:HD11	1:E:351:GLN:HB2	1.96	0.48
1:G:211:ILE:HD13	1:G:274:LYS:HD2	1.96	0.48
1:C:473:ASP:HA	1:C:494:ARG:NH2	2.20	0.48
1:E:75:LEU:HD13	1:E:155:ASP:HA	1.94	0.48
1:F:145:ARG:HB2	1:F:206:TYR:CZ	2.49	0.48
1:G:528:VAL:HG13	1:G:544:ILE:HG22	1.96	0.48
1:H:99:ARG:O	1:H:103:GLU:HG3	2.14	0.48
1:C:460:ALA:HB1	1:C:526:LYS:O	2.12	0.48
1:G:220:LYS:HE3	1:G:250:ALA:HB3	1.95	0.48
1:H:421:ARG:O	1:H:425:HIS:ND1	2.37	0.48
1:G:225:GLN:NE2	1:H:218:ALA:O	2.46	0.48
1:G:373:TYR:O	1:G:375:PRO:HD3	2.13	0.48
1:B:240:ILE:O	1:B:244:LEU:HG	2.13	0.48
1:F:144:LYS:HB3	1:F:201:VAL:HG11	1.94	0.48
1:G:133:CYS:HB2	1:G:348:ALA:HB2	1.94	0.48
1:G:145:ARG:NE	1:H:200:ALA:HB1	2.29	0.48
1:G:345:SER:OG	1:G:349:ASP:OD1	2.21	0.48
1:H:275:LEU:HB3	1:H:280:TYR:HB3	1.95	0.48
1:C:282:ASP:CG	1:C:327:ARG:HE	2.15	0.47
1:G:39:ASP:OD2	1:G:42:HIS:HA	2.13	0.47
1:A:270:MET:HA	1:A:273:VAL:HG12	1.96	0.47
1:A:147:GLU:HA	1:B:145:ARG:NH2	2.29	0.47
1:C:286:THR:HA	1:C:296:ARG:O	2.14	0.47
1:D:286:THR:HA	1:D:296:ARG:O	2.14	0.47
1:F:425:HIS:HD2	1:F:475:TYR:CG	2.32	0.47
1:G:334:HIS:NE2	1:H:135:ASP:OD1	2.43	0.47
1:G:120:LYS:O	1:G:124:ILE:HG12	2.14	0.47
1:A:298:PRO:O	1:A:302:LYS:HG3	2.14	0.47
1:B:494:ARG:NE	1:B:498:VAL:HG11	2.29	0.47
1:C:121:ASN:ND2	1:C:516:PRO:HA	2.28	0.47
1:H:412:MET:SD	1:H:550:PRO:HG3	2.54	0.47
1:H:425:HIS:HD2	1:H:479:PHE:CE2	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:250:ALA:O	1:H:491:LYS:NZ	2.47	0.47
1:D:477:ASP:OD1	1:D:505:HIS:NE2	2.47	0.47
1:E:225:GLN:HG3	1:F:222:TYR:CE1	2.49	0.47
1:G:227:THR:HG21	1:H:471:ARG:CB	2.45	0.47
1:B:178:ALA:HB2	1:B:188:THR:HG22	1.96	0.47
1:F:252:CYS:O	1:F:347:SER:OG	2.23	0.47
1:H:259:LEU:O	1:H:328:VAL:HA	2.14	0.47
1:D:467:THR:HG22	1:D:468:THR:H	1.80	0.47
1:D:503:LYS:HD2	1:D:559:GLY:CA	2.44	0.47
1:G:86:VAL:HG22	1:G:350:ARG:HB3	1.97	0.47
1:G:469:ALA:HB1	1:G:509:TYR:CE1	2.50	0.47
1:H:75:LEU:HB3	1:H:159:LEU:CD2	2.45	0.47
1:H:91:ARG:NH1	1:H:351:GLN:HG3	2.30	0.47
1:H:393:ARG:HH12	1:H:401:GLN:HB2	1.79	0.47
1:D:226:GLU:C	1:D:338:CYS:HB3	2.34	0.47
1:E:467:THR:OG1	1:E:471:ARG:NH1	2.35	0.47
1:F:161:LYS:NZ	1:F:165:ASN:OD1	2.34	0.47
1:G:411:VAL:HG22	1:G:551:ALA:O	2.15	0.47
1:G:93:ASP:OD1	1:G:279:ARG:NH2	2.46	0.47
1:H:416:THR:HA	1:H:544:ILE:O	2.14	0.47
1:A:448:TYR:HD1	1:A:489:LEU:O	1.98	0.47
1:B:142:LEU:O	1:B:208:PHE:HA	2.15	0.47
1:B:223:LEU:HB2	1:B:270:MET:SD	2.55	0.47
1:C:148:LEU:HB2	1:C:204:SER:HB3	1.97	0.47
1:C:252:CYS:SG	1:C:514:GLY:HA3	2.55	0.47
1:E:111:ASP:OD2	1:E:319:GLY:HA3	2.15	0.47
1:E:39:ASP:OD1	1:E:43:HIS:N	2.48	0.47
1:G:219:ASN:O	1:H:225:GLN:HG3	2.14	0.47
1:A:99:ARG:HD3	1:A:373:TYR:HA	1.97	0.47
1:C:464:PHE:HB3	1:C:525:ILE:CD1	2.45	0.47
1:C:532:ALA:HB3	1:C:541:VAL:HB	1.95	0.47
1:G:391:LEU:HB2	1:G:415:GLY:HA3	1.97	0.47
1:H:452:PRO:HB3	1:H:464:PHE:CD2	2.50	0.47
1:B:402:LEU:HD23	1:B:402:LEU:HA	1.72	0.46
1:C:105:PRO:O	1:C:112:ARG:NH2	2.48	0.46
1:C:289:ASP:OD2	1:C:293:ARG:HD3	2.15	0.46
1:G:486:TYR:O	1:G:507:GLY:HA2	2.15	0.46
1:B:36:GLN:O	1:B:285:PRO:HD3	2.15	0.46
1:E:528:VAL:HG22	1:E:544:ILE:CB	2.45	0.46
1:G:193:PRO:HG3	1:H:292:GLY:O	2.15	0.46
1:C:261:ILE:HB	1:C:330:ARG:CD	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:LYS:HD2	1:D:63:PHE:CE1	2.50	0.46
1:E:313:ILE:HG12	1:E:566:THR:HB	1.97	0.46
1:F:263:GLY:HA3	1:F:269:THR:OG1	2.16	0.46
1:F:347:SER:HB2	2:F:601:SF4:S4	2.55	0.46
1:F:419:VAL:HB	1:F:542:TRP:CD1	2.50	0.46
1:E:408:GLY:N	1:E:553:ILE:O	2.30	0.46
1:G:452:PRO:HB3	1:G:464:PHE:CD2	2.51	0.46
1:E:506:GLY:HA2	1:E:557:ASP:HB2	1.97	0.46
1:A:134:GLN:OE1	1:A:517:ALA:HB2	2.15	0.46
1:A:83:PHE:HE1	1:A:210:PHE:CD1	2.34	0.46
1:C:438:LEU:HD12	1:C:439:PRO:HD2	1.97	0.46
1:D:278:CYS:HA	1:D:351:GLN:HE21	1.81	0.46
1:E:144:LYS:CE	1:E:280:TYR:OH	2.64	0.46
1:G:65:ARG:NH1	1:H:150:TRP:HB3	2.31	0.46
1:H:419:VAL:HB	1:H:542:TRP:HD1	1.80	0.46
1:C:425:HIS:HB3	1:C:475:TYR:CG	2.51	0.46
1:F:391:LEU:HB2	1:F:415:GLY:HA3	1.96	0.46
1:F:412:MET:CE	1:F:548:ASP:HB3	2.45	0.46
1:G:183:PHE:HD1	1:H:231:LEU:HB3	1.81	0.46
1:G:215:GLY:HA3	1:H:334:HIS:CG	2.51	0.46
1:G:231:LEU:HD13	1:G:330:ARG:NH2	2.31	0.46
1:H:46:GLU:O	1:H:364:GLU:HA	2.16	0.46
1:C:348:ALA:N	2:C:601:SF4:S3	2.88	0.46
1:D:136:THR:HG21	1:D:173:ARG:H	1.81	0.46
1:H:207:GLU:HG2	1:H:355:HIS:HB3	1.97	0.46
1:B:419:VAL:HA	1:B:448:TYR:O	2.16	0.45
1:C:155:ASP:OD1	1:C:155:ASP:N	2.49	0.45
1:C:248:GLY:HA3	1:C:493:ASN:ND2	2.31	0.45
1:F:119:LEU:HD13	1:F:374:LEU:HD13	1.99	0.45
1:G:452:PRO:HB3	1:G:464:PHE:CE2	2.51	0.45
1:H:29:PHE:CZ	1:H:31:PHE:HB2	2.51	0.45
1:A:76:THR:HG23	1:A:162:GLY:N	2.32	0.45
1:C:531:LEU:N	1:C:541:VAL:O	2.37	0.45
1:E:259:LEU:N	1:E:327:ARG:O	2.43	0.45
1:F:145:ARG:N	1:F:199:LEU:O	2.46	0.45
1:F:89:PHE:CZ	1:F:368:GLN:HG2	2.51	0.45
1:A:240:ILE:O	1:A:244:LEU:HG	2.17	0.45
1:D:166:ALA:O	1:D:170:HIS:HB2	2.16	0.45
1:D:348:ALA:HB1	1:D:350:ARG:CZ	2.45	0.45
1:E:256:HIS:O	1:E:344:VAL:HA	2.15	0.45
1:E:415:GLY:O	1:E:546:VAL:HG22	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:490:ALA:O	1:H:512:SER:N	2.48	0.45
1:A:177:THR:HG22	1:A:185:GLU:HB3	1.97	0.45
1:E:145:ARG:HB2	1:E:206:TYR:CZ	2.51	0.45
1:F:414:ASN:HA	1:F:547:GLU:HA	1.98	0.45
1:H:313:ILE:O	1:H:318:GLY:N	2.41	0.45
1:H:76:THR:HG23	1:H:162:GLY:N	2.31	0.45
1:E:419:VAL:HA	1:E:448:TYR:O	2.17	0.45
1:E:453:ALA:HB3	1:E:463:SER:HB2	1.98	0.45
1:G:145:ARG:HB3	1:H:200:ALA:CB	2.47	0.45
1:A:102:ILE:HG21	1:A:375:PRO:HG2	1.99	0.45
1:A:173:ARG:NH1	1:A:451:GLY:O	2.50	0.45
1:G:556:ASP:OD2	1:G:560:ASN:HB2	2.17	0.45
1:G:55:LYS:HE3	1:G:56:TYR:CZ	2.52	0.45
1:H:88:HIS:HB3	1:H:126:ALA:HA	1.99	0.45
1:A:506:GLY:HA2	1:A:557:ASP:HB2	1.99	0.45
1:B:253:PRO:HG3	1:B:255:TYR:CE2	2.51	0.45
1:B:421:ARG:O	1:B:425:HIS:ND1	2.41	0.45
1:B:90:PHE:HD2	1:B:94:HIS:CD2	2.34	0.45
1:B:91:ARG:HD2	1:B:279:ARG:NH2	2.32	0.45
1:F:250:ALA:O	1:F:491:LYS:NZ	2.43	0.45
1:F:261:ILE:HD13	1:F:340:VAL:HG13	1.99	0.45
1:H:83:PHE:HD2	1:H:167:TYR:HH	1.64	0.45
1:H:254:PRO:HG3	1:H:315:ALA:CB	2.47	0.45
1:H:280:TYR:HD1	1:H:280:TYR:O	2.00	0.45
1:H:419:VAL:HB	1:H:542:TRP:CD1	2.52	0.45
1:A:47:PHE:HD1	1:A:364:GLU:HA	1.82	0.45
1:A:121:ASN:CG	1:A:516:PRO:HA	2.36	0.45
1:B:403:SER:HA	1:B:508:PHE:HZ	1.82	0.45
1:C:164:TRP:CD1	1:C:190:ASP:HB2	2.52	0.45
1:C:374:LEU:HD12	1:C:374:LEU:HA	1.82	0.45
1:E:469:ALA:HB2	1:E:490:ALA:HB3	1.98	0.45
1:G:135:ASP:OD1	1:G:173:ARG:NH2	2.50	0.45
1:H:348:ALA:HB1	1:H:350:ARG:CZ	2.47	0.45
1:C:438:LEU:HD22	1:C:479:PHE:O	2.17	0.45
1:D:91:ARG:HD2	1:D:279:ARG:NH2	2.31	0.45
1:F:174:TYR:O	1:F:187:ASN:ND2	2.41	0.45
1:H:180:LEU:N	1:H:184:LYS:O	2.50	0.45
1:H:333:ARG:HD2	1:H:337:SER:O	2.17	0.45
1:H:392:LYS:NZ	1:H:415:GLY:HA2	2.32	0.45
1:B:134:GLN:NE2	2:B:601:SF4:S4	2.85	0.44
1:C:69:LYS:HD2	1:D:63:PHE:CZ	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:THR:HG21	1:F:172:LEU:HD22	2.00	0.44
1:G:494:ARG:NH1	1:G:509:TYR:CD1	2.77	0.44
1:A:256:HIS:HB2	1:A:345:SER:HB3	1.99	0.44
1:C:83:PHE:HE1	1:C:210:PHE:CD1	2.35	0.44
1:C:480:GLN:HG2	1:C:486:TYR:CD1	2.52	0.44
1:D:224:TYR:O	1:D:340:VAL:N	2.46	0.44
1:E:334:HIS:NE2	1:F:135[B]:ASP:OD1	2.50	0.44
1:G:65:ARG:CZ	1:G:148:LEU:HD11	2.47	0.44
1:C:172:LEU:O	1:C:454:LYS:N	2.49	0.44
1:E:272:THR:HG23	1:E:281:TYR:CE2	2.52	0.44
1:E:254:PRO:HA	1:E:322:PHE:O	2.17	0.44
1:E:334:HIS:NE2	1:F:135[A]:ASP:OD1	2.50	0.44
1:G:253:PRO:HD2	1:G:316:GLN:HG2	1.99	0.44
1:H:47:PHE:HB3	1:H:362:TYR:HB3	2.00	0.44
1:A:490:ALA:N	1:A:509:TYR:HE1	2.14	0.44
1:D:113:TYR:OH	1:D:410:ARG:HD3	2.17	0.44
1:D:421:ARG:HG3	1:D:539:GLU:OE2	2.18	0.44
1:E:419:VAL:O	1:E:541:VAL:HA	2.18	0.44
1:F:325:GLN:OE1	1:F:327:ARG:NH2	2.49	0.44
1:B:449:TYR:CD2	1:B:490:ALA:HB2	2.53	0.44
1:F:392:LYS:HZ3	1:F:415:GLY:HA2	1.83	0.44
1:F:532:ALA:O	1:F:540:ALA:HB1	2.17	0.44
1:G:489:LEU:HA	1:G:510:LEU:HB2	1.99	0.44
1:D:91:ARG:NE	1:D:364:GLU:OE2	2.45	0.44
1:E:150:TRP:HB3	1:F:65:ARG:NH1	2.31	0.44
1:F:214:GLY:HA3	2:F:601:SF4:S3	2.58	0.44
1:G:219:ASN:HA	1:H:225:GLN:CD	2.37	0.44
1:B:94:HIS:CE1	1:B:256:HIS:HE2	2.34	0.44
1:B:424:ALA:O	1:B:428:ILE:HG13	2.18	0.44
1:D:143:GLY:O	1:D:199:LEU:N	2.43	0.44
1:E:240:ILE:O	1:E:244:LEU:HG	2.17	0.44
1:G:255:TYR:O	1:G:323:ALA:HA	2.17	0.44
1:A:209:LEU:HD11	1:A:351:GLN:HB2	1.98	0.44
1:B:210:PHE:O	1:B:351:GLN:HA	2.18	0.44
1:B:403:SER:OG	1:B:557:ASP:OD2	2.26	0.44
1:C:173:ARG:HD2	1:C:538:MET:SD	2.58	0.44
1:C:251:ALA:HB3	1:C:255:TYR:CE1	2.52	0.44
1:C:531:LEU:HD22	1:C:543:LYS:HE3	1.98	0.44
1:F:466:PRO:HG2	1:F:491:LYS:HG2	1.99	0.44
1:C:543:LYS:HE3	1:C:543:LYS:HB2	1.76	0.44
1:E:438:LEU:HD12	1:E:439:PRO:HD2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:418:ILE:HG12	1:E:445:SER:HB2	2.00	0.44
1:F:62:VAL:HG11	1:F:150:TRP:CH2	2.44	0.44
1:E:346:CYS:CB	2:E:601:SF4:S4	3.06	0.43
1:C:120:LYS:O	1:C:124:ILE:HG12	2.19	0.43
1:E:193:PRO:HG3	1:F:292:GLY:O	2.17	0.43
1:F:419:VAL:HB	1:F:542:TRP:HB2	2.00	0.43
1:B:316:GLN:CD	1:B:514:GLY:H	2.20	0.43
1:C:131:PRO:HD2	1:C:463:SER:OG	2.18	0.43
1:C:264:THR:OG1	1:D:195:GLN:HB2	2.17	0.43
1:C:256:HIS:O	1:C:344:VAL:HA	2.18	0.43
1:C:385:THR:C	1:C:410:ARG:HB3	2.39	0.43
1:F:192:LEU:HB3	1:F:193:PRO:HA	1.99	0.43
1:F:210:PHE:HE1	1:F:354:ALA:HB3	1.83	0.43
1:C:531:LEU:HD22	1:C:543:LYS:HB2	2.01	0.43
1:D:102:ILE:O	1:D:112:ARG:HD3	2.18	0.43
1:D:469:ALA:HB1	1:D:494:ARG:CZ	2.49	0.43
1:F:75:LEU:HB3	1:F:159:LEU:CD2	2.48	0.43
1:F:177:THR:CG2	1:F:185:GLU:HB3	2.47	0.43
1:F:250:ALA:HB1	1:F:468:THR:HG23	2.00	0.43
1:C:124:ILE:HD12	1:C:522:LYS:CD	2.49	0.43
1:E:88:HIS:CE1	1:E:128:ARG:HA	2.54	0.43
1:E:219:ASN:HD21	1:F:337:SER:HA	1.83	0.43
1:H:133:CYS:HB3	1:H:350:ARG:HH22	1.84	0.43
1:H:480:GLN:HE22	1:H:486:TYR:HA	1.83	0.43
1:B:489:LEU:HD21	1:B:549:PHE:CE1	2.54	0.43
1:E:88:HIS:ND1	1:E:125:ALA:O	2.39	0.43
1:G:133:CYS:SG	1:G:134:GLN:N	2.91	0.43
1:H:171:ASN:CA	1:H:454:LYS:HB2	2.47	0.43
1:B:425:HIS:CD2	1:B:472:MET:HG2	2.52	0.43
1:E:233:PRO:HA	1:E:300:TRP:CZ2	2.54	0.43
1:A:93:ASP:OD1	1:A:94:HIS:N	2.52	0.43
1:C:42:HIS:HE2	1:C:280:TYR:HE1	1.65	0.43
1:E:262:GLY:C	1:E:339:PRO:HG2	2.39	0.43
1:F:57:VAL:HA	1:F:69:LYS:O	2.18	0.43
1:G:57:VAL:HB	1:G:68:LEU:HD11	2.00	0.43
1:H:88:HIS:CD2	1:H:128:ARG:HA	2.53	0.43
1:E:91:ARG:HH21	1:E:364:GLU:CD	2.22	0.43
1:F:285:PRO:O	1:F:295:PHE:HB2	2.18	0.43
1:F:473:ASP:HA	1:F:494:ARG:HH21	1.83	0.43
1:G:425:HIS:ND1	1:G:472:MET:HG3	2.34	0.43
1:G:410:ARG:HB3	1:G:552:PHE:CZ	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LEU:HB3	1:A:280:TYR:HB3	1.99	0.43
1:B:529:THR:N	1:B:543:LYS:O	2.46	0.43
1:D:94:HIS:CE1	1:D:256:HIS:HE2	2.37	0.43
1:D:429:LYS:NZ	1:D:433:ASP:OD2	2.33	0.43
1:F:418:ILE:HG13	1:F:441:TYR:O	2.19	0.43
1:G:446:PRO:HG3	1:G:487:ILE:HD11	2.00	0.43
1:G:480:GLN:OE1	1:G:505:HIS:HB2	2.19	0.43
1:H:98:TRP:CZ2	1:H:118:LEU:HB3	2.54	0.43
1:D:438:LEU:HD12	1:D:439:PRO:HD2	2.00	0.42
1:D:428:ILE:HD11	1:D:441:TYR:HE1	1.84	0.42
1:H:425:HIS:CD2	1:H:479:PHE:HE2	2.28	0.42
1:A:300:TRP:CZ2	1:B:183:PHE:HZ	2.38	0.42
1:F:134:GLN:HA	1:F:463:SER:HB3	2.00	0.42
1:G:279:ARG:HH12	1:G:351:GLN:HE22	1.67	0.42
1:H:268:MET:SD	1:H:331:LEU:HD13	2.59	0.42
1:H:415:GLY:O	1:H:546:VAL:HG22	2.19	0.42
1:B:47:PHE:HB3	1:B:362:TYR:HB3	2.01	0.42
1:C:168:ARG:HG3	1:C:169:TYR:CD1	2.54	0.42
1:E:409:THR:HB	1:E:553:ILE:HD12	2.00	0.42
1:F:452:PRO:HD2	1:F:538:MET:HA	2.00	0.42
1:G:136:THR:OG1	1:G:173:ARG:O	2.33	0.42
1:G:272:THR:HG21	1:G:331:LEU:HD11	2.01	0.42
1:H:158:TYR:HA	1:H:158:TYR:HD1	1.68	0.42
1:H:239:PHE:CE1	1:H:243:LYS:HE2	2.54	0.42
1:H:452:PRO:HD2	1:H:538:MET:HA	2.01	0.42
1:E:467:THR:O	1:E:490:ALA:HB1	2.19	0.42
1:A:468:THR:HA	1:A:491:LYS:O	2.20	0.42
1:D:289:ASP:OD2	1:D:293:ARG:HD3	2.19	0.42
1:D:259:LEU:O	1:D:328:VAL:HA	2.19	0.42
1:E:313:ILE:O	1:E:318:GLY:N	2.50	0.42
1:G:209:LEU:HD22	1:G:280:TYR:CD1	2.55	0.42
1:A:164:TRP:CD1	1:A:190:ASP:HB2	2.54	0.42
1:A:259:LEU:HA	1:A:341:GLY:O	2.20	0.42
1:B:178:ALA:N	1:B:186:CYS:O	2.51	0.42
1:B:432:MET:HA	1:B:436:GLU:O	2.20	0.42
1:C:314:GLY:O	1:C:322:PHE:HD1	2.03	0.42
1:F:419:VAL:HB	1:F:542:TRP:HD1	1.85	0.42
1:A:111:ASP:OD2	1:A:320:LYS:N	2.52	0.42
1:B:499:THR:HG21	1:B:561:ASP:HB2	2.01	0.42
1:B:448:TYR:CZ	1:B:549:PHE:HZ	2.38	0.42
1:B:95:LEU:HD23	1:B:98:TRP:CZ3	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:LEU:HA	1:C:150:TRP:NE1	2.35	0.42
1:C:150:TRP:HB3	1:D:65:ARG:NH1	2.33	0.42
1:D:34:ILE:O	1:D:294:ALA:N	2.31	0.42
1:E:233:PRO:HA	1:E:300:TRP:HZ2	1.83	0.42
1:F:80:HIS:ND1	1:F:80:HIS:O	2.52	0.42
1:G:473:ASP:CG	1:G:498:VAL:HG21	2.40	0.42
1:H:309:GLN:HG2	1:H:320:LYS:O	2.20	0.42
1:A:158:TYR:HA	1:A:158:TYR:HD1	1.68	0.42
1:A:392:LYS:HE3	1:A:415:GLY:HA2	2.00	0.42
1:B:435:GLY:O	1:B:437:PRO:HD3	2.19	0.42
1:F:120:LYS:O	1:F:124:ILE:HG12	2.20	0.42
1:A:464:PHE:N	1:A:517:ALA:HB1	2.35	0.42
1:B:261:ILE:HD13	1:B:340:VAL:HG13	2.02	0.42
1:B:316:GLN:OE1	1:B:514:GLY:N	2.39	0.42
1:B:389:VAL:HG21	1:B:413:LEU:HD23	2.01	0.42
1:C:245:LYS:NZ	1:C:568:ALA:HB3	2.35	0.42
1:C:430:GLU:O	1:C:434:ASN:ND2	2.46	0.42
1:E:230:LEU:HD11	1:E:236:LEU:HA	2.00	0.42
1:E:220:LYS:CE	1:E:250:ALA:HB3	2.47	0.42
1:G:520:LEU:HD23	1:G:520:LEU:HA	1.93	0.42
1:A:254:PRO:HB2	1:A:324:HIS:CG	2.55	0.42
1:B:133:CYS:HB3	1:B:350:ARG:NH2	2.35	0.42
1:B:494:ARG:HD3	1:B:498:VAL:HG11	2.01	0.42
1:E:529:THR:O	1:E:543:LYS:N	2.40	0.42
1:E:533:PHE:N	1:E:534:PRO:HD3	2.34	0.42
1:F:156:GLU:HG3	1:F:198:LEU:HD11	2.02	0.42
1:H:166:ALA:HA	1:H:170:HIS:CE1	2.55	0.42
1:A:211:ILE:CG2	1:A:213:LYS:HG2	2.50	0.41
1:B:520:LEU:HD21	1:B:550:PRO:HD2	2.02	0.41
1:E:94:HIS:NE2	1:E:347:SER:O	2.50	0.41
1:E:245:LYS:HZ1	1:E:568:ALA:HB2	1.85	0.41
1:F:456:PRO:HB2	1:F:459:TYR:CD2	2.54	0.41
1:F:134:GLN:CB	1:F:465:GLY:H	2.30	0.41
1:B:438:LEU:HA	1:B:439:PRO:HD3	1.94	0.41
1:C:200:ALA:HB1	1:D:145:ARG:CZ	2.50	0.41
1:C:88:HIS:CG	1:C:128:ARG:HA	2.55	0.41
1:G:167:TYR:HB3	1:G:174:TYR:CE1	2.55	0.41
1:C:104:ASP:OD2	1:C:106:GLU:HB2	2.20	0.41
1:D:357:ASN:HB2	1:D:358:LYS:HD3	2.02	0.41
1:G:136:THR:O	1:G:167:TYR:OH	2.35	0.41
1:G:139:ALA:HB1	1:G:163:ILE:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:THR:HB	1:G:167:TYR:HE2	1.85	0.41
1:G:494:ARG:NH1	1:G:509:TYR:HD1	2.11	0.41
1:B:155:ASP:OD1	1:B:155:ASP:N	2.54	0.41
1:E:36:GLN:O	1:E:285:PRO:HD3	2.20	0.41
1:E:395:ILE:C	1:E:397:LYS:N	2.74	0.41
1:F:87:HIS:CE1	1:F:136:THR:HB	2.54	0.41
1:H:294:ALA:HA	1:H:330:ARG:O	2.21	0.41
1:A:90:PHE:HE1	1:A:348:ALA:HA	1.86	0.41
1:C:425:HIS:HB3	1:C:475:TYR:CZ	2.55	0.41
1:D:391:LEU:C	1:D:393:ARG:H	2.23	0.41
1:D:452:PRO:HB3	1:D:464:PHE:CD2	2.56	0.41
1:F:417:LEU:HD12	1:F:546:VAL:HG11	2.02	0.41
1:C:334:HIS:CE1	1:D:175:SER:HB3	2.55	0.41
1:D:532:ALA:O	1:D:540:ALA:HB1	2.21	0.41
1:F:254:PRO:HB2	1:F:324:HIS:ND1	2.35	0.41
1:H:166:ALA:O	1:H:170:HIS:ND1	2.54	0.41
1:H:510:LEU:CD2	1:H:553:ILE:HA	2.50	0.41
1:H:508:PHE:CD1	1:H:556:ASP:HA	2.53	0.41
1:A:446:PRO:HA	1:A:487:ILE:O	2.21	0.41
1:A:449:TYR:HD2	1:A:469:ALA:HA	1.85	0.41
1:C:148:LEU:HD22	1:C:150:TRP:HZ2	1.85	0.41
1:C:42:HIS:HB3	1:C:45:THR:HB	2.02	0.41
1:H:300:TRP:O	1:H:304:VAL:HG23	2.21	0.41
1:A:86:VAL:HG22	1:A:350:ARG:HB3	2.03	0.41
1:B:83:PHE:CE2	1:B:210:PHE:HD2	2.38	0.41
1:B:466:PRO:HB2	1:B:491:LYS:HG2	2.01	0.41
1:C:37:PRO:HA	1:C:284:LEU:HD23	2.02	0.41
1:E:245:LYS:HZ2	1:E:568:ALA:HB2	1.86	0.41
1:H:65:ARG:NE	1:H:148:LEU:HD11	2.35	0.41
1:B:105:PRO:HA	1:B:112:ARG:HH12	1.86	0.41
1:C:447:ILE:O	1:C:489:LEU:N	2.53	0.41
1:G:193:PRO:HD3	1:H:291:TYR:O	2.21	0.41
1:B:223:LEU:HD12	1:B:340:VAL:O	2.20	0.41
1:B:422:ASP:OD1	1:B:471:ARG:NH1	2.47	0.41
1:D:78:LEU:HD22	1:D:356:ILE:HD11	2.03	0.41
1:F:467:THR:O	1:F:490:ALA:HB1	2.21	0.41
1:F:97:GLY:HA3	1:F:324:HIS:CD2	2.48	0.41
1:H:164:TRP:O	1:H:168:ARG:HB3	2.20	0.41
1:D:96:GLU:HG3	1:D:373:TYR:HE1	1.86	0.41
1:H:280:TYR:CD1	1:H:280:TYR:O	2.73	0.41
1:A:111:ASP:OD2	1:A:319:GLY:HA3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LEU:HD23	1:A:192:LEU:HA	1.87	0.40
1:C:254:PRO:HA	1:C:322:PHE:O	2.20	0.40
1:C:325:GLN:OE1	1:C:327:ARG:NH2	2.53	0.40
1:E:233:PRO:O	1:E:300:TRP:HH2	2.04	0.40
1:E:259:LEU:HD12	1:E:341:GLY:O	2.21	0.40
1:E:65:ARG:NH1	1:F:152:GLY:HA2	2.36	0.40
1:F:158:TYR:HA	1:F:158:TYR:HD1	1.69	0.40
1:F:479:PHE:HD2	1:F:485:SER:HB2	1.86	0.40
1:F:412:MET:HB3	1:F:548:ASP:HA	2.02	0.40
1:A:75:LEU:CD1	1:A:155:ASP:HA	2.51	0.40
1:B:421:ARG:NH1	1:B:451:GLY:HA3	2.15	0.40
1:C:185:GLU:OE2	1:D:333:ARG:NH2	2.46	0.40
1:C:285:PRO:O	1:C:296:ARG:N	2.36	0.40
1:C:317:PHE:HA	1:C:562:MET:HE2	2.03	0.40
1:C:259:LEU:HA	1:C:341:GLY:O	2.21	0.40
1:D:358:LYS:CD	1:D:358:LYS:H	2.26	0.40
1:E:312:GLY:O	1:E:318:GLY:HA2	2.21	0.40
1:F:256:HIS:O	1:F:344:VAL:HA	2.21	0.40
1:G:65:ARG:NH1	1:G:148:LEU:HD21	2.36	0.40
1:A:121:ASN:HB2	1:A:516:PRO:HA	2.02	0.40
1:C:463:SER:HB3	1:C:517:ALA:HB1	2.04	0.40
1:C:520:LEU:O	1:C:525:ILE:HG13	2.22	0.40
1:D:374:LEU:HA	1:D:374:LEU:HD12	1.86	0.40
1:F:554:VAL:O	1:F:561:ASP:HA	2.21	0.40
1:H:164:TRP:CH2	1:H:168:ARG:HG2	2.56	0.40
1:A:78:LEU:HD13	1:A:361:ILE:CG2	2.51	0.40
1:A:418:ILE:HG12	1:A:445:SER:HB2	2.04	0.40
1:B:167:TYR:HA	1:B:172:LEU:HD12	2.03	0.40
1:D:148:LEU:HA	1:D:150:TRP:NE1	2.36	0.40
1:F:391:LEU:N	1:F:414:ASN:O	2.38	0.40
1:G:50:VAL:HB	1:G:53:SER:HB3	2.03	0.40
1:G:528:VAL:HG22	1:G:544:ILE:HG22	2.03	0.40
1:G:218:ALA:O	1:H:225:GLN:NE2	2.55	0.40
1:G:179:ALA:HB2	1:H:330:ARG:CZ	2.52	0.40
1:H:37:PRO:HA	1:H:284:LEU:HD23	2.03	0.40
1:H:452:PRO:HB3	1:H:464:PHE:CG	2.56	0.40
1:A:410:ARG:HA	1:A:552:PHE:HA	2.03	0.40
1:C:533:PHE:N	1:C:534:PRO:HD3	2.36	0.40
1:D:110:ASN:HA	1:D:113:TYR:HB3	2.04	0.40
1:F:266:ALA:O	1:F:270:MET:HG2	2.22	0.40
1:H:248:GLY:HA3	1:H:493:ASN:OD1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	535/604 (89%)	513 (96%)	20 (4%)	2 (0%)	34	69
1	B	530/604 (88%)	511 (96%)	17 (3%)	2 (0%)	34	69
1	C	528/604 (87%)	512 (97%)	16 (3%)	0	100	100
1	D	526/604 (87%)	508 (97%)	17 (3%)	1 (0%)	47	79
1	E	527/604 (87%)	506 (96%)	17 (3%)	4 (1%)	19	58
1	F	528/604 (87%)	510 (97%)	16 (3%)	2 (0%)	34	69
1	G	528/604 (87%)	513 (97%)	15 (3%)	0	100	100
1	H	527/604 (87%)	510 (97%)	16 (3%)	1 (0%)	47	79
All	All	4229/4832 (88%)	4083 (96%)	134 (3%)	12 (0%)	41	74

