



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:39 PM UTC

PDB ID : 4JC0 / pdb_00004jc0
Title : Crystal structure of Thermotoga maritima holo RimO in complex with penta-sulfide, Northeast Structural Genomics Consortium Target VR77
Authors : Forouhar, F.; Hussain, M.; Seetharaman, J.; Fang, Y.; Chen, C.X.; Cunningham, K.; Conover, K.; Ma, L.-C.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2013-02-20
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

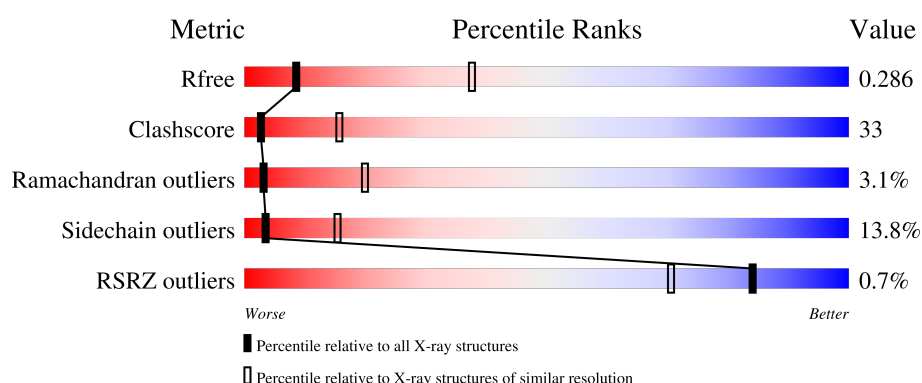
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	A	438	% 40% 46% 10% .
1	B	438	% 39% 47% 10% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6850 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.

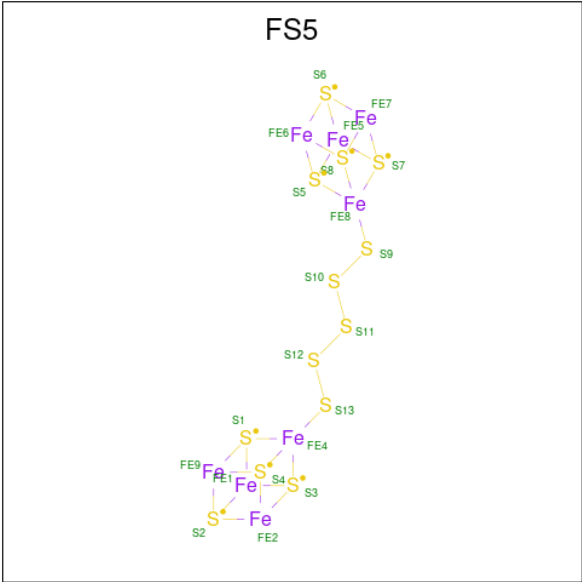
- Molecule 1 is a protein called Ribosomal protein S12 methylthiotransferase RimO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3419	2179	570	657	13			
1	B	421	Total	C	N	O	S	0	0	0
			3389	2162	562	652	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	LEU	-	expression tag	UNP Q9X2H6
A	432	GLU	-	expression tag	UNP Q9X2H6
A	433	HIS	-	expression tag	UNP Q9X2H6
A	434	HIS	-	expression tag	UNP Q9X2H6
A	435	HIS	-	expression tag	UNP Q9X2H6
A	436	HIS	-	expression tag	UNP Q9X2H6
A	437	HIS	-	expression tag	UNP Q9X2H6
A	438	HIS	-	expression tag	UNP Q9X2H6
B	431	LEU	-	expression tag	UNP Q9X2H6
B	432	GLU	-	expression tag	UNP Q9X2H6
B	433	HIS	-	expression tag	UNP Q9X2H6
B	434	HIS	-	expression tag	UNP Q9X2H6
B	435	HIS	-	expression tag	UNP Q9X2H6
B	436	HIS	-	expression tag	UNP Q9X2H6
B	437	HIS	-	expression tag	UNP Q9X2H6
B	438	HIS	-	expression tag	UNP Q9X2H6

- Molecule 2 is IRON/SULFUR PENTA-SULFIDE CONNECTED CLUSTERS (CCD ID: FS5) (formula: Fe₈S₁₃).

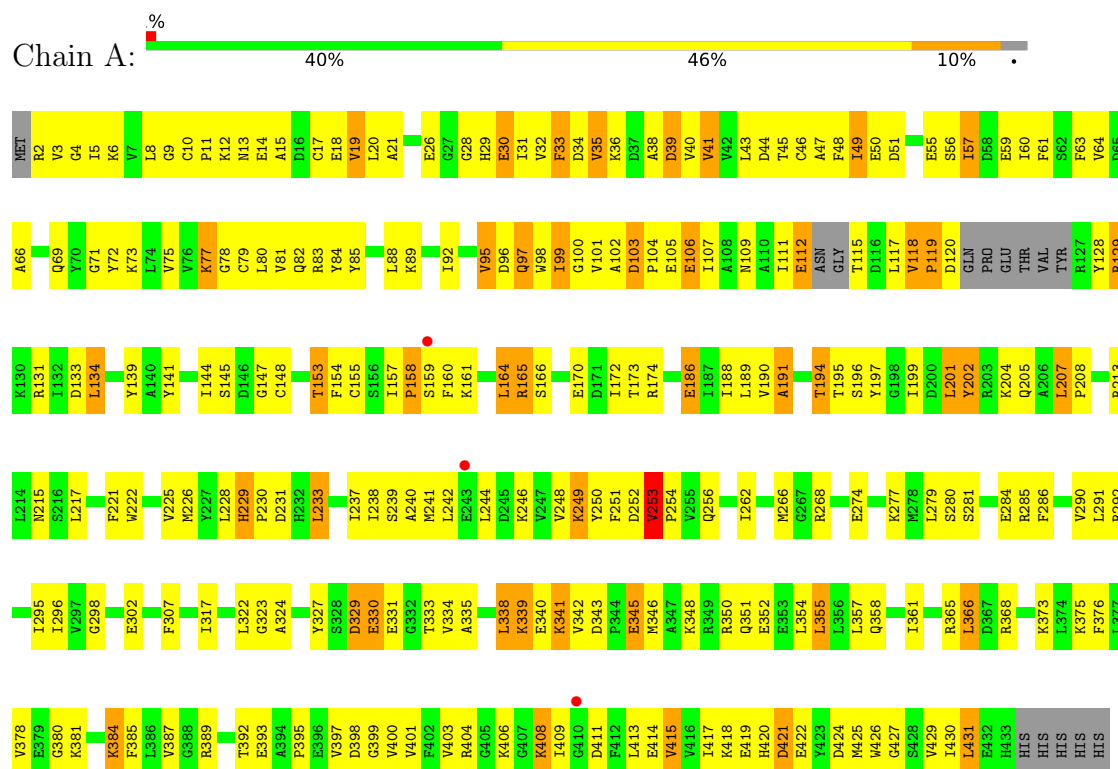


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			21	8	13		
2	B	1	Total	Fe	S	0	0
			21	8	13		