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	387	VAL
1	B	438	LEU
1	E	386	SER
1	E	395	ILE
1	H	374	LEU
1	D	536	LEU
1	E	396	ASP
1	F	79	ALA
1	A	27	ALA
1	F	536	LEU
1	E	438	LEU
1	A	25	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/492 (74%)	355 (98%)	8 (2%)	52	79
1	B	369/492 (75%)	363 (98%)	6 (2%)	62	84
1	C	347/492 (70%)	342 (99%)	5 (1%)	67	86
1	D	362/492 (74%)	353 (98%)	9 (2%)	47	77
1	E	363/492 (74%)	357 (98%)	6 (2%)	60	83
1	F	391/492 (80%)	383 (98%)	8 (2%)	55	80
1	G	357/492 (73%)	353 (99%)	4 (1%)	73	88
1	H	365/492 (74%)	358 (98%)	7 (2%)	57	81
All	All	2917/3936 (74%)	2864 (98%)	53 (2%)	59	82

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LEU
1	A	206	TYR
1	A	274	LYS
1	A	351	GLN
1	A	374	LEU
1	A	464	PHE
1	A	538	MET
1	A	548	ASP
1	B	206	TYR
1	B	274	LYS
1	B	358	LYS
1	B	374	LEU
1	B	457	GLU
1	B	464	PHE
1	C	206	TYR
1	C	374	LEU
1	C	464	PHE
1	C	491	LYS
1	C	538	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	80	HIS
1	D	170	HIS
1	D	206	TYR
1	D	351	GLN
1	D	358	LYS
1	D	374	LEU
1	D	464	PHE
1	D	491	LYS
1	D	538	MET
1	E	144	LYS
1	E	206	TYR
1	E	386	SER
1	E	410	ARG
1	E	464	PHE
1	E	538	MET
1	F	206	TYR
1	F	274	LYS
1	F	351	GLN
1	F	374	LEU
1	F	410	ARG
1	F	464	PHE
1	F	491	LYS
1	F	538	MET
1	G	206	TYR
1	G	464	PHE
1	G	467	THR
1	G	538	MET
1	H	206	TYR
1	H	280	TYR
1	H	374	LEU
1	H	392	LYS
1	H	464	PHE
1	H	467	THR
1	H	491	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	F	170	HIS
1	F	324	HIS
1	H	480	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	B	602	-	5,5,5	0.98	0	5,5,5	0.94	0
2	SF4	F	601	1	0,12,12	0.00	-	-		
2	SF4	E	601	1	0,12,12	0.00	-	-		
2	SF4	G	601	1	0,12,12	0.00	-	-		
2	SF4	B	601	1	0,12,12	0.00	-	-		
2	SF4	A	601	1	0,12,12	0.00	-	-		
2	SF4	D	601	1	0,12,12	0.00	-	-		
2	SF4	C	601	1	0,12,12	0.00	-	-		
3	GOL	E	602	-	5,5,5	0.94	0	5,5,5	1.16	1 (20%)
2	SF4	H	601	1	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	602	-	-	2/4/4/4	-
2	SF4	F	601	1	-	-	0/6/5/5
2	SF4	E	601	1	-	-	0/6/5/5
2	SF4	G	601	1	-	-	0/6/5/5
2	SF4	B	601	1	-	-	0/6/5/5
2	SF4	A	601	1	-	-	0/6/5/5
2	SF4	D	601	1	-	-	0/6/5/5
2	SF4	C	601	1	-	-	0/6/5/5
3	GOL	E	602	-	-	2/4/4/4	-
2	SF4	H	601	1	-	-	0/6/5/5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	E	602	GOL	C3-C2-C1	-2.01	103.91	111.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	602	GOL	C1-C2-C3-O3
3	B	602	GOL	O1-C1-C2-O2
3	B	602	GOL	O1-C1-C2-C3
3	E	602	GOL	O2-C2-C3-O3

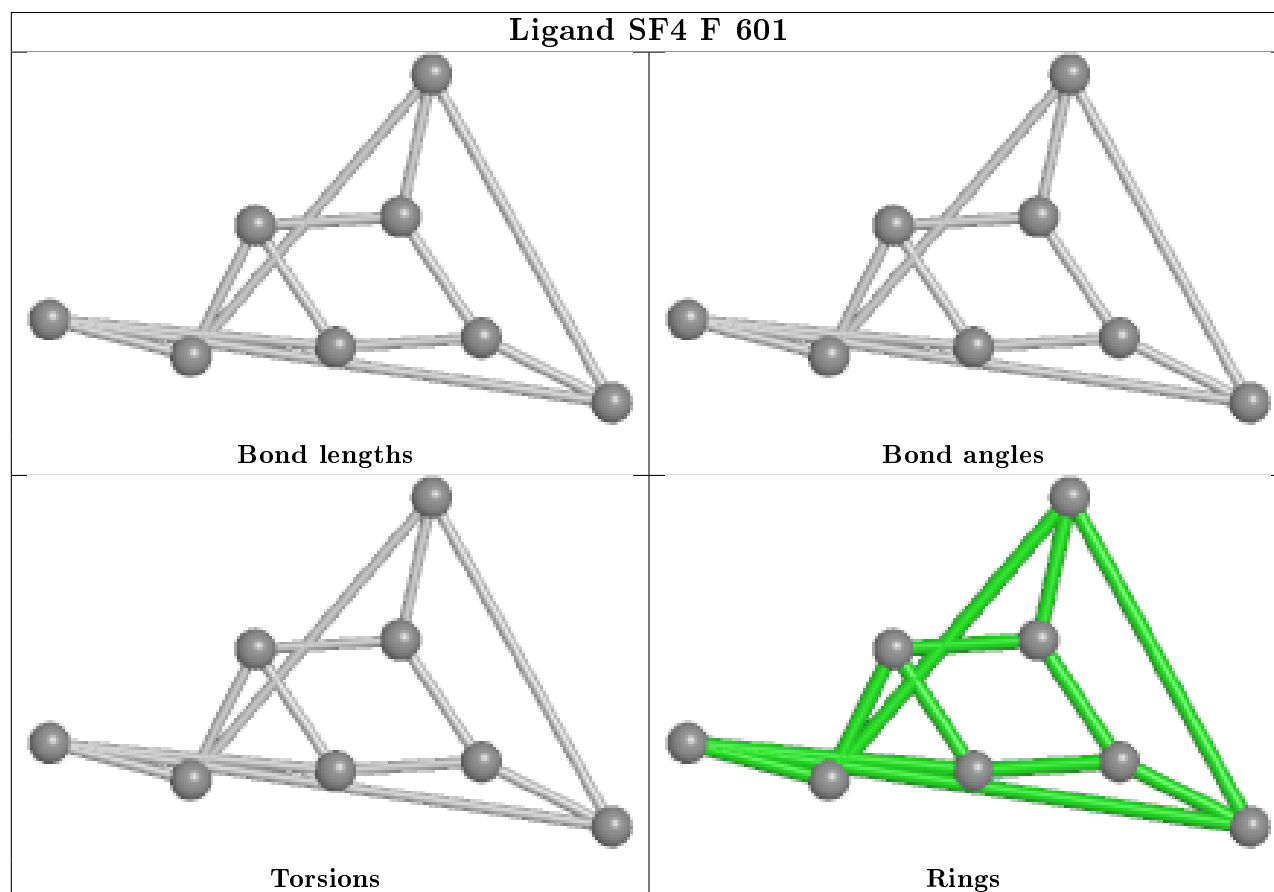
There are no ring outliers.

7 monomers are involved in 15 short contacts:

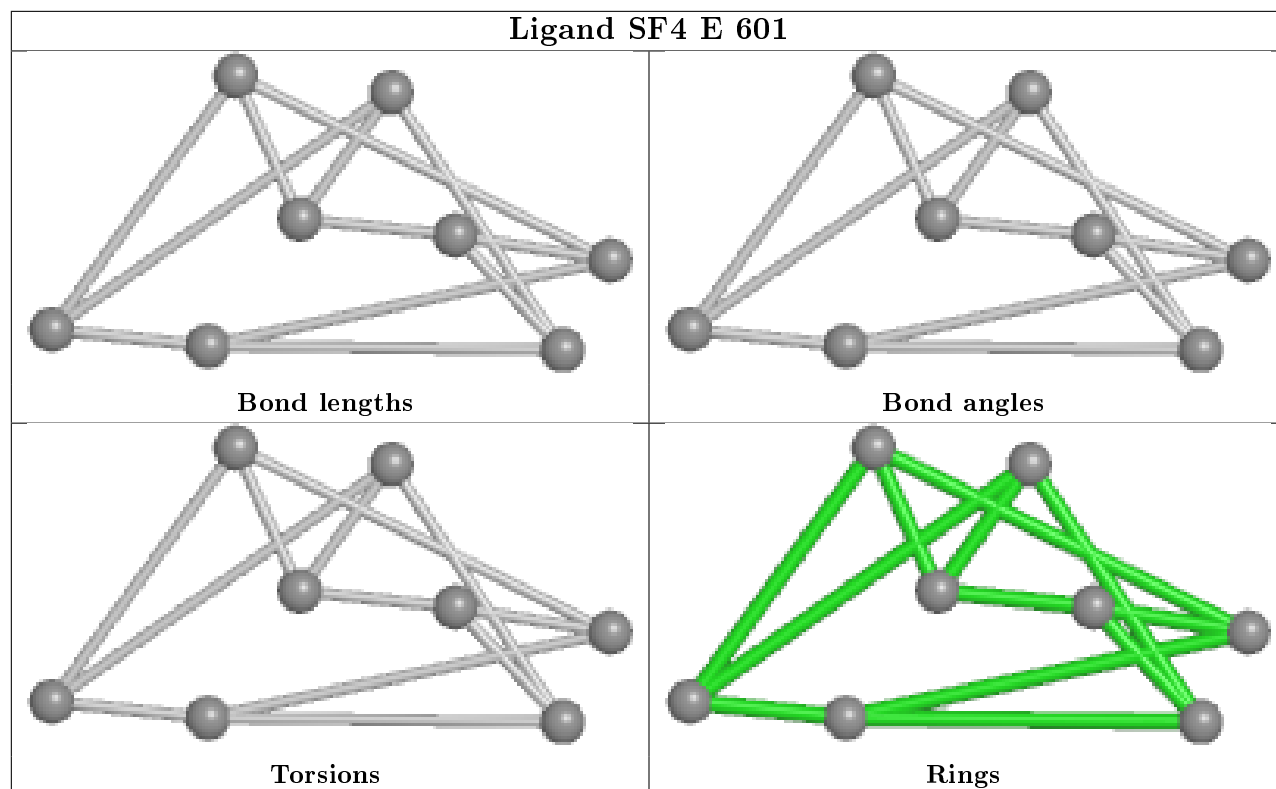
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	GOL	2	0
2	F	601	SF4	3	0
2	E	601	SF4	1	0
2	B	601	SF4	2	0
2	A	601	SF4	1	0
2	C	601	SF4	5	0
3	E	602	GOL	1	0

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

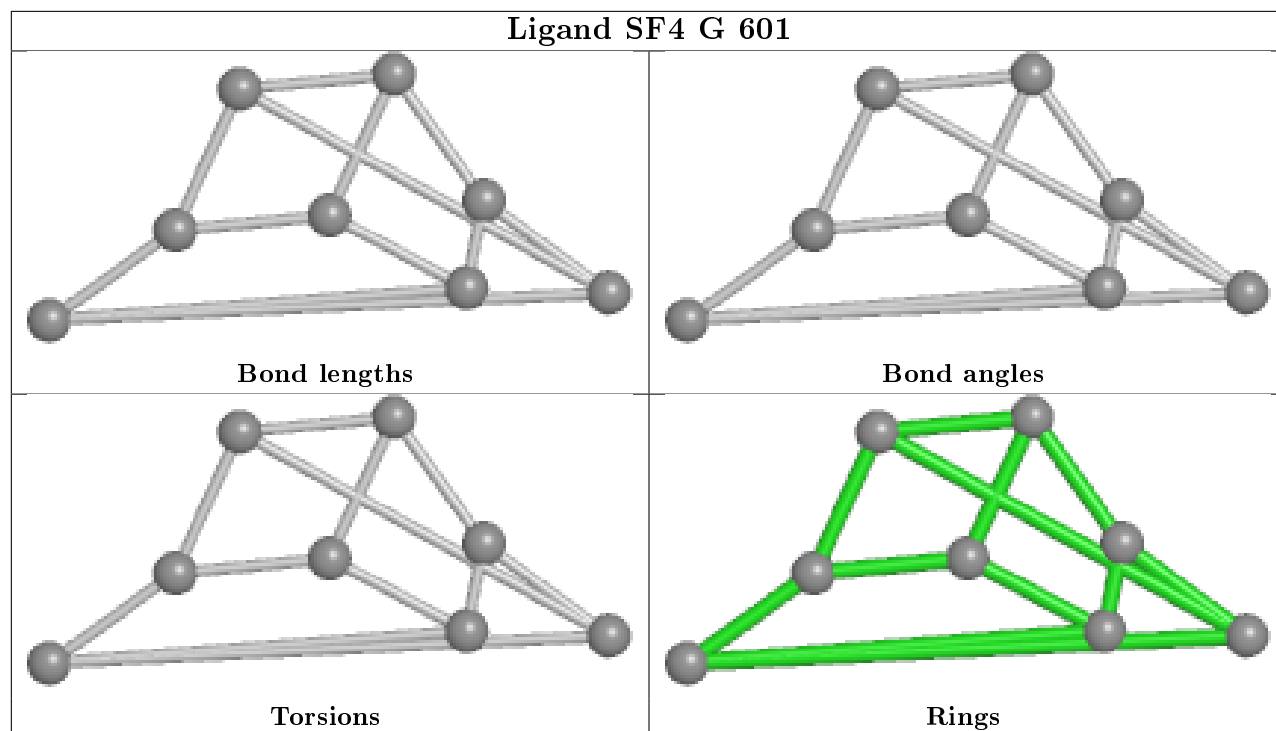
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