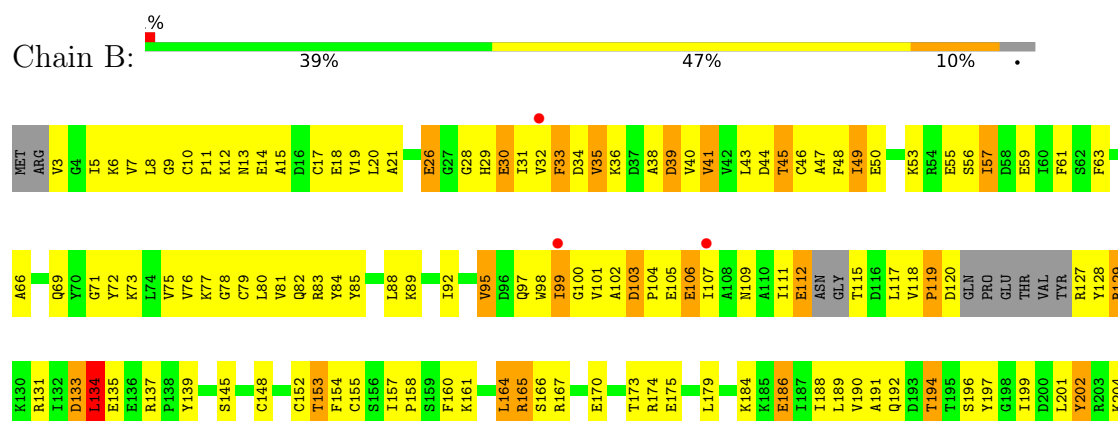
3 Residue-property plots

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

- Molecule 1: Ribosomal protein S12 methylthiotransferase RimO



- Molecule 1: Ribosomal protein S12 methylthiotransferase RimO



L430	L431	GLU	HIS	HIS	HIS	HIS	HIS	HIS	L361	R365	L366	D367	R368	K373	L374	K375	F376	G380	K381	K384	F385	L386	F387	G388	R389	T392	K393	A394	F396	E396	F397	D398	G399	V400	V401	F402	V403	R404	G405	K406	G407	K408	L409	G410	D411	E414	V415	V416	L417	K418	E419	H420	D421	E422	V423	D424	V425	V426	G427	S428	V429
L207	P208	S280	S281	E284	R285	F286	V290	L291	R292	T293	T296	V297	G298	E302	F307	F313	T317	Q318	L322	G323	A324	F327	S328	D329	E330	E331	G332	T333	V334	A335	L338	K339	E340	K341	V342	D343	F344	E345	K346	A347	K348	R349	R350	Q351	E352	E353	L354	L355	L356	L357	Q358										

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.72Å 86.95Å 172.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.46 – 3.30 41.46 – 3.30	Depositor EDS
% Data completeness (in resolution range)	83.1 (41.46-3.30) 83.0 (41.46-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.32Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.245 , 0.296 0.229 , 0.286	Depositor DCC
R_{free} test set	1344 reflections (10.29%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6850	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: FS5

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	0.60	0/3476	0.89	3/4676 (0.1%)
1	B	0.60	0/3445	0.88	5/4635 (0.1%)
All	All	0.60	0/6921	0.88	8/9311 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	VAL	N-CA-C	6.60	114.69	108.15
1	B	134	LEU	N-CA-C	-6.44	105.49	113.15
1	B	253	VAL	N-CA-C	5.71	113.81	108.15
1	A	229	HIS	CA-C-N	5.65	125.76	119.32
1	A	229	HIS	C-N-CA	5.65	125.76	119.32
1	B	229	HIS	CA-C-N	5.51	125.61	119.32
1	B	229	HIS	C-N-CA	5.51	125.61	119.32
1	B	45	THR	N-CA-C	5.02	117.30	109.52

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	3419	0	3420	220	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3389	0	3394	239	0
2	A	21	0	0	2	0
2	B	21	0	0	5	0
All	All	6850	0	6814	456	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 33.

All (456) 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:B:32:VAL:HG21	1:B:38:ALA:HB2	1.38	1.06
1:A:32:VAL:HG21	1:A:38:ALA:HB2	1.38	1.04
1:B:81:VAL:HG21	1:B:99:ILE:O	1.66	0.94
1:B:131:ARG:HD3	1:B:179:LEU:HD21	1.48	0.92
1:A:81:VAL:HG21	1:A:99:ILE:O	1.73	0.89
1:A:322:LEU:HB3	1:A:358:GLN:HG2	1.55	0.87
1:B:9:GLY:HA2	1:B:46:CYS:HB2	1.59	0.85
1:A:408:LYS:HD3	1:A:409:ILE:H	1.43	0.84
1:A:9:GLY:HA2	1:A:46:CYS:HB2	1.60	0.83
1:B:40:VAL:HG13	1:B:73:LYS:HB3	1.59	0.83
1:B:13:ASN:ND2	2:B:501:FS5:S6	2.52	0.83
1:B:408:LYS:HD3	1:B:409:ILE:H	1.42	0.83
1:B:5:ILE:HD11	1:B:134:LEU:HD22	1.61	0.83
1:B:322:LEU:HB3	1:B:358:GLN:HG2	1.62	0.82
1:A:420:HIS:O	1:A:421:ASP:HB2	1.80	0.82
1:A:188:ILE:HD11	1:A:395:PRO:HG2	1.63	0.80
1:B:420:HIS:O	1:B:421:ASP:HB2	1.79	0.80
1:A:20:LEU:HD11	1:A:106:GLU:HB2	1.64	0.78
1:B:188:ILE:HD11	1:B:395:PRO:HG2	1.66	0.78
1:B:10:CYS:SG	1:B:12:LYS:HE3	2.24	0.77
1:B:5:ILE:HD12	1:B:17:CYS:HB3	1.67	0.76
1:A:279:LEU:HD12	1:A:317:ILE:HD13	1.67	0.76
1:A:40:VAL:HG13	1:A:73:LYS:HB3	1.66	0.76
1:A:128:TYR:CE2	1:A:174:ARG:HD2	2.22	0.75
1:A:32:VAL:HG21	1:A:38:ALA:CB	2.17	0.74
1:A:48:PHE:CE2	1:A:330:GLU:HG2	2.23	0.74
1:A:5:ILE:HD12	1:A:17:CYS:HB3	1.70	0.73
1:A:10:CYS:SG	1:A:12:LYS:HE3	2.27	0.73
1:B:32:VAL:HG21	1:B:38:ALA:CB	2.17	0.73
1:A:307:PHE:CE2	1:A:350:ARG:HB3	2.23	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:LEU:HD11	1:B:106:GLU:HB2	1.71	0.73
1:A:103:ASP:HB3	1:A:104:PRO:HD3	1.69	0.72
1:B:241:MET:HE3	1:B:251:PHE:CE2	2.24	0.72
1:B:417:ILE:HD12	1:B:425:MET:HB3	1.71	0.72
1:A:13:ASN:ND2	2:A:501:FS5:S6	2.60	0.71
1:B:6:LYS:HB3	1:B:43:LEU:HD12	1.73	0.70
1:B:251:PHE:HB2	1:B:291:LEU:HD23	1.73	0.70
1:A:417:ILE:HD12	1:A:425:MET:HB3	1.73	0.69
1:B:17:CYS:SG	1:B:44:ASP:CG	2.75	0.69
1:B:105:GLU:O	1:B:109:ASN:HB2	1.93	0.69
1:B:279:LEU:HD12	1:B:317:ILE:HD13	1.73	0.69
1:A:201:LEU:HB3	1:A:202:TYR:CD2	2.28	0.68
1:B:165:ARG:HB3	1:B:165:ARG:HH21	1.58	0.68
1:A:422:GLU:HG3	1:B:418:LYS:HE3	1.76	0.68
1:A:201:LEU:HD23	1:A:202:TYR:CE2	2.29	0.68
1:B:307:PHE:CE2	1:B:350:ARG:HB3	2.29	0.68
1:A:201:LEU:HD23	1:A:202:TYR:HE2	1.59	0.68
1:A:268:ARG:HG2	1:A:268:ARG:HH11	1.60	0.67
1:B:201:LEU:HB3	1:B:202:TYR:CD2	2.30	0.67
1:B:79:CYS:SG	1:B:161:LYS:HE3	2.35	0.67
1:B:268:ARG:HH11	1:B:268:ARG:HG2	1.60	0.67
1:A:342:VAL:HG23	1:A:346:MET:HE3	1.75	0.67
1:B:418:LYS:HD3	1:B:427:GLY:HA2	1.76	0.67
1:A:165:ARG:HH21	1:A:165:ARG:HB3	1.59	0.67
1:B:83:ARG:HB2	1:B:160:PHE:CE2	2.30	0.66
1:A:418:LYS:HD3	1:A:427:GLY:HA2	1.76	0.66
1:A:415:VAL:HG12	1:A:429:VAL:HG22	1.77	0.66
1:B:103:ASP:HB3	1:B:104:PRO:HD3	1.77	0.66
1:A:322:LEU:C	1:A:322:LEU:HD23	2.21	0.66
1:A:393:GLU:OE2	1:A:398:ASP:HB3	1.96	0.66
1:A:194:THR:HG21	1:A:225:VAL:CG1	2.26	0.65
1:B:139:TYR:CB	1:B:186:GLU:HB3	2.27	0.65
1:A:327:TYR:CE2	1:A:329:ASP:HB3	2.31	0.65
1:B:201:LEU:HD23	1:B:202:TYR:HE2	1.62	0.65
1:B:342:VAL:HG23	1:B:346:MET:HE3	1.77	0.65
1:A:78:GLY:O	1:A:81:VAL:HG22	1.96	0.65
1:A:251:PHE:HB2	1:A:291:LEU:HD23	1.78	0.65
1:A:49:ILE:HG22	1:A:49:ILE:O	1.98	0.64
1:A:105:GLU:O	1:A:109:ASN:HB2	1.97	0.64
1:A:400:VAL:HG22	1:A:401:VAL:H	1.63	0.64
1:B:12:LYS:HD3	1:B:191:ALA:C	2.22	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:TYR:CE1	1:B:395:PRO:HB3	2.33	0.64
1:B:78:GLY:O	1:B:81:VAL:HG22	1.97	0.63
1:A:215:ASN:ND2	1:A:244:LEU:HD22	2.14	0.63
1:A:415:VAL:HG12	1:A:429:VAL:CG2	2.28	0.63
1:A:148:CYS:HA	1:A:164:LEU:HD23	1.80	0.63
1:A:422:GLU:HG3	1:B:418:LYS:CE	2.29	0.63
1:B:194:THR:HG21	1:B:225:VAL:CG1	2.29	0.62
1:A:241:MET:HE3	1:A:251:PHE:CE2	2.34	0.62
1:B:83:ARG:NE	1:B:83:ARG:HA	2.12	0.62
1:B:201:LEU:HD23	1:B:202:TYR:CE2	2.34	0.62
1:B:75:VAL:HG22	1:B:97:GLN:HB2	1.81	0.62
1:A:2:ARG:HA	1:A:30:GLU:O	1.99	0.62
1:A:222:TRP:HZ2	1:A:375:LYS:HB3	1.65	0.62
1:B:322:LEU:C	1:B:322:LEU:HD23	2.24	0.62
1:A:298:GLY:HA2	1:A:342:VAL:HG11	1.81	0.62
1:A:109:ASN:C	1:A:111:ILE:H	2.06	0.62
1:B:32:VAL:C	1:B:34:ASP:H	2.08	0.61
1:A:117:LEU:O	1:A:118:VAL:HG13	1.99	0.61