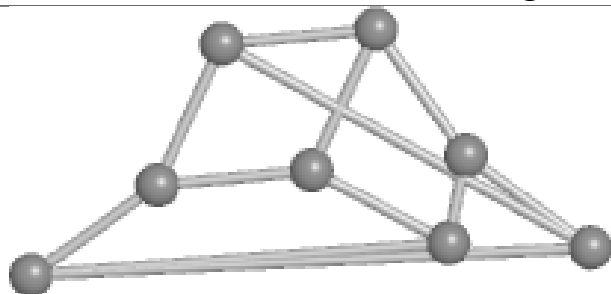
Ligand SF4 E 601



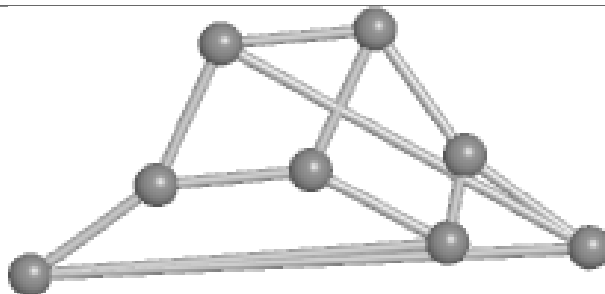
Ligand SF4 G 601



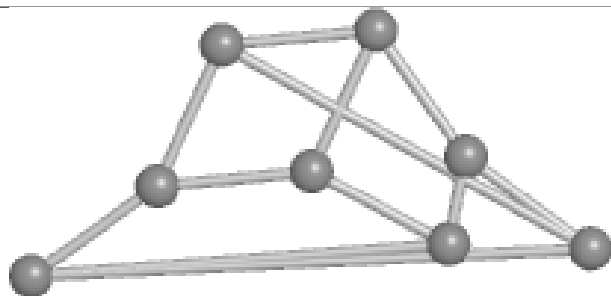
Ligand SF4 B 601



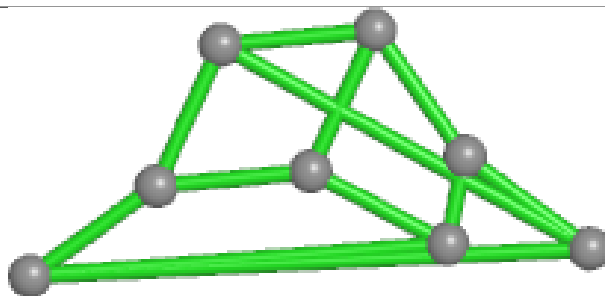
Bond lengths



Bond angles

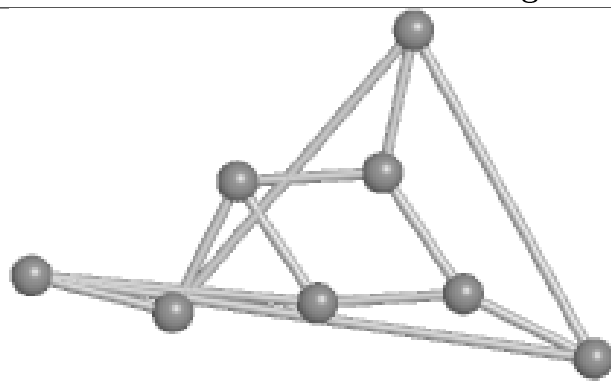


Torsions

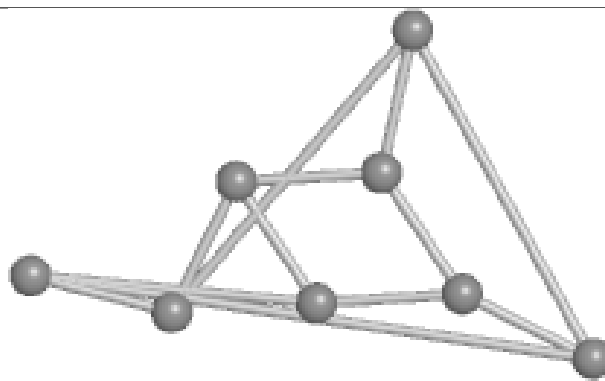


Rings

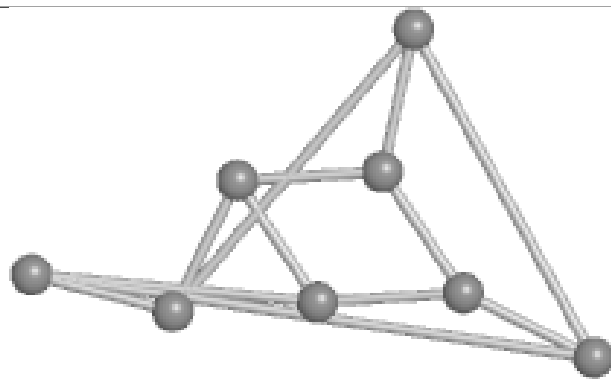
Ligand SF4 A 601



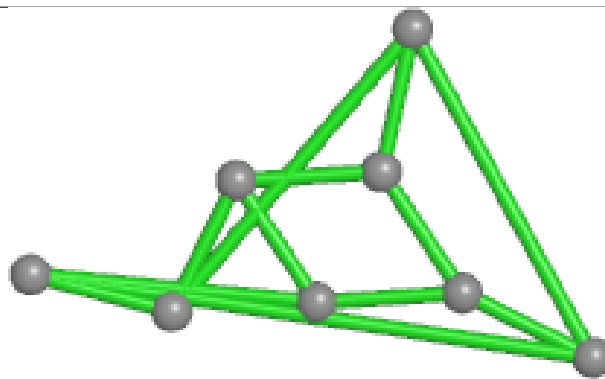
Bond lengths



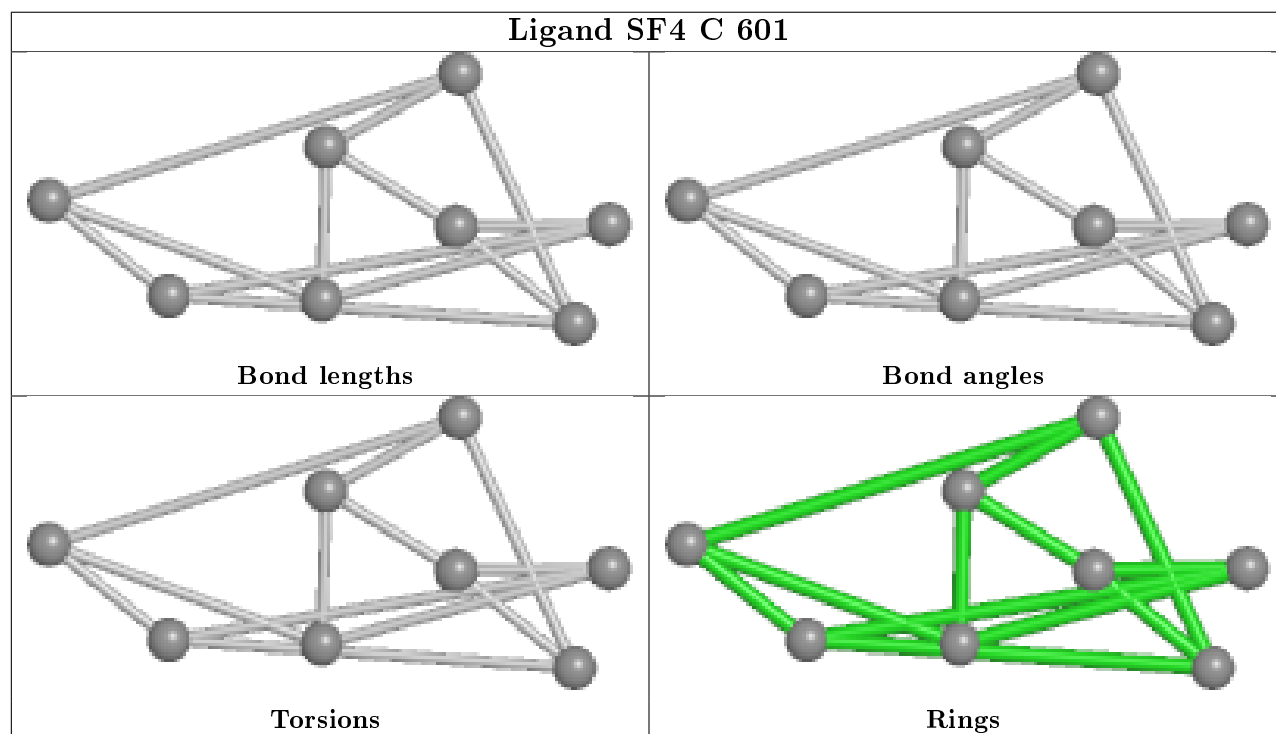
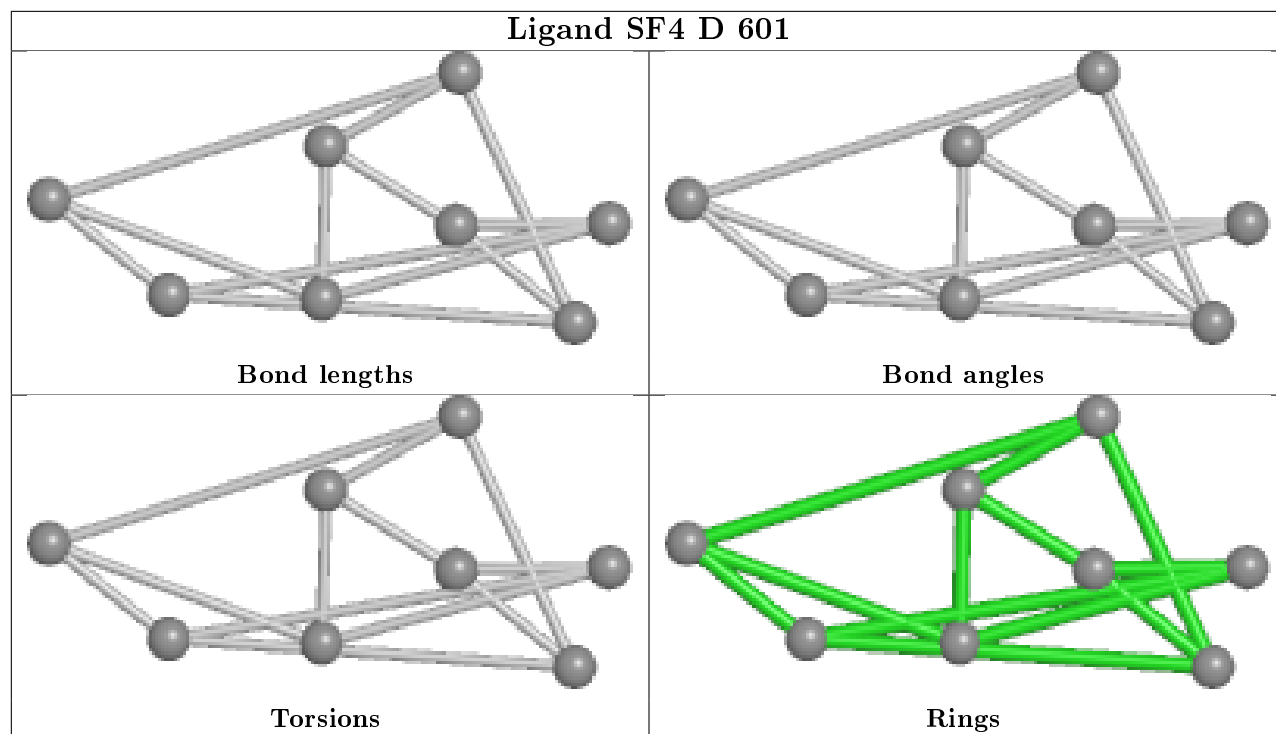
Bond angles

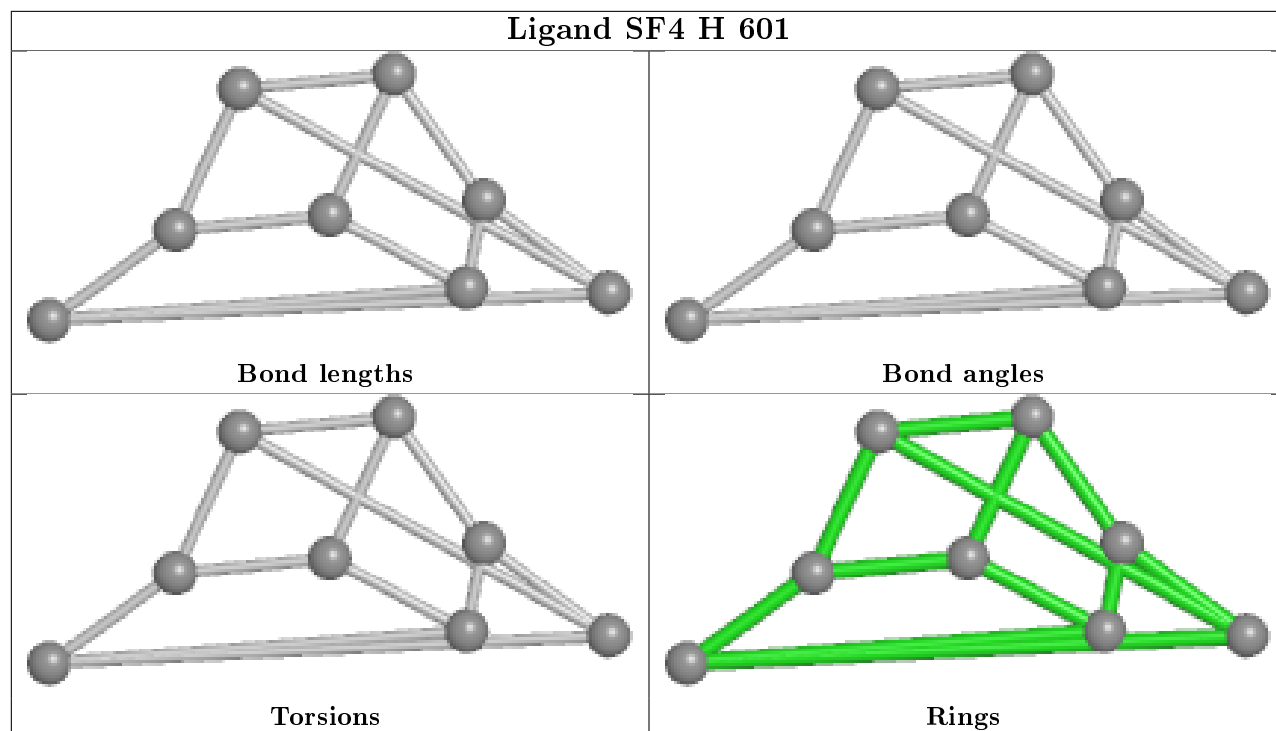


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	539/604 (89%)	1.50	133 (24%) 0 0	23, 58, 89, 106	0
1	B	534/604 (88%)	1.39	121 (22%) 0 0	24, 50, 79, 89	0
1	C	532/604 (88%)	1.68	173 (32%) 0 0	37, 80, 91, 100	0
1	D	530/604 (87%)	1.66	168 (31%) 0 0	29, 72, 89, 102	0
1	E	531/604 (87%)	1.76	177 (33%) 0 0	34, 65, 92, 103	0
1	F	531/604 (87%)	1.28	118 (22%) 0 0	34, 57, 71, 81	0
1	G	532/604 (88%)	1.71	173 (32%) 0 0	28, 66, 91, 102	0
1	H	531/604 (87%)	1.52	153 (28%) 0 0	22, 65, 88, 111	0
All	All	4260/4832 (88%)	1.56	1216 (28%) 0 0	22, 64, 89, 111	0