1:A:5:ILE:HD11	1:A:134:LEU:CD2	2.31	0.61
1:B:7:VAL:HG11	1:B:134:LEU:HD21	1.83	0.61
1:B:66:ALA:HB1	1:B:69:GLN:HG3	1.83	0.61
1:B:79:CYS:HB3	1:B:160:PHE:HZ	1.64	0.61
1:A:66:ALA:HB1	1:A:69:GLN:HG3	1.83	0.61
1:A:83:ARG:HA	1:A:83:ARG:NE	2.15	0.61
1:B:215:ASN:ND2	1:B:244:LEU:HD22	2.16	0.61
1:B:201:LEU:HB3	1:B:202:TYR:HD2	1.66	0.61
1:B:148:CYS:HA	1:B:164:LEU:HD23	1.83	0.60
1:B:79:CYS:HB3	1:B:160:PHE:CZ	2.37	0.60
1:A:400:VAL:HG22	1:A:401:VAL:N	2.16	0.60
1:A:17:CYS:SG	1:A:44:ASP:CG	2.85	0.60
1:A:242:LEU:HA	1:A:249:LYS:HE3	1.84	0.60
1:A:290:VAL:HG21	1:A:392:THR:HB	1.84	0.60
1:B:242:LEU:HA	1:B:249:LYS:HE3	1.82	0.60
1:B:109:ASN:C	1:B:111:ILE:H	2.09	0.60
1:A:262:ILE:O	1:A:266:MET:HG3	2.02	0.60
1:B:32:VAL:HG11	1:B:38:ALA:HA	1.84	0.60
1:B:207:LEU:HB3	1:B:208:PRO:HD3	1.84	0.60
1:A:75:VAL:HG22	1:A:97:GLN:HB2	1.83	0.59
1:B:327:TYR:OH	1:B:329:ASP:HB3	2.01	0.59
1:A:155:CYS:HB2	2:A:501:FS5:S3	2.41	0.59
1:A:166:SER:HB2	1:A:197:TYR:CD1	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:CD1	1:A:317:ILE:HD13	2.32	0.59
1:B:222:TRP:HZ2	1:B:375:LYS:HB3	1.67	0.59
1:B:233:LEU:HD22	1:B:238:ILE:HG13	1.84	0.59
1:B:393:GLU:OE2	1:B:398:ASP:HB3	2.01	0.59
1:A:32:VAL:C	1:A:34:ASP:H	2.10	0.59
1:B:17:CYS:SG	1:B:44:ASP:OD2	2.61	0.59
1:B:80:LEU:O	1:B:84:TYR:HB2	2.02	0.59
1:A:343:ASP:HB3	1:A:345:GLU:HG3	1.85	0.59
1:A:49:ILE:O	1:A:49:ILE:CG2	2.51	0.59
1:B:400:VAL:HG22	1:B:401:VAL:H	1.67	0.59
1:B:327:TYR:CE2	1:B:329:ASP:HB3	2.38	0.59
1:B:55:GLU:O	1:B:59:GLU:HB2	2.02	0.58
1:B:83:ARG:HB2	1:B:160:PHE:CD2	2.37	0.58
1:B:322:LEU:HD23	1:B:323:GLY:N	2.18	0.58
1:A:153:THR:OG1	1:A:266:MET:HA	2.03	0.58
1:A:207:LEU:HB3	1:A:208:PRO:HD3	1.84	0.58
1:B:21:ALA:O	1:B:31:ILE:HD11	2.04	0.58
1:B:49:ILE:O	1:B:49:ILE:HG22	2.03	0.58
1:A:408:LYS:HD3	1:A:409:ILE:N	2.18	0.58
1:B:408:LYS:HD3	1:B:409:ILE:N	2.16	0.58
1:A:32:VAL:HG11	1:A:38:ALA:HA	1.85	0.58
1:A:400:VAL:HG12	1:A:424:ASP:OD2	2.04	0.58
1:B:117:LEU:O	1:B:118:VAL:HG13	2.04	0.58
1:A:92:ILE:O	1:A:95:VAL:HG13	2.03	0.58
1:A:249:LYS:HG2	1:A:286:PHE:CD2	2.38	0.58
1:A:281:SER:O	1:A:285:ARG:HG3	2.03	0.58
1:A:5:ILE:HD11	1:A:134:LEU:HD22	1.85	0.58
1:B:186:GLU:OE1	1:B:222:TRP:HE3	1.87	0.57
1:B:290:VAL:HG21	1:B:392:THR:HB	1.85	0.57
1:A:322:LEU:HD23	1:A:323:GLY:N	2.19	0.57
1:A:201:LEU:HB3	1:A:202:TYR:HD2	1.70	0.57
1:B:3:VAL:HG23	1:B:40:VAL:O	2.04	0.57
1:A:80:LEU:O	1:A:84:TYR:HB2	2.04	0.57
1:B:112:GLU:HG3	1:B:115:THR:OG1	2.03	0.56
1:B:327:TYR:CZ	1:B:329:ASP:HB3	2.40	0.56
1:A:157:ILE:N	1:A:158:PRO:CD	2.68	0.56
1:A:229:HIS:CE1	1:A:231:ASP:HB2	2.40	0.56
1:A:327:TYR:CZ	1:A:329:ASP:HB3	2.40	0.56
1:B:98:TRP:C	1:B:99:ILE:HG12	2.30	0.56
1:B:157:ILE:N	1:B:158:PRO:CD	2.67	0.56
1:A:9:GLY:CA	1:A:46:CYS:HB2	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:HG22	1:A:77:LYS:O	2.06	0.56
1:A:49:ILE:O	1:A:50:GLU:HG2	2.05	0.56
1:A:117:LEU:HD23	1:A:117:LEU:N	2.21	0.56
1:B:3:VAL:C	1:B:32:VAL:HG22	2.30	0.56
1:B:157:ILE:HG23	1:B:161:LYS:HB2	1.88	0.56
1:B:45:THR:HG22	1:B:77:LYS:O	2.05	0.56
1:A:48:PHE:O	1:A:49:ILE:HG12	2.06	0.56
1:A:186:GLU:OE1	1:A:222:TRP:HE3	1.89	0.56
1:B:18:GLU:CD	1:B:134:LEU:HD23	2.31	0.56
1:A:55:GLU:O	1:A:59:GLU:HB2	2.05	0.55
1:B:81:VAL:CG2	1:B:99:ILE:O	2.47	0.55
1:B:279:LEU:CD1	1:B:317:ILE:HD13	2.36	0.55
1:B:17:CYS:SG	1:B:44:ASP:OD1	2.65	0.55
1:B:343:ASP:HB3	1:B:345:GLU:HG3	1.86	0.55
1:A:112:GLU:HG3	1:A:115:THR:OG1	2.06	0.55
1:B:139:TYR:HB2	1:B:186:GLU:HG2	1.89	0.55
1:A:6:LYS:HB3	1:A:43:LEU:HD12	1.87	0.55
1:B:129:ARG:HG2	1:B:129:ARG:HH11	1.71	0.55
1:A:233:LEU:HD22	1:A:238:ILE:HG13	1.89	0.55
1:A:327:TYR:OH	1:A:329:ASP:HB3	2.06	0.55
1:B:49:ILE:O	1:B:49:ILE:CG2	2.55	0.55
1:B:192:GLN:O	2:B:501:FS5:S12	2.65	0.55
1:B:12:LYS:HD3	1:B:191:ALA:O	2.07	0.54
1:B:281:SER:O	1:B:285:ARG:HG3	2.07	0.54
1:B:400:VAL:HG22	1:B:401:VAL:N	2.23	0.54
1:A:98:TRP:C	1:A:99:ILE:HG12	2.31	0.54
1:B:400:VAL:HG12	1:B:424:ASP:OD2	2.06	0.54
1:A:57:ILE:CD1	1:A:80:LEU:HD21	2.36	0.54
1:B:202:TYR:CD2	1:B:202:TYR:N	2.76	0.54
1:A:389:ARG:NH2	1:A:395:PRO:HG3	2.23	0.54
1:A:81:VAL:CG2	1:A:99:ILE:O	2.52	0.54
1:B:92:ILE:O	1:B:95:VAL:HG13	2.08	0.54
1:B:153:THR:OG1	1:B:266:MET:HA	2.08	0.54
1:B:12:LYS:NZ	2:B:501:FS5:S11	2.80	0.54
1:B:324:ALA:HB2	1:B:354:LEU:HD23	1.90	0.54
1:A:21:ALA:O	1:A:31:ILE:HD11	2.07	0.53
1:B:49:ILE:O	1:B:50:GLU:HG2	2.08	0.53
1:A:188:ILE:CD1	1:A:395:PRO:HG2	2.37	0.53
1:A:420:HIS:O	1:A:421:ASP:CB	2.55	0.53
1:B:417:ILE:HD12	1:B:425:MET:CB	2.38	0.53
1:A:298:GLY:CA	1:A:342:VAL:HG11	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLN:O	1:A:355:LEU:HB2	2.07	0.53
1:B:139:TYR:HB3	1:B:186:GLU:HB3	1.90	0.53
1:B:221:PHE:O	1:B:246:LYS:HG2	2.08	0.53
1:A:11:PRO:HB3	1:A:141:TYR:CD2	2.44	0.53
1:B:117:LEU:N	1:B:117:LEU:HD23	2.24	0.52
1:B:133:ASP:OD1	1:B:184:LYS:HE2	2.08	0.52
1:B:18:GLU:OE1	1:B:134:LEU:HD23	2.09	0.52
1:B:57:ILE:CD1	1:B:80:LEU:HD21	2.40	0.52
1:B:48:PHE:O	1:B:49:ILE:HG12	2.09	0.52
1:B:53:LYS:NZ	1:B:330:GLU:OE1	2.42	0.52
1:B:128:TYR:CE2	1:B:175:GLU:HA	2.45	0.52
1:A:18:GLU:OE1	1:A:133:ASP:HA	2.09	0.52
1:A:139:TYR:HA	1:A:186:GLU:HB3	1.92	0.52
1:B:18:GLU:O	1:B:131:ARG:HB2	2.10	0.52
1:B:302:GLU:HG2	1:B:350:ARG:NH2	2.24	0.52
1:A:5:ILE:HG13	1:A:5:ILE:O	2.10	0.51
1:B:389:ARG:NH2	1:B:395:PRO:HG3	2.25	0.51
1:A:221:PHE:O	1:A:246:LYS:HG2	2.11	0.51
1:A:366:LEU:N	1:A:366:LEU:HD23	2.26	0.51
1:A:154:PHE:HZ	1:A:256:GLN:HG3	1.76	0.51
1:A:403:VAL:HA	1:A:427:GLY:O	2.10	0.51
1:B:85:TYR:CD1	1:B:118:VAL:HG21	2.45	0.51
1:A:35:VAL:C	1:A:36:LYS:HG2	2.35	0.51
1:A:330:GLU:O	1:A:333:THR:HG23	2.10	0.51
1:B:39:ASP:O	1:B:72:TYR:HA	2.11	0.51
1:A:154:PHE:CZ	1:A:256:GLN:HG3	2.46	0.50
1:A:365:ARG:O	1:A:368:ARG:HG2	2.11	0.50
1:B:248:VAL:O	1:B:250:TYR:N	2.39	0.50
1:B:421:ASP:O	1:B:422:GLU:HB2	2.11	0.50
1:A:11:PRO:HB2	1:A:190:VAL:HG11	1.93	0.50
1:A:109:ASN:C	1:A:111:ILE:N	2.69	0.50
1:A:421:ASP:O	1:A:422:GLU:HB2	2.12	0.50
1:B:166:SER:HB2	1:B:197:TYR:CD1	2.46	0.50
1:A:139:TYR:HB3	1:A:186:GLU:HB3	1.93	0.50
1:A:157:ILE:HG23	1:A:161:LYS:HB2	1.93	0.50
1:B:229:HIS:CE1	1:B:231:ASP:HB2	2.46	0.50
1:A:207:LEU:HD12	1:A:237:ILE:HG23	1.94	0.50
1:B:250:TYR:OH	1:B:292:ARG:HD2	2.12	0.50
1:B:35:VAL:C	1:B:36:LYS:HG2	2.36	0.50
1:B:342:VAL:CG2	1:B:346:MET:HE3	2.42	0.50
1:A:39:ASP:O	1:A:72:TYR:HA	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:CYS:SG	1:A:157:ILE:HG12	2.52	0.50
1:A:153:THR:HG1	1:A:266:MET:HA	1.76	0.50
1:A:202:TYR:CD2	1:A:202:TYR:N	2.80	0.50
1:B:48:PHE:HE1	1:B:160:PHE:CG	2.30	0.50
1:B:82:GLN:OE1	1:B:100:GLY:HA3	2.12	0.50
1:B:351:GLN:O	1:B:355:LEU:HB2	2.11	0.50
1:B:365:ARG:O	1:B:368:ARG:HG2	2.11	0.50
1:B:139:TYR:CD2	1:B:139:TYR:C	2.90	0.49
1:B:207:LEU:HD12	1:B:237:ILE:HG23	1.94	0.49
1:B:242:LEU:HD21	1:B:251:PHE:CZ	2.48	0.49
1:B:280:SER:O	1:B:284:GLU:HG3	2.12	0.49
1:B:420:HIS:O	1:B:421:ASP:CB	2.53	0.49
1:A:139:TYR:CB	1:A:186:GLU:HB3	2.42	0.49
1:B:48:PHE:HE1	1:B:160:PHE:CD2	2.29	0.49
1:B:77:LYS:HA	1:B:99:ILE:O	2.12	0.49
1:A:250:TYR:OH	1:A:292:ARG:HD2	2.13	0.49
1:B:152:CYS:HB2	2:B:501:FS5:S2	2.52	0.49
1:A:28:GLY:C	1:A:30:GLU:H	2.21	0.49
1:A:196:SER:O	1:A:199:ILE:HG13	2.13	0.49
1:B:226:MET:CE	1:B:250:TYR:HE2	2.25	0.49
1:A:111:ILE:HG13	1:A:112:GLU:OE1	2.13	0.49
1:B:298:GLY:HA2	1:B:342:VAL:HG11	1.93	0.49
1:A:324:ALA:HB2	1:A:354:LEU:HD23	1.93	0.49
1:B:393:GLU:OE2	1:B:399:GLY:N	2.45	0.48
1:A:242:LEU:HD23	1:A:249:LYS:HG3	1.94	0.48
1:B:119:PRO:HG2	1:B:120:ASP:H	1.78	0.48
1:A:302:GLU:HG2	1:A:350:ARG:NH2	2.27	0.48
1:B:242:LEU:HD21	1:B:251:PHE:HZ	1.78	0.48
1:A:82:GLN:OE1	1:A:118:VAL:HG12	2.14	0.48
1:A:194:THR:HG21	1:A:225:VAL:HG11	1.94	0.48
1:A:215:ASN:CG	1:A:244:LEU:HD22	2.39	0.48
1:B:128:TYR:HB2	1:B:167:ARG:NH1	2.28	0.48
1:A:393:GLU:OE2	1:A:399:GLY:N	2.42	0.48
1:A:11:PRO:CB	1:A:190:VAL:HG11	2.44	0.48
1:A:380:GLY:CA	1:A:387:VAL:HG12	2.43	0.48
1:A:85:TYR:CD1	1:A:118:VAL:HG21	2.49	0.48
1:A:95:VAL:HG21	1:A:98:TRP:CE2	2.49	0.48
1:B:14:GLU:O	1:B:18:GLU:HG2	2.14	0.48
1:B:109:ASN:C	1:B:111:ILE:N	2.72	0.48