All (1216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	ALA	13.7
1	C	437	PRO	12.8
1	E	489	LEU	12.8
1	E	547	GLU	12.7
1	A	480	GLN	12.7
1	G	490	ALA	10.7
1	F	427	LYS	9.5
1	E	488	THR	8.6
1	G	369	ASN	8.2
1	D	332	PRO	8.2
1	E	409	THR	8.2
1	C	439	PRO	8.1
1	E	490	ALA	8.0
1	H	140	ILE	7.9
1	E	118	LEU	7.9
1	E	264	THR	7.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	400	GLN	7.8
1	H	475	TYR	7.8
1	A	482	HIS	7.7
1	D	506	GLY	7.6
1	C	419	VAL	7.6
1	A	395	ILE	7.6
1	A	525	ILE	7.4
1	D	141	VAL	7.3
1	D	435	GLY	7.3
1	D	259	LEU	7.2
1	H	189	GLY	7.2
1	D	36	GLN	7.1
1	G	249	THR	7.1
1	G	534	PRO	7.1
1	G	507	GLY	7.0
1	E	116	THR	6.9
1	A	130	LEU	6.9
1	A	536	LEU	6.9
1	E	509	TYR	6.9
1	E	372	GLN	6.9
1	H	530	CYS	6.8
1	D	371	ALA	6.8
1	A	483	GLY	6.8
1	A	396	ASP	6.7
1	E	415	GLY	6.7
1	G	79	ALA	6.7
1	D	255	TYR	6.7
1	G	413	LEU	6.7
1	D	253	PRO	6.7
1	G	535	GLU	6.7
1	F	475	TYR	6.7
1	E	125	ALA	6.6
1	E	560	ASN	6.6
1	G	117	THR	6.5
1	G	508	PHE	6.5
1	F	450	ALA	6.5
1	C	522	LYS	6.5
1	B	470	GLY	6.5
1	E	469	ALA	6.5
1	B	530	CYS	6.5
1	G	390	ASP	6.5
1	E	446	PRO	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	287	THR	6.4
1	G	118	LEU	6.4
1	B	33	ALA	6.4
1	H	101	ALA	6.4
1	H	188	THR	6.3
1	A	193	PRO	6.3
1	G	500	ASP	6.3
1	H	449	TYR	6.2
1	H	507	GLY	6.2
1	C	193	PRO	6.2
1	H	316	GLN	6.2
1	G	524	SER	6.2
1	D	248	GLY	6.1
1	G	468	THR	6.1
1	D	227	THR	6.1
1	D	254	PRO	6.0
1	B	259	LEU	6.0
1	B	507	GLY	6.0
1	A	458	GLY	6.0
1	H	456	PRO	6.0
1	D	434	ASN	6.0
1	D	436	GLU	5.9
1	G	442	MET	5.9
1	E	430	GLU	5.9
1	B	429	LYS	5.9
1	A	178	ALA	5.9
1	A	342	LEU	5.9
1	H	535	GLU	5.9
1	G	512	SER	5.9
1	G	153	GLY	5.9
1	F	430	GLU	5.8
1	B	403	SER	5.8
1	D	411	VAL	5.8
1	A	485	SER	5.8
1	A	484	GLY	5.8
1	D	322	PHE	5.8
1	F	563	TYR	5.8
1	C	486	TYR	5.8
1	E	484	GLY	5.8
1	E	480	GLN	5.8
1	E	419	VAL	5.8
1	A	420	ALA	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	441	TYR	5.7
1	D	142	LEU	5.7
1	B	557	ASP	5.7
1	G	316	GLN	5.7
1	G	525	ILE	5.7
1	E	520	LEU	5.6
1	A	432	MET	5.6
1	A	111	ASP	5.6
1	C	223	LEU	5.6
1	C	224	TYR	5.5
1	C	537	GLY	5.5
1	E	40	PRO	5.5
1	C	168	ARG	5.5
1	G	559	GLY	5.5
1	H	184	LYS	5.5
1	C	523	ASP	5.5
1	G	416	THR	5.5
1	D	493	ASN	5.5
1	H	427	LYS	5.5
1	G	511	GLY	5.4
1	A	543	LYS	5.4
1	A	535	GLU	5.4
1	H	540	ALA	5.4
1	F	507	GLY	5.4
1	B	482	HIS	5.4
1	F	426	ALA	5.4
1	D	412	MET	5.4
1	C	519	ILE	5.4
1	D	242	GLU	5.4
1	H	470	GLY	5.4
1	H	317	PHE	5.4
1	G	564	SER	5.3
1	D	468	THR	5.3
1	C	392	LYS	5.3
1	E	471	ARG	5.3
1	C	517	ALA	5.3
1	A	131	PRO	5.3
1	G	163	ILE	5.3
1	C	263	GLY	5.3
1	B	404	GLN	5.3
1	A	481	SER	5.2
1	E	532	ALA	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	394	PRO	5.2
1	H	411	VAL	5.2
1	E	117	THR	5.2
1	B	542	TRP	5.2
1	A	343	ALA	5.2
1	D	401	GLN	5.2
1	E	394	PRO	5.2
1	E	548	ASP	5.2
1	C	75	LEU	5.1
1	B	419	VAL	5.1
1	H	48	ALA	5.1
1	D	247	LEU	5.1
1	C	501	ALA	5.1
1	C	225	GLN	5.1
1	E	375	PRO	5.1
1	G	114	VAL	5.1
1	E	371	ALA	5.1
1	D	266	ALA	5.1
1	A	552	PHE	5.1
1	B	508	PHE	5.1
1	B	141	VAL	5.1
1	H	533	PHE	5.0
1	E	132	SER	5.0
1	C	500	ASP	5.0
1	C	385	THR	5.0
1	B	387	VAL	5.0
1	B	405	TYR	5.0
1	A	413	LEU	5.0
1	D	33	ALA	5.0
1	F	527	GLN	5.0
1	H	486	TYR	5.0
1	D	68	LEU	4.9
1	G	443	LYS	4.9
1	E	524	SER	4.9
1	E	432	MET	4.9
1	A	438	LEU	4.9
1	B	566	THR	4.9
1	G	315	ALA	4.9
1	D	88	HIS	4.8
1	G	298	PRO	4.8
1	H	195	GLN	4.8
1	B	227	THR	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	450	ALA	4.7
1	G	520	LEU	4.7
1	H	541	VAL	4.7
1	E	559	GLY	4.7
1	H	415	GLY	4.7
1	H	261	ILE	4.7
1	D	257	ILE	4.7
1	H	416	THR	4.7
1	G	105	PRO	4.7
1	C	411	VAL	4.7
1	F	359	SER	4.7
1	H	455	THR	4.6
1	A	175	SER	4.6
1	C	190	ASP	4.6
1	H	229	ALA	4.6
1	B	451	GLY	4.6
1	G	375	PRO	4.6
1	B	539	GLU	4.6
1	B	295	PHE	4.6
1	D	540	ALA	4.6
1	A	98	TRP	4.6
1	H	433	ASP	4.6
1	E	445	SER	4.6
1	G	132	SER	4.6
1	B	284	LEU	4.6
1	C	347	SER	4.5
1	D	239	PHE	4.5
1	F	389	VAL	4.5
1	B	345	SER	4.5
1	C	169	TYR	4.5
1	F	186	CYS	4.5
1	A	341	GLY	4.5
1	D	246	THR	4.5
1	B	426	ALA	4.5
1	D	105	PRO	4.5
1	E	413	LEU	4.5
1	E	422	ASP	4.5
1	G	513	ILE	4.5
1	C	50	VAL	4.4
1	F	467	THR	4.4
1	G	469	ALA	4.4
1	D	405	TYR	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	485	SER	4.4
1	C	74	ALA	4.4
1	B	492	GLY	4.4
1	H	167	TYR	4.4
1	C	119	LEU	4.4
1	C	130	LEU	4.4
1	D	260	VAL	4.4
1	E	339	PRO	4.4
1	E	417	LEU	4.4
1	D	508	PHE	4.4
1	E	373	TYR	4.4
1	A	556	ASP	4.4
1	D	281	TYR	4.3
1	D	502	CYS	4.3
1	E	534	PRO	4.3
1	E	368	GLN	4.3
1	B	386	SER	4.3
1	E	102	ILE	4.3
1	E	218	ALA	4.3
1	C	402	LEU	4.3
1	H	422	ASP	4.3
1	F	455	THR	4.3
1	H	227	THR	4.3
1	D	490	ALA	4.3
1	C	165	ASN	4.3
1	G	396	ASP	4.3
1	E	400	GLN	4.3
1	C	484	GLY	4.3
1	B	233	PRO	4.3
1	H	426	ALA	4.3
1	H	511	GLY	4.3
1	A	479	PHE	4.3
1	C	346	CYS	4.3
1	H	185	GLU	4.2
1	B	390	ASP	4.2
1	G	548	ASP	4.2
1	C	222	TYR	4.2
1	E	475	TYR	4.2
1	E	429	LYS	4.2
1	G	172	LEU	4.2
1	B	499	THR	4.2
1	G	488	THR	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	212	ALA	4.2
1	H	442	MET	4.2
1	G	516	PRO	4.2
1	G	540	ALA	4.2
1	G	339	PRO	4.2
1	B	396	ASP	4.2
1	H	333	ARG	4.2
1	E	511	GLY	4.2
1	F	506	GLY	4.2
1	F	528	VAL	4.2
1	A	90	PHE	4.1
1	D	533	PHE	4.1
1	G	528	VAL	4.1
1	H	487	ILE	4.1
1	E	500	ASP	4.1
1	F	478	LEU	4.1
1	D	398	VAL	4.1
1	E	241	GLU	4.1
1	G	486	TYR	4.1
1	C	203	GLY	4.1
1	G	317	PHE	4.1
1	G	509	TYR	4.1
1	H	203	GLY	4.1
1	E	98	TRP	4.1
1	H	453	ALA	4.1
1	C	117	THR	4.1
1	C	502	CYS	4.1
1	D	359	SER	4.1
1	A	462	GLY	4.1
1	G	541	VAL	4.1
1	B	255	TYR	4.1
1	B	485	SER	4.1
1	H	38	THR	4.1
1	E	399	ARG	4.1
1	D	209	LEU	4.1
1	E	406	PRO	4.0
1	E	124	ILE	4.0
1	G	441	TYR	4.0
1	E	508	PHE	4.0
1	H	439	PRO	4.0
1	B	336	ALA	4.0
1	E	416	THR	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	180	LEU	4.0
1	C	264	THR	4.0
1	H	483	GLY	4.0
1	F	532	ALA	4.0
1	A	412	MET	4.0
1	B	45	THR	4.0
1	B	477	ASP	4.0
1	G	409	THR	4.0
1	B	402	LEU	4.0
1	G	78	LEU	4.0
1	H	126	ALA	4.0
1	C	221	ALA	4.0
1	F	125	ALA	4.0
1	H	454	LYS	4.0
1	G	510	LEU	4.0
1	C	457	GLU	3.9
1	E	514	GLY	3.9
1	A	419	VAL	3.9
1	H	234	LYS	3.9
1	C	166	ALA	3.9
1	D	194	ALA	3.9
1	D	336	ALA	3.9
1	H	413	LEU	3.9
1	A	24	ALA	3.9
1	D	425	HIS	3.9
1	B	406	PRO	3.9
1	E	456	PRO	3.9
1	G	110	ASN	3.9
1	A	421	ARG	3.9
1	A	137	GLY	3.9
1	B	463	SER	3.9
1	H	432	MET	3.8
1	D	389	VAL	3.8
1	D	426	ALA	3.8
1	G	555	VAL	3.8
1	G	362	TYR	3.8
1	D	59	GLU	3.8
1	B	493	ASN	3.8
1	C	77	ILE	3.8
1	A	442	MET	3.8
1	C	481	SER	3.8
1	D	67	ALA	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	483	GLY	3.8
1	C	122	ALA	3.8
1	E	115	ALA	3.8
1	E	496	LYS	3.8
1	G	251	ALA	3.8
1	D	64	GLY	3.8
1	G	31	PHE	3.8
1	C	405	TYR	3.8
1	A	317	PHE	3.8
1	H	322	PHE	3.8
1	H	478	LEU	3.8
1	C	324	HIS	3.8
1	C	490	ALA	3.8
1	G	385	THR	3.8
1	C	438	LEU	3.8
1	F	484	GLY	3.8
1	C	182	MET	3.7
1	F	477	ASP	3.7
1	E	317	PHE	3.7
1	G	181	ASP	3.7
1	G	323	ALA	3.7
1	C	463	SER	3.7
1	H	465	GLY	3.7
1	B	427	LYS	3.7
1	C	338	CYS	3.7
1	G	304	VAL	3.7
1	B	431	MET	3.7
1	G	250	ALA	3.7
1	A	328	VAL	3.7
1	H	476	VAL	3.7
1	C	512	SER	3.7
1	D	215	GLY	3.7
1	E	340	VAL	3.7
1	E	175	SER	3.7
1	C	136	THR	3.7
1	C	525	ILE	3.7
1	D	56	TYR	3.7
1	A	315	ALA	3.6
1	C	418	ILE	3.6
1	D	338	CYS	3.6
1	H	129	VAL	3.6
1	C	51	GLU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	440	GLU	3.6
1	G	368	GLN	3.6
1	E	566	THR	3.6
1	F	508	PHE	3.6
1	A	156	GLU	3.6
1	B	189	GLY	3.6
1	E	316	GLN	3.6
1	C	460	ALA	3.6
1	E	515	GLY	3.6
1	E	331	LEU	3.6
1	A	560	ASN	3.6
1	G	357	ASN	3.6
1	B	258	ALA	3.6
1	D	111	ASP	3.6
1	E	320	LYS	3.6
1	A	257	ILE	3.6
1	D	492	GLY	3.6
1	A	538	MET	3.6
1	D	454	LYS	3.6
1	E	563	TYR	3.6
1	D	108	SER	3.6
1	A	441	TYR	3.6
1	A	435	GLY	3.6
1	E	567	LEU	3.6
1	B	209	LEU	3.6
1	E	252	CYS	3.6
1	G	487	ILE	3.5
1	F	441	TYR	3.5
1	G	429	LYS	3.5
1	B	438	LEU	3.5
1	C	518	ALA	3.5
1	G	221	ALA	3.5
1	G	232	ASN	3.5
1	H	534	PRO	3.5
1	C	410	ARG	3.5
1	C	478	LEU	3.5
1	C	491	LYS	3.5
1	D	483	GLY	3.5
1	E	343	ALA	3.5
1	E	472	MET	3.5
1	C	462	GLY	3.5
1	H	125	ALA	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	485	SER	3.5
1	E	90	PHE	3.5
1	H	294	ALA	3.5
1	B	224	TYR	3.5
1	E	525	ILE	3.5
1	A	80	HIS	3.5
1	G	97	GLY	3.5
1	H	508	PHE	3.5
1	A	488	THR	3.5
1	G	283	SER	3.5
1	C	303	ILE	3.5
1	D	462	GLY	3.5
1	D	284	LEU	3.5
1	H	423	ILE	3.5
1	C	197	ASP	3.4
1	D	198	LEU	3.4
1	B	194	ALA	3.4
1	A	467	THR	3.4
1	C	529	THR	3.4
1	H	83	PHE	3.4
1	E	79	ALA	3.4
1	E	531	LEU	3.4
1	H	473	ASP	3.4
1	A	403	SER	3.4
1	D	214	GLY	3.4
1	C	188	THR	3.4
1	G	538	MET	3.4
1	E	105	PRO	3.4
1	F	254	PRO	3.4
1	F	551	ALA	3.4
1	A	422	ASP	3.4
1	B	545	GLU	3.4
1	C	547	GLU	3.4
1	B	490	ALA	3.4
1	F	489	LEU	3.4
1	F	483	GLY	3.4
1	D	285	PRO	3.4
1	A	436	GLU	3.4
1	A	177	THR	3.4
1	C	199	LEU	3.3
1	C	365	GLN	3.3
1	F	444	THR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	479	PHE	3.3
1	A	168	ARG	3.3
1	C	422	ASP	3.3
1	C	458	GLY	3.3
1	E	390	ASP	3.3
1	C	493	ASN	3.3
1	G	480	GLN	3.3
1	C	528	VAL	3.3
1	G	322	PHE	3.3
1	G	321	TYR	3.3
1	H	539	GLU	3.3
1	A	461	SER	3.3
1	G	489	LEU	3.3
1	E	329	ILE	3.3
1	C	137	GLY	3.3
1	F	210	PHE	3.3
1	G	464	PHE	3.3
1	H	505	HIS	3.3
1	D	289	ASP	3.3
1	B	355	HIS	3.3
1	D	191	ASN	3.3
1	F	530	CYS	3.3
1	G	372	GLN	3.3
1	D	318	GLY	3.3
1	G	473	ASP	3.3
1	G	186	CYS	3.2
1	B	337	SER	3.2
1	B	246	THR	3.2
1	D	29	PHE	3.2
1	H	561	ASP	3.2
1	C	172	LEU	3.2
1	C	444	THR	3.2
1	F	409	THR	3.2
1	B	282	ASP	3.2
1	E	555	VAL	3.2
1	G	493	ASN	3.2
1	D	31	PHE	3.2
1	B	93	ASP	3.2
1	H	568	ALA	3.2
1	A	493	ASN	3.2
1	B	347	SER	3.2
1	C	226	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	567	LEU	3.2
1	F	195	GLN	3.2
1	D	476	VAL	3.2
1	C	132	SER	3.2
1	C	431	MET	3.2
1	E	420	ALA	3.2
1	F	541	VAL	3.2
1	G	426	ALA	3.2
1	A	478	LEU	3.2
1	B	32	SER	3.2
1	F	388	LYS	3.2
1	C	386	SER	3.2
1	E	564	SER	3.2
1	C	123	CYS	3.2
1	D	461	SER	3.1
1	H	434	ASN	3.1
1	A	106	GLU	3.1
1	A	249	THR	3.1
1	D	155	ASP	3.1
1	G	391	LEU	3.1
1	E	356	ILE	3.1
1	H	447	ILE	3.1
1	B	568	ALA	3.1
1	D	400	GLN	3.1
1	D	564	SER	3.1
1	B	300	TRP	3.1
1	E	503	LYS	3.1
1	G	484	GLY	3.1
1	B	399	ARG	3.1
1	H	253	PRO	3.1
1	C	126	ALA	3.1
1	A	159	LEU	3.1
1	D	152	GLY	3.1
1	H	506	GLY	3.1
1	F	485	SER	3.1
1	G	485	SER	3.1
1	C	459	TYR	3.1
1	F	531	LEU	3.1
1	C	401	GLN	3.1
1	H	389	VAL	3.1
1	D	366	LEU	3.1
1	E	231	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	471	ARG	3.1
1	H	513	ILE	3.1
1	A	345	SER	3.1
1	E	321	TYR	3.1
1	D	211	ILE	3.1
1	G	407	VAL	3.1
1	A	540	ALA	3.1
1	B	193	PRO	3.1
1	D	232	ASN	3.1
1	D	481	SER	3.1
1	D	272	THR	3.1
1	H	127	GLY	3.1
1	H	262	GLY	3.1
1	C	353	LEU	3.1
1	E	421	ARG	3.1
1	A	339	PRO	3.0
1	C	562	MET	3.0
1	C	194	ALA	3.0
1	F	479	PHE	3.0
1	B	434	ASN	3.0
1	F	126	ALA	3.0
1	D	37	PRO	3.0
1	E	444	THR	3.0
1	E	60	VAL	3.0
1	G	119	LEU	3.0
1	B	535	GLU	3.0
1	A	431	MET	3.0
1	B	67	ALA	3.0
1	B	242	GLU	3.0
1	H	558	LYS	3.0
1	D	319	GLY	3.0
1	H	509	TYR	3.0
1	C	546	VAL	3.0
1	C	368	GLN	3.0
1	A	28	ASP	3.0
1	F	403	SER	3.0
1	F	472	MET	3.0
1	B	420	ALA	3.0
1	F	486	TYR	3.0
1	G	313	ILE	3.0
1	C	236	LEU	3.0
1	F	373	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	159	LEU	3.0