1:B:257:HIS:ND1	1:B:258:GLY:N	2.58	0.48
1:A:82:GLN:OE1	1:A:100:GLY:HA3	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:GLU:O	1:B:333:THR:HG23	2.13	0.47
1:B:5:ILE:O	1:B:5:ILE:HG13	2.14	0.47
1:A:101:VAL:O	1:A:102:ALA:HB3	2.14	0.47
1:A:12:LYS:HD3	1:A:191:ALA:C	2.40	0.47
1:A:77:LYS:HA	1:A:99:ILE:O	2.13	0.47
1:B:381:LYS:NZ	1:B:406:LYS:HE3	2.29	0.47
1:A:3:VAL:HG23	1:A:40:VAL:O	2.14	0.47
1:A:17:CYS:SG	1:A:44:ASP:OD2	2.73	0.47
1:A:280:SER:O	1:A:284:GLU:HG3	2.14	0.47
1:A:103:ASP:C	1:A:105:GLU:H	2.23	0.47
1:B:28:GLY:C	1:B:30:GLU:H	2.23	0.47
1:B:157:ILE:HA	1:B:160:PHE:HB3	1.96	0.47
1:B:348:LYS:O	1:B:352:GLU:HG3	2.15	0.47
1:A:426:TRP:CH2	1:B:419:GLU:OE1	2.68	0.47
1:B:366:LEU:N	1:B:366:LEU:HD23	2.29	0.47
1:B:335:ALA:O	1:B:338:LEU:HB2	2.15	0.47
1:A:190:VAL:O	1:A:191:ALA:HB2	2.15	0.46
1:A:335:ALA:O	1:A:338:LEU:HB2	2.16	0.46
1:B:242:LEU:HD23	1:B:249:LYS:HG3	1.96	0.46
1:A:84:TYR:O	1:A:88:LEU:HG	2.15	0.46
1:A:242:LEU:CD2	1:A:249:LYS:HG3	2.45	0.46
1:A:381:LYS:NZ	1:A:406:LYS:HE3	2.29	0.46
1:A:119:PRO:HG2	1:A:120:ASP:H	1.79	0.46
1:B:255:VAL:C	1:B:257:HIS:H	2.24	0.46
1:A:14:GLU:O	1:A:18:GLU:HG2	2.15	0.46
1:A:147:GLY:O	1:A:148:CYS:HB2	2.14	0.46
1:B:9:GLY:O	1:B:10:CYS:HB3	2.14	0.46
1:B:95:VAL:HG21	1:B:98:TRP:CE2	2.51	0.46
1:B:365:ARG:CZ	1:B:368:ARG:HD3	2.45	0.46
1:A:413:LEU:HD13	1:A:429:VAL:HG21	1.97	0.46
1:B:417:ILE:HG23	1:B:425:MET:HB3	1.97	0.46
1:B:101:VAL:O	1:B:102:ALA:HB3	2.16	0.46
1:B:249:LYS:HG2	1:B:286:PHE:CD2	2.50	0.46
1:A:226:MET:CE	1:A:250:TYR:HE2	2.29	0.46
1:A:35:VAL:O	1:A:35:VAL:HG22	2.16	0.46
1:A:82:GLN:HB3	1:A:160:PHE:CE2	2.51	0.46
1:B:57:ILE:HD13	1:B:80:LEU:HD21	1.98	0.46
1:B:194:THR:HG21	1:B:225:VAL:HG11	1.98	0.46
1:B:329:ASP:OD1	1:B:329:ASP:N	2.47	0.46
1:B:5:ILE:CD1	1:B:134:LEU:HD22	2.41	0.45
1:B:298:GLY:CA	1:B:342:VAL:HG11	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:THR:OG1	1:B:393:GLU:N	2.49	0.45
1:B:403:VAL:HA	1:B:427:GLY:O	2.16	0.45
1:A:228:LEU:O	1:A:254:PRO:HD2	2.16	0.45
1:A:57:ILE:HD13	1:A:80:LEU:HD21	1.98	0.45
1:B:61:PHE:C	1:B:63:PHE:N	2.74	0.45
1:B:18:GLU:OE2	1:B:137:ARG:NH2	2.50	0.45
1:B:82:GLN:OE1	1:B:118:VAL:HG12	2.16	0.45
1:B:215:ASN:CG	1:B:244:LEU:HD22	2.41	0.45
1:B:155:CYS:HB2	2:B:501:FS5:S3	2.57	0.45
1:B:341:LYS:HB3	1:B:342:VAL:H	1.52	0.45
1:A:106:GLU:OE1	1:A:106:GLU:N	2.50	0.45
1:B:103:ASP:C	1:B:105:GLU:H	2.24	0.45
1:A:195:THR:O	1:A:205:GLN:NE2	2.45	0.45
1:B:15:ALA:C	1:B:17:CYS:N	2.75	0.45
1:B:84:TYR:O	1:B:88:LEU:HG	2.17	0.45
1:A:39:ASP:OD2	1:A:39:ASP:N	2.50	0.44
1:A:365:ARG:CZ	1:A:368:ARG:HD3	2.48	0.44
1:B:231:ASP:OD1	1:B:270:LYS:HB2	2.18	0.44
1:A:40:VAL:HG12	1:A:41:VAL:N	2.31	0.44
1:A:248:VAL:O	1:A:250:TYR:N	2.46	0.44
1:A:358:GLN:HA	1:A:361:ILE:HD12	1.99	0.44
1:A:268:ARG:HG2	1:A:268:ARG:NH1	2.30	0.44
1:A:417:ILE:HD12	1:A:425:MET:CB	2.45	0.44
1:B:9:GLY:CA	1:B:46:CYS:HB2	2.39	0.44
1:B:329:ASP:OD2	1:B:341:LYS:NZ	2.50	0.44
1:A:30:GLU:HG3	1:A:31:ILE:N	2.28	0.44
1:B:34:ASP:C	1:B:36:LYS:H	2.25	0.44
1:B:188:ILE:CD1	1:B:395:PRO:HG2	2.42	0.44
1:B:139:TYR:HA	1:B:186:GLU:HB3	2.00	0.44
1:A:61:PHE:C	1:A:63:PHE:N	2.75	0.44
1:B:30:GLU:HG3	1:B:31:ILE:N	2.30	0.44
1:B:32:VAL:O	1:B:34:ASP:N	2.48	0.44
1:B:89:LYS:HE3	1:B:89:LYS:HB3	1.77	0.44
1:B:39:ASP:OD2	1:B:39:ASP:N	2.51	0.43
1:A:48:PHE:HE2	1:A:330:GLU:HG2	1.81	0.43
1:B:15:ALA:C	1:B:17:CYS:H	2.25	0.43
1:B:47:ALA:HB2	1:B:79:CYS:C	2.42	0.43
1:A:139:TYR:CA	1:A:186:GLU:HB3	2.48	0.43
1:A:253:VAL:O	1:A:253:VAL:HG22	2.17	0.43
1:B:242:LEU:CD2	1:B:251:PHE:HZ	2.31	0.43
1:A:34:ASP:C	1:A:36:LYS:H	2.27	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:O	1:A:64:VAL:HG23	2.19	0.43
1:B:154:PHE:HZ	1:B:256:GLN:HG3	1.83	0.43
1:A:144:ILE:HG22	1:A:172:ILE:HD13	2.01	0.43
1:A:153:THR:HG22	1:A:334:VAL:HB	2.00	0.43
1:B:35:VAL:HG22	1:B:35:VAL:O	2.18	0.43
1:B:135:GLU:HG2	1:B:137:ARG:HD3	2.01	0.43
1:B:83:ARG:NE	1:B:83:ARG:CA	2.80	0.43
1:B:254:PRO:HA	1:B:293:THR:OG1	2.17	0.43
1:B:419:GLU:HG2	1:B:420:HIS:N	2.34	0.43
1:A:348:LYS:O	1:A:352:GLU:HG3	2.19	0.43
1:B:133:ASP:C	1:B:135:GLU:H	2.25	0.43
1:B:242:LEU:CD2	1:B:249:LYS:HG3	2.49	0.43
1:B:342:VAL:O	1:B:342:VAL:HG13	2.18	0.43
1:A:47:ALA:HB2	1:A:79:CYS:C	2.44	0.43
1:B:135:GLU:HB3	1:B:137:ARG:NE	2.34	0.43
1:A:83:ARG:NE	1:A:83:ARG:CA	2.81	0.43
1:A:392:THR:OG1	1:A:393:GLU:N	2.51	0.43
1:A:17:CYS:SG	1:A:44:ASP:OD1	2.77	0.42
1:A:217:LEU:N	1:A:217:LEU:HD23	2.34	0.42
1:A:329:ASP:N	1:A:329:ASP:OD1	2.49	0.42
1:B:76:VAL:HG12	1:B:81:VAL:CG1	2.48	0.42
1:B:210:LEU:O	1:B:213:ARG:HB3	2.19	0.42
1:B:262:ILE:O	1:B:266:MET:HG3	2.19	0.42
1:A:19:VAL:HA	1:A:131:ARG:HB3	2.01	0.42
1:A:95:VAL:HG23	1:A:96:ASP:N	2.33	0.42
1:A:295:ILE:CG2	1:A:296:ILE:N	2.82	0.42
1:B:40:VAL:HG12	1:B:41:VAL:N	2.33	0.42
1:A:242:LEU:HD21	1:A:251:PHE:HZ	1.85	0.42
1:A:338:LEU:HD13	1:A:339:LYS:H	1.83	0.42
1:B:106:GLU:CD	1:B:106:GLU:H	2.28	0.42
1:B:252:ASP:HA	1:B:292:ARG:O	2.20	0.42
1:A:49:ILE:C	1:A:51:ASP:H	2.27	0.42
1:A:145:SER:HB2	1:A:166:SER:CB	2.50	0.42
1:B:380:GLY:CA	1:B:387:VAL:HG12	2.49	0.42
1:B:154:PHE:CZ	1:B:256:GLN:HG3	2.55	0.42
1:A:15:ALA:C	1:A:17:CYS:N	2.78	0.42
1:A:104:PRO:HG3	1:A:129:ARG:NH1	2.34	0.42
1:B:47:ALA:HB2	1:B:80:LEU:N	2.34	0.42
1:B:83:ARG:HB2	1:B:160:PHE:HE2	1.77	0.42
1:A:322:LEU:C	1:A:322:LEU:CD2	2.92	0.42
1:A:342:VAL:CG2	1:A:346:MET:HE3	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLU:CD	1:B:26:GLU:N	2.77	0.42
1:A:157:ILE:O	1:A:159:SER:N	2.53	0.42
1:B:313:PHE:CZ	1:B:317:ILE:HD11	2.55	0.42
1:B:196:SER:O	1:B:199:ILE:HG13	2.19	0.42
1:A:56:SER:O	1:A:60:ILE:HG13	2.19	0.41
1:A:57:ILE:HD12	1:A:80:LEU:HD21	2.01	0.41
1:A:242:LEU:HD21	1:A:251:PHE:CZ	2.55	0.41
1:B:11:PRO:HB2	1:B:190:VAL:HG11	2.02	0.41
1:B:111:ILE:HG13	1:B:112:GLU:OE1	2.20	0.41
1:B:145:SER:HB2	1:B:166:SER:CB	2.49	0.41
1:A:376:PHE:HE1	1:A:378:VAL:HG22	1.84	0.41
1:B:139:TYR:CA	1:B:186:GLU:HB3	2.50	0.41
1:B:376:PHE:CB	1:B:415:VAL:HG13	2.50	0.41
1:B:45:THR:OG1	1:B:56:SER:HB3	2.20	0.41
1:B:61:PHE:C	1:B:63:PHE:H	2.27	0.41
1:B:268:ARG:HG2	1:B:268:ARG:NH1	2.33	0.41
1:B:273:GLU:OE2	1:B:273:GLU:CA	2.69	0.41
1:A:237:ILE:O	1:A:240:ALA:HB3	2.20	0.41
1:B:358:GLN:HA	1:B:361:ILE:HD12	2.03	0.41
1:A:157:ILE:C	1:A:159:SER:H	2.29	0.41
1:A:373:LYS:HD2	1:A:414:GLU:OE1	2.20	0.41
1:A:417:ILE:HG23	1:A:425:MET:HB3	2.02	0.41
1:B:66:ALA:CB	1:B:69:GLN:HG3	2.48	0.41
1:B:202:TYR:HD2	1:B:202:TYR:N	2.17	0.41
1:B:338:LEU:HD13	1:B:339:LYS:H	1.86	0.41
1:B:415:VAL:HA	1:B:429:VAL:HA	2.02	0.41
1:A:2:ARG:HB2	1:A:39:ASP:CG	2.46	0.41
1:A:47:ALA:HB2	1:A:80:LEU:N	2.36	0.41
1:A:89:LYS:HE3	1:A:89:LYS:HB3	1.82	0.41
1:A:174:ARG:HB2	1:A:174:ARG:CZ	2.50	0.41
1:A:322:LEU:CB	1:A:358:GLN:HG2	2.38	0.41
1:A:419:GLU:HG2	1:A:420:HIS:N	2.36	0.41
1:B:11:PRO:CB	1:B:190:VAL:HG11	2.51	0.41
1:B:106:GLU:N	1:B:106:GLU:OE1	2.53	0.41
1:A:15:ALA:C	1:A:17:CYS:H	2.28	0.41
1:A:61:PHE:C	1:A:63:PHE:H	2.28	0.41
1:A:66:ALA:CB	1:A:69:GLN:HG3	2.49	0.41
1:A:106:GLU:CD	1:A:106:GLU:H	2.29	0.41
1:B:384:LYS:NZ	1:B:404:ARG:NH1	2.69	0.41
1:A:230:PRO:HB3	1:A:253:VAL:CG2	2.51	0.41
1:B:6:LYS:HA	1:B:6:LYS:HD2	1.99	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:HG	1:B:88:LEU:HD11	2.02	0.41
1:B:174:ARG:CZ	1:B:174:ARG:HB2	2.50	0.41
1:B:174:ARG:HH11	1:B:174:ARG:HG3	1.86	0.41
1:A:3:VAL:HG22	1:A:4:GLY:N	2.36	0.40
1:A:341:LYS:HB3	1:A:342:VAL:H	1.55	0.40
1:A:384:LYS:NZ	1:A:404:ARG:NH1	2.70	0.40
1:A:351:GLN:O	1:A:351:GLN:HG2	2.19	0.40
1:B:103:ASP:H	1:B:104:PRO:CD	2.35	0.40
1:B:256:GLN:OE1	1:B:296:ILE:HG13	2.22	0.40
1:B:273:GLU:OE2	1:B:273:GLU:HA	2.21	0.40
1:B:317:ILE:O	1:B:318:GLN:HB2	2.21	0.40
1:B:211:LEU:O	1:B:212:ARG:C	2.63	0.40
1:A:252:ASP:OD1	1:A:292:ARG:HG2	2.21	0.40
1:A:295:ILE:HG22	1:A:296:ILE:N	2.36	0.40
1:B:32:VAL:C	1:B:34:ASP:N	2.75	0.40
1:B:373:LYS:HD2	1:B:414:GLU:OE1	2.21	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	418/438 (95%)	351 (84%)	52 (12%)	15 (4%)	2	17
1	B	415/438 (95%)	348 (84%)	56 (14%)	11 (3%)	4	22
All	All	833/876 (95%)	699 (84%)	108 (13%)	26 (3%)	3	20