1	C	342	LEU	3.0
1	E	402	LEU	3.0
1	F	534	PRO	3.0
1	B	388	LYS	2.9
1	B	253	PRO	2.9
1	B	346	CYS	2.9
1	H	462	GLY	2.9
1	C	243	LYS	2.9
1	D	424	ALA	2.9
1	D	297	ASP	2.9
1	H	235	SER	2.9
1	D	437	PRO	2.9
1	A	537	GLY	2.9
1	A	548	ASP	2.9
1	B	433	ASP	2.9
1	H	435	GLY	2.9
1	E	481	SER	2.9
1	F	524	SER	2.9
1	A	308	ALA	2.9
1	E	33	ALA	2.9
1	G	460	ALA	2.9
1	F	529	THR	2.9
1	G	113	TYR	2.9
1	H	113	TYR	2.9
1	D	282	ASP	2.9
1	A	568	ALA	2.9
1	C	113	TYR	2.9
1	C	461	SER	2.9
1	D	238	ALA	2.9
1	D	250	ALA	2.9
1	E	171	ASN	2.9
1	G	482	HIS	2.9
1	G	297	ASP	2.9
1	F	466	PRO	2.9
1	H	324	HIS	2.9
1	F	164	TRP	2.9
1	G	138	THR	2.9
1	G	269	THR	2.9
1	A	490	ALA	2.9
1	C	357	ASN	2.9
1	F	488	THR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	352	ILE	2.9
1	G	115	ALA	2.9
1	D	213	LYS	2.9
1	D	544	ILE	2.9
1	E	499	THR	2.9
1	B	509	TYR	2.9
1	G	224	TYR	2.9
1	D	355	HIS	2.9
1	C	432	MET	2.9
1	C	536	LEU	2.9
1	F	369	ASN	2.9
1	E	47	PHE	2.9
1	G	494	ARG	2.9
1	E	366	LEU	2.9
1	H	528	VAL	2.8
1	F	139	ALA	2.8
1	H	420	ALA	2.8
1	D	484	GLY	2.8
1	H	163	ILE	2.8
1	A	521	ALA	2.8
1	E	205	ASP	2.8
1	A	406	PRO	2.8
1	C	423	ILE	2.8
1	G	471	ARG	2.8
1	B	84	SER	2.8
1	F	177	THR	2.8
1	E	510	LEU	2.8
1	C	257	ILE	2.8
1	C	150	TRP	2.8
1	G	551	ALA	2.8
1	G	515	GLY	2.8
1	G	365	GLN	2.8
1	E	38	THR	2.8
1	F	476	VAL	2.8
1	H	482	HIS	2.8
1	A	122	ALA	2.8
1	D	150	TRP	2.8
1	G	366	LEU	2.8
1	F	519	ILE	2.8
1	G	546	VAL	2.8
1	E	354	ALA	2.8
1	F	560	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	258	ALA	2.8
1	E	348	ALA	2.8
1	G	211	ILE	2.8
1	A	174	TYR	2.8
1	C	415	GLY	2.8
1	E	137	GLY	2.8
1	E	298	PRO	2.8
1	G	343	ALA	2.8
1	G	187	ASN	2.8
1	B	262	GLY	2.8
1	C	492	GLY	2.8
1	A	340	VAL	2.8
1	E	355	HIS	2.8
1	H	181	ASP	2.8
1	C	128	ARG	2.8
1	C	230	LEU	2.8
1	A	197	ASP	2.8
1	F	411	VAL	2.7
1	H	549	PHE	2.7
1	D	447	ILE	2.7
1	H	529	THR	2.7
1	F	141	VAL	2.7
1	F	446	PRO	2.7
1	H	187	ASN	2.7
1	A	164	TRP	2.7
1	H	259	LEU	2.7
1	C	479	PHE	2.7
1	A	332	PRO	2.7
1	G	309	GLN	2.7
1	F	127	GLY	2.7
1	E	407	VAL	2.7
1	H	114	VAL	2.7
1	B	235	SER	2.7
1	H	440	GLU	2.7
1	C	433	ASP	2.7
1	D	390	ASP	2.7
1	G	533	PHE	2.7
1	C	64	GLY	2.7
1	F	511	GLY	2.7
1	E	220	LYS	2.7
1	E	239	PHE	2.7
1	B	444	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	100	ARG	2.7
1	F	443	LYS	2.7
1	C	129	VAL	2.7
1	E	260	VAL	2.7
1	G	400	GLN	2.7
1	C	445	SER	2.7
1	C	428	ILE	2.7
1	E	418	ILE	2.7
1	E	401	GLN	2.7
1	A	344	VAL	2.7
1	C	79	ALA	2.7
1	G	459	TYR	2.7
1	C	227	THR	2.7
1	E	468	THR	2.7
1	E	464	PHE	2.7
1	E	465	GLY	2.7
1	F	129	VAL	2.7
1	F	291	TYR	2.6
1	G	449	TYR	2.6
1	G	521	ALA	2.7
1	B	510	LEU	2.6
1	F	410	ARG	2.6
1	G	444	THR	2.6
1	A	466	PRO	2.6
1	B	222	TYR	2.6
1	D	256	HIS	2.6
1	A	387	VAL	2.6
1	D	408	GLY	2.6
1	F	114	VAL	2.6
1	F	429	LYS	2.6
1	H	260	VAL	2.6
1	F	317	PHE	2.6
1	E	473	ASP	2.6
1	A	409	THR	2.6
1	B	272	THR	2.6
1	F	46	GLU	2.6
1	H	134	GLN	2.6
1	H	538	MET	2.6
1	C	358	LYS	2.6
1	E	512	SER	2.6
1	C	242	GLU	2.6
1	F	249	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	280	TYR	2.6
1	D	293	ARG	2.6
1	F	456	PRO	2.6
1	B	263	GLY	2.6
1	F	542	TRP	2.6
1	B	223	LEU	2.6
1	F	561	ASP	2.6
1	G	363	ILE	2.6
1	D	258	ALA	2.6
1	E	410	ARG	2.6
1	C	406	PRO	2.6
1	D	465	GLY	2.6
1	D	507	GLY	2.6
1	G	514	GLY	2.6
1	G	342	LEU	2.6
1	G	549	PHE	2.6
1	B	344	VAL	2.6
1	B	452	PRO	2.6
1	E	96	GLU	2.6
1	F	52	GLY	2.6
1	A	78	LEU	2.6
1	G	65	ARG	2.6
1	E	450	ALA	2.6
1	F	123	CYS	2.6
1	A	242	GLU	2.6
1	F	264	THR	2.6
1	B	257	ILE	2.6
1	A	321	TYR	2.6
1	C	229	ALA	2.6
1	G	373	TYR	2.6
1	A	338	CYS	2.6
1	E	114	VAL	2.6
1	A	439	PRO	2.6
1	C	90	PHE	2.6
1	F	89	PHE	2.6
1	A	169	TYR	2.6
1	G	294	ALA	2.6
1	A	474	SER	2.6
1	H	545	GLU	2.6
1	C	393	ARG	2.6
1	E	398	VAL	2.6
1	E	523	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	466	PRO	2.6
1	G	46	GLU	2.5
1	B	279	ARG	2.5
1	C	181	ASP	2.5
1	D	417	LEU	2.5
1	H	488	THR	2.5
1	D	164	TRP	2.5
1	G	364	GLU	2.5
1	E	236	LEU	2.5
1	E	391	LEU	2.5
1	B	394	PRO	2.5
1	G	553	ILE	2.5
1	E	191	ASN	2.5
1	E	369	ASN	2.5
1	A	566	THR	2.5
1	H	269	THR	2.5
1	G	465	GLY	2.5
1	D	231	LEU	2.5
1	E	536	LEU	2.5
1	G	479	PHE	2.5
1	C	81	ARG	2.5
1	G	399	ARG	2.5
1	B	425	HIS	2.5
1	A	312	GLY	2.5
1	F	492	GLY	2.5
1	H	404	GLN	2.5
1	D	478	LEU	2.5
1	H	186	CYS	2.5
1	A	246	THR	2.5
1	G	318	GLY	2.5
1	G	223	LEU	2.5
1	G	417	LEU	2.5
1	A	549	PHE	2.5
1	G	412	MET	2.5
1	C	299	GLU	2.5
1	G	40	PRO	2.5
1	F	74	ALA	2.5
1	C	244	LEU	2.5
1	C	127	GLY	2.5
1	D	32	SER	2.5
1	G	314	GLY	2.5
1	C	159	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	309	GLN	2.5
1	B	150	TRP	2.5
1	B	416	THR	2.5
1	F	221	ALA	2.5
1	G	64	GLY	2.5
1	H	57	VAL	2.5
1	F	132	SER	2.5
1	H	550	PRO	2.5
1	A	91	ARG	2.5
1	A	398	VAL	2.5
1	C	420	ALA	2.5
1	A	368	GLN	2.5
1	A	394	PRO	2.5
1	C	69	LYS	2.5
1	A	559	GLY	2.5
1	F	415	GLY	2.5
1	F	449	TYR	2.5
1	A	40	PRO	2.5
1	B	365	GLN	2.5
1	E	439	PRO	2.5
1	H	516	PRO	2.5
1	C	43	HIS	2.5
1	E	386	SER	2.5
1	C	98	TRP	2.5
1	G	286	THR	2.5
1	B	439	PRO	2.5
1	F	37	PRO	2.5
1	D	292	GLY	2.4
1	G	419	VAL	2.4
1	G	354	ALA	2.4
1	G	499	THR	2.4
1	E	295	PHE	2.4
1	E	479	PHE	2.4
1	A	102	ILE	2.4
1	C	340	VAL	2.4
1	D	236	LEU	2.4
1	B	264	THR	2.4
1	F	502	CYS	2.4
1	E	452	PRO	2.4
1	H	452	PRO	2.4
1	A	397	LYS	2.4
1	E	349	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	337	SER	2.4
1	B	142	LEU	2.4
1	D	345	SER	2.4
1	E	180	LEU	2.4
1	E	541	VAL	2.4
1	G	200	ALA	2.4
1	A	116	THR	2.4
1	A	404	GLN	2.4
1	F	51	GLU	2.4
1	F	131	PRO	2.4
1	D	349	ASP	2.4
1	H	477	ASP	2.4
1	D	251	ALA	2.4
1	B	395	ILE	2.4
1	E	304	VAL	2.4
1	B	349	ASP	2.4
1	D	45	THR	2.4
1	E	516	PRO	2.4
1	H	172	LEU	2.4
1	F	559	GLY	2.4
1	C	504	LYS	2.4
1	D	278	CYS	2.4
1	D	326	ALA	2.4
1	D	352	ILE	2.4
1	A	198	LEU	2.4
1	E	527	GLN	2.4
1	G	259	LEU	2.4
1	A	285	PRO	2.4
1	D	302	LYS	2.4
1	E	136	THR	2.4
1	B	229	ALA	2.4
1	C	282	ASP	2.4
1	G	561	ASP	2.4
1	H	557	ASP	2.4
1	C	252	CYS	2.4
1	H	338	CYS	2.4
1	F	510	LEU	2.4
1	B	239	PHE	2.4
1	B	430	GLU	2.4
1	E	449	TYR	2.4
1	G	563	TYR	2.4
1	H	206	TYR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	491	LYS	2.4
1	B	537	GLY	2.4
1	H	401	GLN	2.4
1	C	96	GLU	2.4
1	C	112	ARG	2.4
1	E	414	ASN	2.4
1	F	107	ALA	2.4
1	G	184	LYS	2.4
1	B	29	PHE	2.4
1	A	191	ASN	2.4
1	A	434	ASN	2.4
1	E	165	ASN	2.4
1	F	280	TYR	2.4
1	A	417	LEU	2.4
1	E	280	TYR	2.4
1	F	298	PRO	2.4
1	H	238	ALA	2.4
1	H	160	SER	2.3
1	B	551	ALA	2.3
1	G	356	ILE	2.3
1	G	395	ILE	2.3
1	D	151	THR	2.3
1	E	91	ARG	2.3
1	E	206	TYR	2.3
1	G	167	TYR	2.3
1	C	209	LEU	2.3
1	D	353	LEU	2.3
1	F	566	THR	2.3
1	D	501	ALA	2.3
1	H	417	LEU	2.3
1	H	469	ALA	2.3
1	C	499	THR	2.3
1	E	431	MET	2.3
1	F	562	MET	2.3
1	G	116	THR	2.3
1	H	110	ASN	2.3
1	A	349	ASP	2.3
1	H	44	GLN	2.3
1	E	328	VAL	2.3
1	A	515	GLY	2.3
1	D	499	THR	2.3
1	E	365	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	313	ILE	2.3
1	C	345	SER	2.3
1	C	451	GLY	2.3
1	H	474	SER	2.3
1	D	168	ARG	2.3
1	D	459	TYR	2.3
1	F	93	ASP	2.3
1	G	476	VAL	2.3
1	D	431	MET	2.3
1	A	414	ASN	2.3
1	B	155	ASP	2.3
1	C	258	ALA	2.3
1	D	34	ILE	2.3
1	F	211	ILE	2.3
1	C	344	VAL	2.3
1	D	477	ASP	2.3
1	F	218	ALA	2.3
1	H	551	ALA	2.3
1	H	559	GLY	2.3
1	G	332	PRO	2.3
1	A	508	PHE	2.3
1	E	443	LYS	2.3
1	H	106	GLU	2.3
1	C	66	GLN	2.3
1	F	509	TYR	2.3
1	H	291	TYR	2.3
1	H	542	TRP	2.3
1	B	519	ILE	2.3
1	E	99	ARG	2.3
1	B	546	VAL	2.3
1	D	210	PHE	2.3
1	F	554	VAL	2.3
1	C	319	GLY	2.3
1	D	130	LEU	2.3
1	D	279	ARG	2.3
1	E	412	MET	2.3
1	F	417	LEU	2.3
1	G	446	PRO	2.3
1	B	277	SER	2.3
1	D	160	SER	2.3
1	D	328	VAL	2.3
1	D	482	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	354	ALA	2.3
1	C	133	CYS	2.2
1	B	562	MET	2.2
1	D	104	ASP	2.2
1	H	489	LEU	2.2
1	A	447	ILE	2.2
1	C	456	PRO	2.2
1	A	222	TYR	2.2
1	F	546	VAL	2.2
1	B	283	SER	2.2
1	H	204	SER	2.2
1	D	197	ASP	2.2
1	D	491	LYS	2.2
1	A	487	ILE	2.2
1	A	509	TYR	2.2
1	H	304	VAL	2.2
1	D	368	GLN	2.2
1	E	539	GLU	2.2
1	G	299	GLU	2.2
1	H	460	ALA	2.2
1	E	53	SER	2.2
1	H	520	LEU	2.2
1	H	123	CYS	2.2
1	B	486	TYR	2.2
1	F	73	GLU	2.2
1	H	320	LYS	2.2
1	D	495	SER	2.2
1	G	472	MET	2.2
1	H	546	VAL	2.2
1	B	558	LYS	2.2
1	C	308	ALA	2.2
1	D	568	ALA	2.2
1	G	386	SER	2.2
1	H	445	SER	2.2
1	E	554	VAL	2.2
1	E	207	GLU	2.2
1	F	113	TYR	2.2
1	B	247	LEU	2.2
1	C	391	LEU	2.2
1	D	445	SER	2.2
1	F	445	SER	2.2
1	H	240	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	59	GLU	2.2
1	A	501	ALA	2.2
1	D	548	ASP	2.2
1	E	460	ALA	2.2
1	F	402	LEU	2.2
1	H	309	GLN	2.2
1	H	332	PRO	2.2
1	C	88	HIS	2.2
1	E	307	VAL	2.2
1	D	497	GLN	2.2
1	F	413	LEU	2.2
1	C	558	LYS	2.2
1	F	71	ASN	2.2
1	C	34	ILE	2.2
1	B	72	PRO	2.2
1	C	105	PRO	2.2
1	C	202	PRO	2.2
1	C	516	PRO	2.2
1	G	439	PRO	2.2
1	H	63	PHE	2.2
1	G	152	GLY	2.2
1	E	251	ALA	2.2
1	E	556	ASP	2.2
1	D	97	GLY	2.2
1	D	335	GLY	2.2
1	D	514	GLY	2.2
1	C	180	LEU	2.2
1	D	556	ASP	2.2
1	D	470	GLY	2.2
1	D	374	LEU	2.1
1	E	404	GLN	2.1
1	D	545	GLU	2.1
1	E	546	VAL	2.1
1	E	530	CYS	2.1
1	G	556	ASP	2.1
1	H	73	GLU	2.1
1	C	151	THR	2.1
1	D	475	TYR	2.1
1	E	448	TYR	2.1
1	F	258	ALA	2.1
1	H	224	TYR	2.1
1	H	255	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	88	HIS	2.1
1	B	468	THR	2.1
1	D	208	PHE	2.1
1	D	455	THR	2.1
1	D	479	PHE	2.1
1	F	468	THR	2.1
1	H	424	ALA	2.1
1	A	463	SER	2.1
1	D	361	ILE	2.1
1	D	527	GLN	2.1
1	G	70	VAL	2.1
1	B	312	GLY	2.1
1	F	153	GLY	2.1
1	F	514	GLY	2.1
1	G	233	PRO	2.1
1	C	448	TYR	2.1
1	G	434	ASN	2.1
1	G	467	THR	2.1
1	C	337	SER	2.1
1	F	244	LEU	2.1
1	H	202	PRO	2.1
1	H	277	SER	2.1
1	H	311	SER	2.1
1	D	505	HIS	2.1
1	A	411	VAL	2.1
1	G	340	VAL	2.1
1	D	186	CYS	2.1
1	E	186	CYS	2.1
1	C	175	SER	2.1
1	E	233	PRO	2.1
1	H	564	SER	2.1
1	F	222	TYR	2.1
1	G	371	ALA	2.1
1	C	527	GLN	2.1
1	A	95	LEU	2.1
1	A	209	LEU	2.1
1	F	393	ARG	2.1
1	G	270	MET	2.1
1	G	83	PHE	2.1
1	C	436	GLU	2.1
1	D	539	GLU	2.1
1	G	389	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	388	LYS	2.1
1	G	183	PHE	2.1
1	E	557	ASP	2.1
1	H	387	VAL	2.1
1	D	327	ARG	2.1
1	E	393	ARG	2.1
1	F	412	MET	2.1
1	A	468	THR	2.1
1	D	101	ALA	2.1
1	A	327	ARG	2.1
1	D	525	ILE	2.1
1	C	80	HIS	2.1
1	C	189	GLY	2.1
1	C	442	MET	2.1
1	E	89	PHE	2.1
1	E	139	ALA	2.1
1	F	550	PRO	2.1
1	H	139	ALA	2.1
1	H	371	ALA	2.1
1	G	461	SER	2.1
1	E	83	PHE	2.1
1	H	193	PRO	2.1
1	C	204	SER	2.1
1	C	538	MET	2.1
1	H	270	MET	2.1
1	B	333	ARG	2.0
1	G	222	TYR	2.0
1	C	254	PRO	2.0
1	G	432	MET	2.0
1	C	57	VAL	2.0
1	H	56	TYR	2.0
1	C	488	THR	2.0
1	D	72	PRO	2.0
1	D	240	ILE	2.0
1	F	496	LYS	2.0
1	A	347	SER	2.0
1	C	477	ASP	2.0
1	H	158	TYR	2.0
1	B	95	LEU	2.0
1	B	525	ILE	2.0
1	H	180	LEU	2.0
1	H	312	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	325	GLN	2.0
1	G	277	SER	2.0
1	A	224	TYR	2.0
1	A	491	LYS	2.0
1	D	69	LYS	2.0
1	D	220	LYS	2.0
1	F	320	LYS	2.0
1	G	567	LEU	2.0
1	H	315	ALA	2.0
1	A	452	PRO	2.0
1	C	555	VAL	2.0
1	D	407	VAL	2.0
1	E	561	ASP	2.0
1	F	243	LYS	2.0
1	F	548	ASP	2.0
1	G	425	HIS	2.0
1	A	212	ALA	2.0
1	D	356	ILE	2.0
1	B	35	PHE	2.0
1	B	147	GLU	2.0
1	B	472	MET	2.0
1	E	188	THR	2.0
1	F	187	ASN	2.0
1	G	547	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

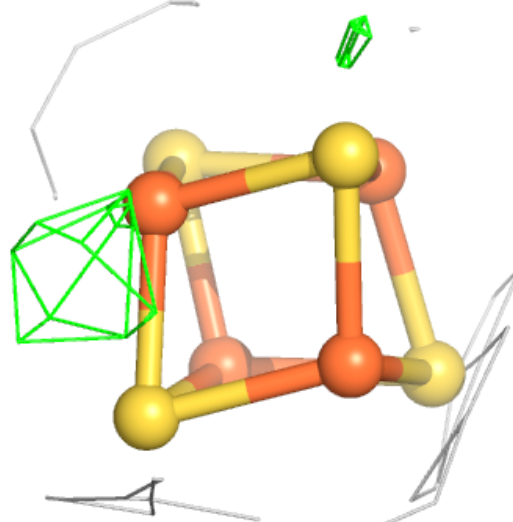
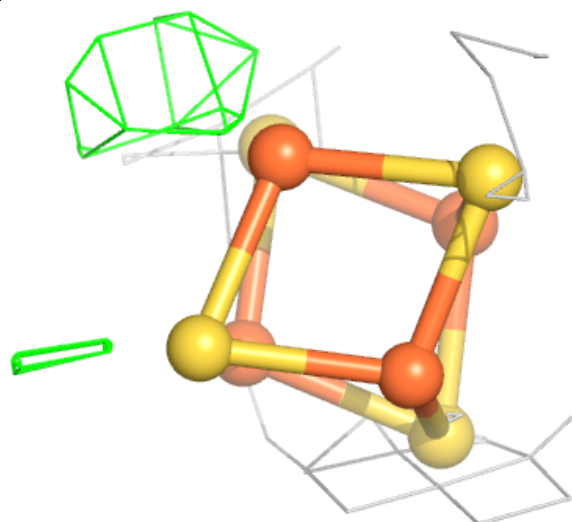
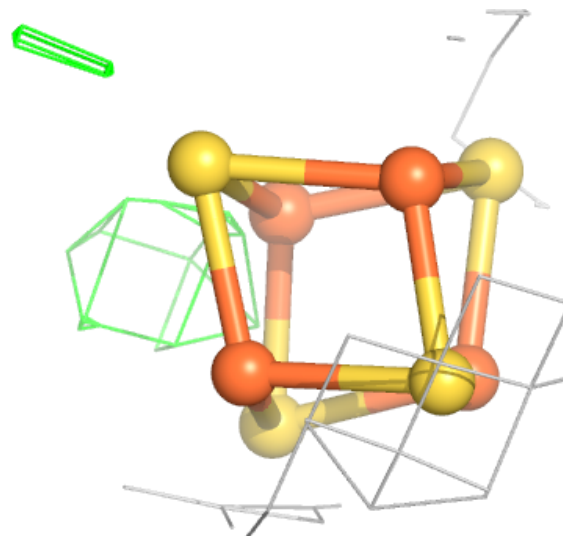
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	E	602	6/6	0.65	0.26	58,59,65,65	0
3	GOL	B	602	6/6	0.66	0.36	35,37,41,41	0
2	SF4	C	601	8/8	0.88	0.14	80,84,105,116	0
2	SF4	F	601	8/8	0.89	0.13	51,77,94,94	0
2	SF4	E	601	8/8	0.90	0.13	55,69,89,96	0
2	SF4	G	601	8/8	0.90	0.16	48,80,92,96	0
2	SF4	H	601	8/8	0.91	0.12	65,70,94,94	0
2	SF4	A	601	8/8	0.93	0.13	53,65,77,81	0
2	SF4	B	601	8/8	0.93	0.18	29,40,52,74	0
2	SF4	D	601	8/8	0.95	0.16	52,59,78,85	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.

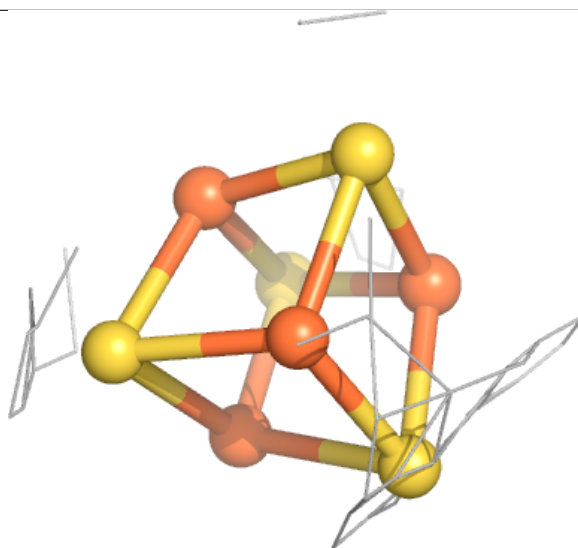
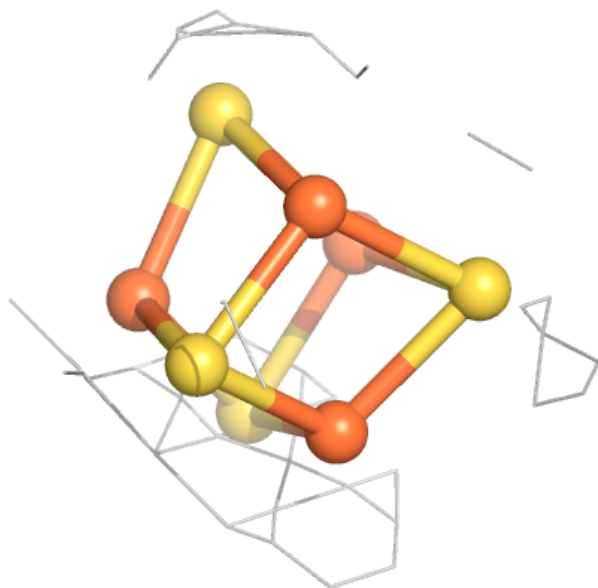
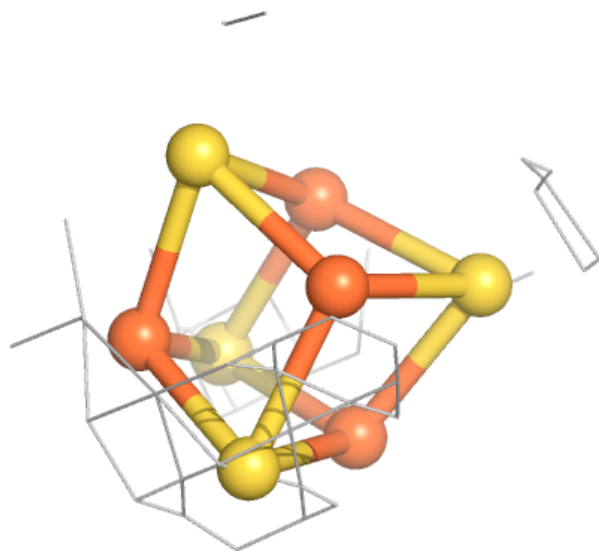
Electron density around SF4 C 601:

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



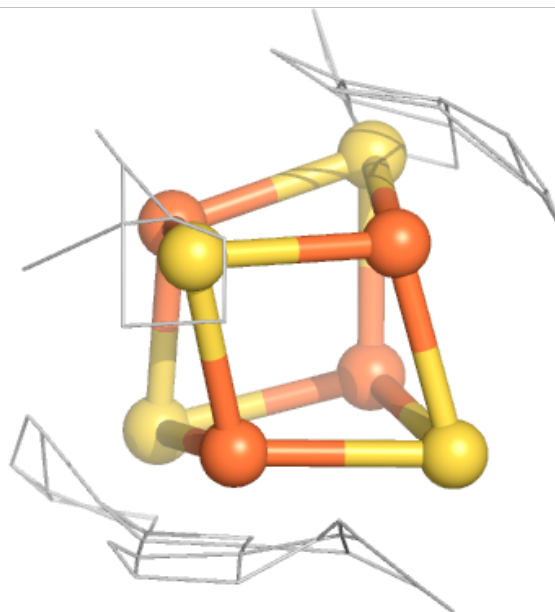
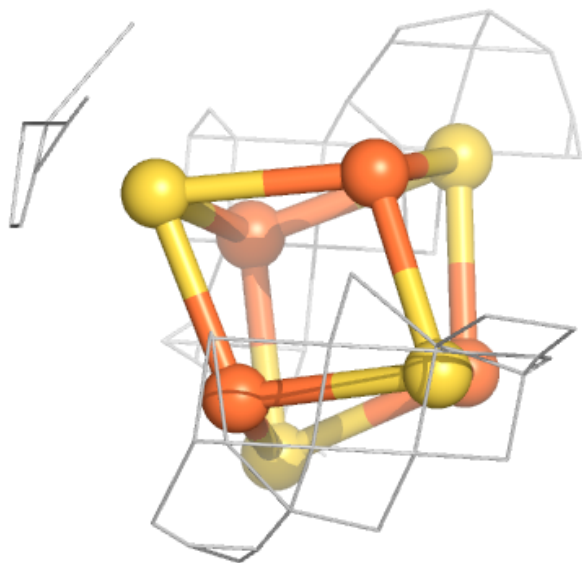
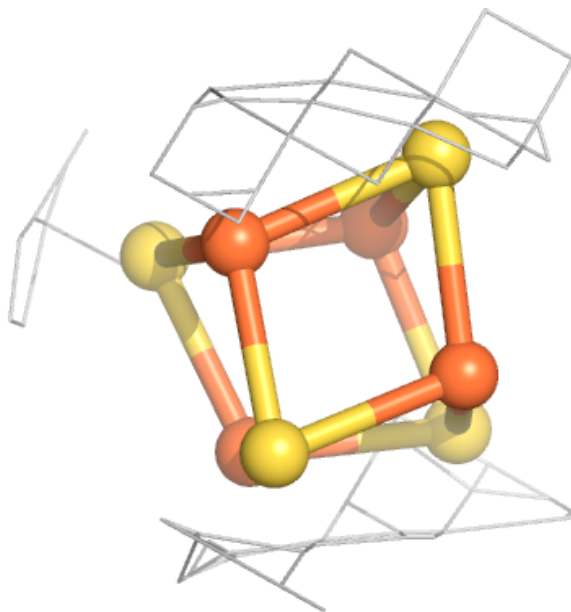
Electron density around SF4 F 601:

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



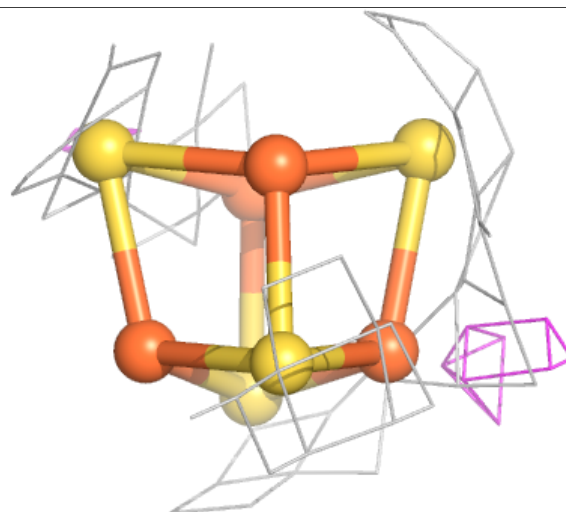
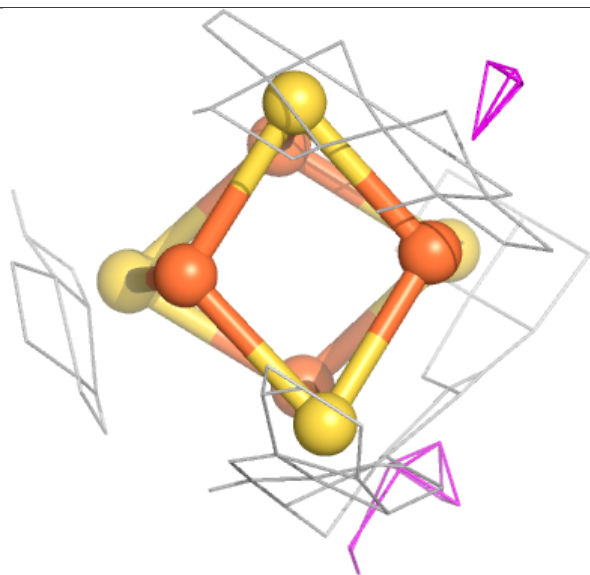
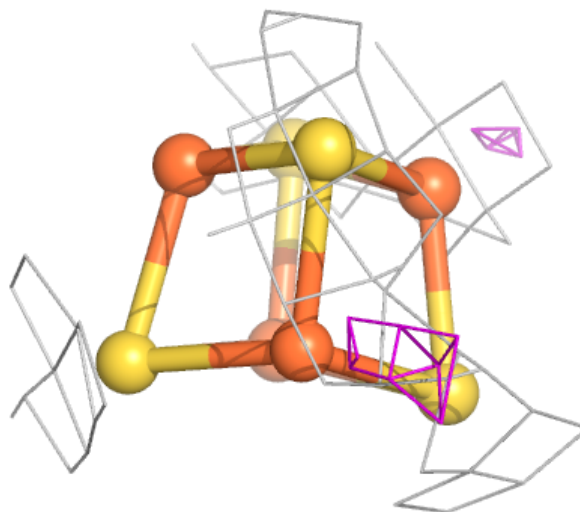
Electron density around SF4 E 601:

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



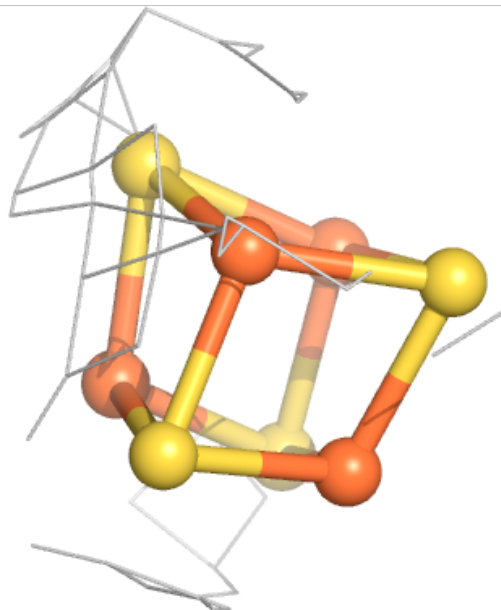
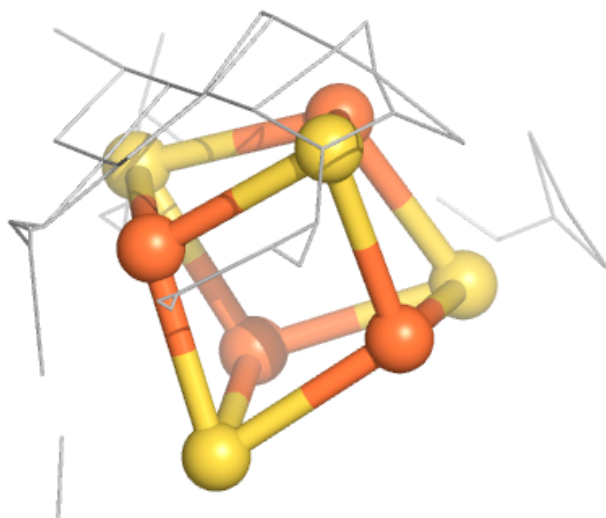
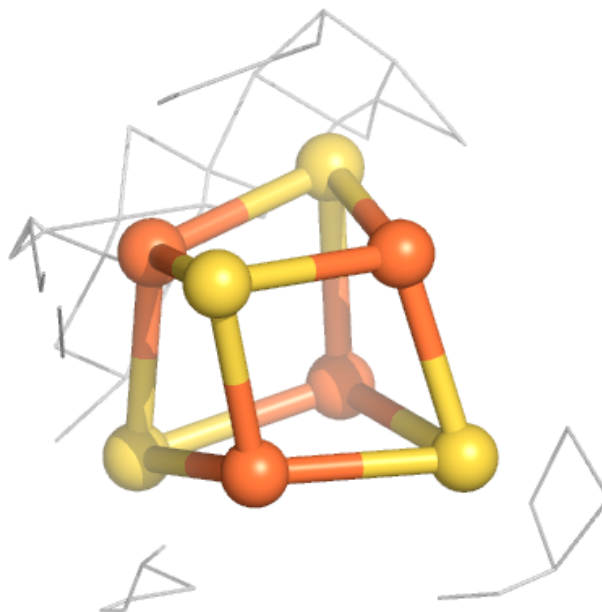
Electron density around SF4 G 601:

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



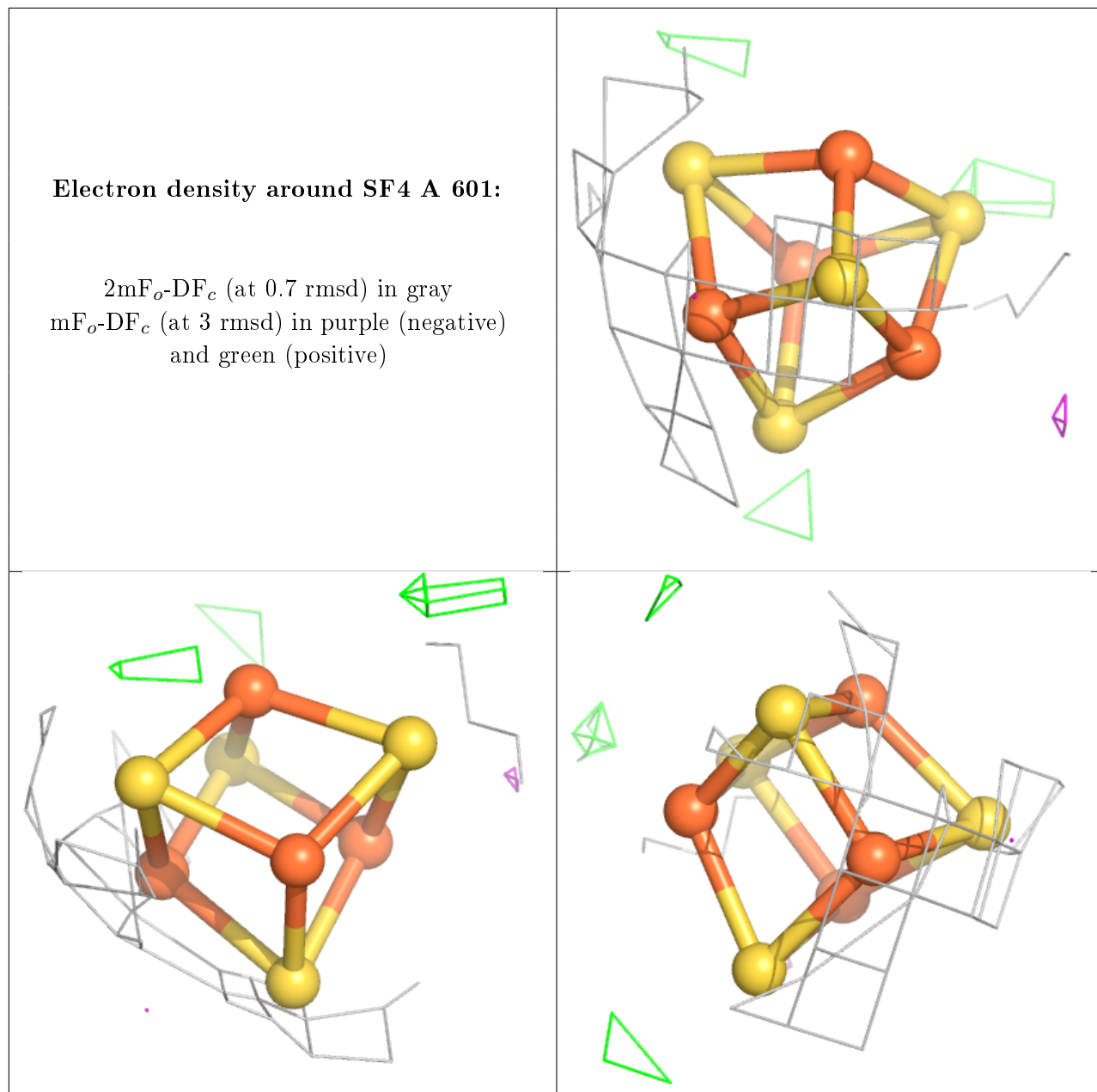
Electron density around SF4 H 601:

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



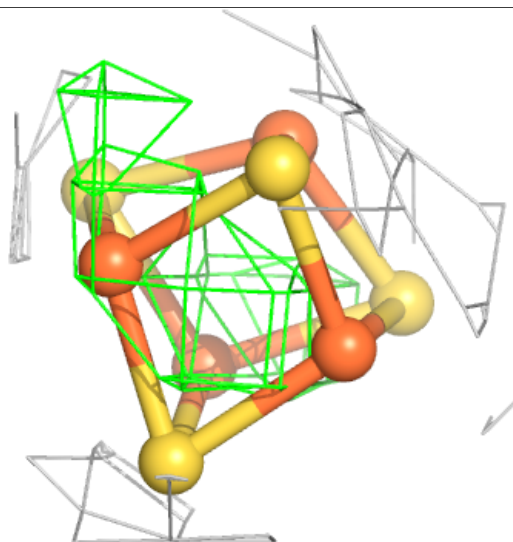
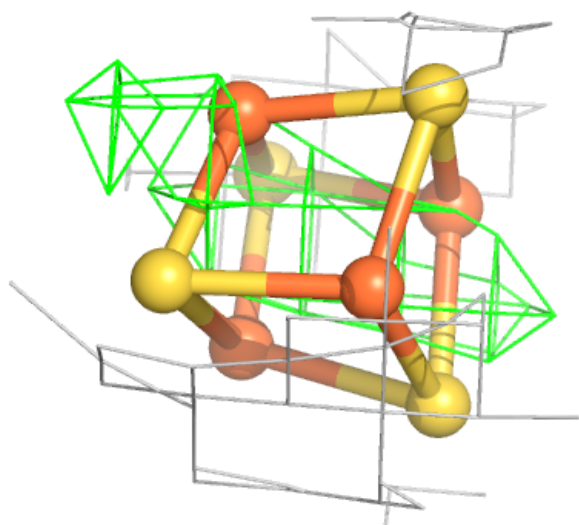
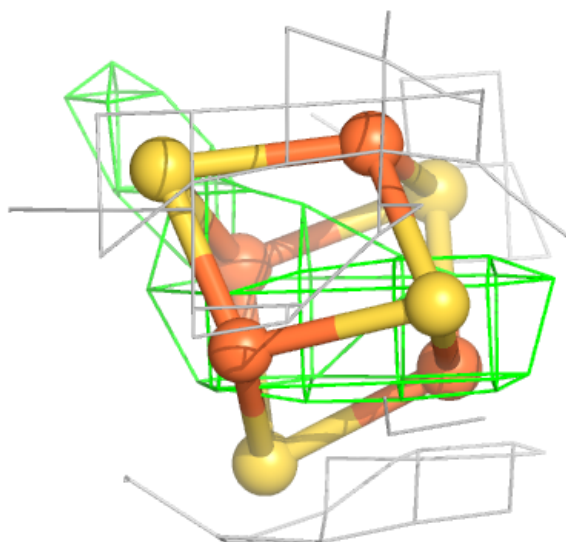
Electron density around SF4 A 601:

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



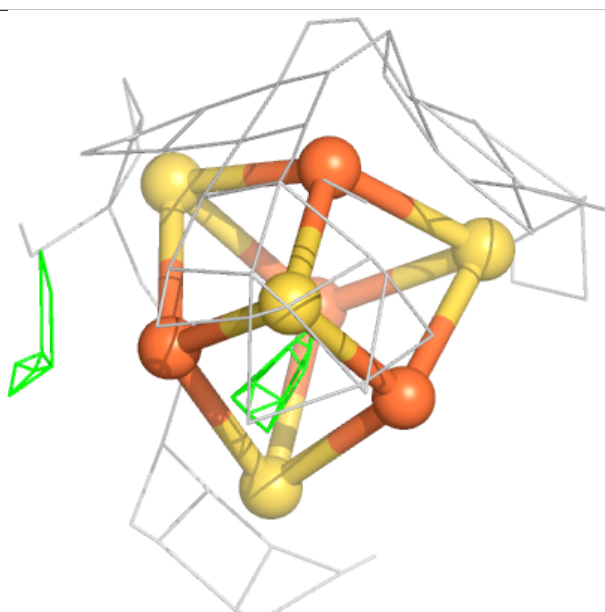
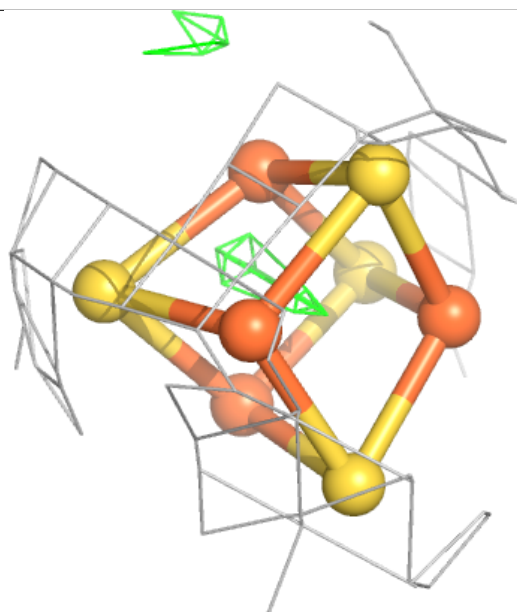
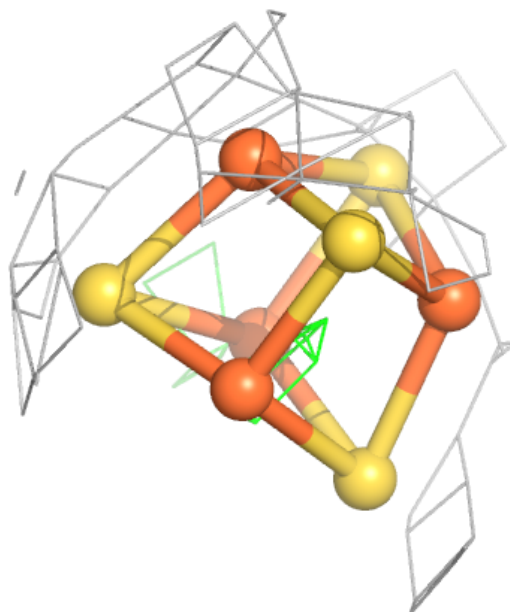
Electron density around SF4 B 601:

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



Electron density around SF4 D 601:

$2mF_o - DF_c$ (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.