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	ILE
1	A	421	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	421	ASP
1	A	341	LYS
1	A	431	LEU
1	B	49	ILE
1	B	249	LYS
1	B	341	LYS
1	A	33	PHE
1	A	103	ASP
1	A	119	PRO
1	A	191	ALA
1	A	340	GLU
1	B	33	PHE
1	B	103	ASP
1	B	119	PRO
1	B	340	GLU
1	A	35	VAL
1	A	397	VAL
1	A	249	LYS
1	B	35	VAL
1	B	397	VAL
1	A	158	PRO
1	A	329	ASP
1	B	71	GLY
1	A	71	GLY

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	376/389 (97%)	324 (86%)	52 (14%)	3	15
1	B	373/389 (96%)	322 (86%)	51 (14%)	3	16
All	All	749/778 (96%)	646 (86%)	103 (14%)	3	15

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	19	VAL
1	A	26	GLU
1	A	29	HIS
1	A	30	GLU
1	A	33	PHE
1	A	39	ASP
1	A	41	VAL
1	A	57	ILE
1	A	77	LYS
1	A	95	VAL
1	A	97	GLN
1	A	99	ILE
1	A	106	GLU
1	A	107	ILE
1	A	112	GLU
1	A	118	VAL
1	A	129	ARG
1	A	134	LEU
1	A	153	THR
1	A	164	LEU
1	A	165	ARG
1	A	170	GLU
1	A	173	THR
1	A	186	GLU
1	A	189	LEU
1	A	194	THR
1	A	201	LEU
1	A	202	TYR
1	A	204	LYS
1	A	207	LEU
1	A	213	ARG
1	A	233	LEU
1	A	239	SER
1	A	253	VAL
1	A	274	GLU
1	A	277	LYS
1	A	330	GLU
1	A	331	GLU
1	A	338	LEU
1	A	339	LYS
1	A	345	GLU
1	A	355	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	357	LEU
1	A	366	LEU
1	A	384	LYS
1	A	385	PHE
1	A	408	LYS
1	A	411	ASP
1	A	415	VAL
1	A	430	ILE
1	A	431	LEU
1	B	8	LEU
1	B	19	VAL
1	B	26	GLU
1	B	29	HIS
1	B	30	GLU
1	B	33	PHE
1	B	39	ASP
1	B	41	VAL
1	B	57	ILE
1	B	95	VAL
1	B	99	ILE
1	B	106	GLU
1	B	107	ILE
1	B	112	GLU
1	B	127	ARG
1	B	129	ARG
1	B	133	ASP
1	B	134	LEU
1	B	153	THR
1	B	164	LEU
1	B	165	ARG
1	B	170	GLU
1	B	173	THR
1	B	186	GLU
1	B	189	LEU
1	B	194	THR
1	B	202	TYR
1	B	204	LYS
1	B	207	LEU
1	B	213	ARG
1	B	233	LEU
1	B	239	SER
1	B	265	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	268	ARG
1	B	277	LYS
1	B	285	ARG
1	B	330	GLU
1	B	331	GLU
1	B	338	LEU
1	B	339	LYS
1	B	345	GLU
1	B	355	LEU
1	B	357	LEU
1	B	366	LEU
1	B	384	LYS
1	B	385	PHE
1	B	408	LYS
1	B	411	ASP
1	B	415	VAL
1	B	429	VAL
1	B	431	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	A	232	HIS
1	B	192	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 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	$\# Z > 2$
2	FS5	B	501	1	8,30,30	4.06	6 (75%)	1,59,59	3.41	1 (100%)
2	FS5	A	501	1	8,30,30	4.89	6 (75%)	1,59,59	2.97	1 (100%)

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
2	FS5	B	501	1	-	0/0/118/118	0/12/10/10
2	FS5	A	501	1	-	0/0/118/118	0/12/10/10

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FS5	S3-FE4	-8.21	2.15	2.28
2	A	501	FS5	S4-FE4	-6.80	2.17	2.28
2	B	501	FS5	S5-FE8	-6.59	2.17	2.28
2	B	501	FS5	S8-FE8	-5.60	2.19	2.28
2	A	501	FS5	S7-FE8	-5.22	2.19	2.28
2	A	501	FS5	S8-FE8	-4.96	2.20	2.28
2	B	501	FS5	S7-FE8	-4.65	2.20	2.28
2	A	501	FS5	S5-FE8	-4.60	2.20	2.28
2	B	501	FS5	S1-FE4	-3.95	2.21	2.28
2	B	501	FS5	S4-FE4	-3.43	2.22	2.28
2	B	501	FS5	S3-FE4	-2.79	2.23	2.28
2	A	501	FS5	S1-FE4	-2.04	2.24	2.28

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FS5	S10-S11-S12	3.41	120.00	106.31
2	A	501	FS5	S10-S11-S12	2.97	118.25	106.31

There are no chirality outliers.

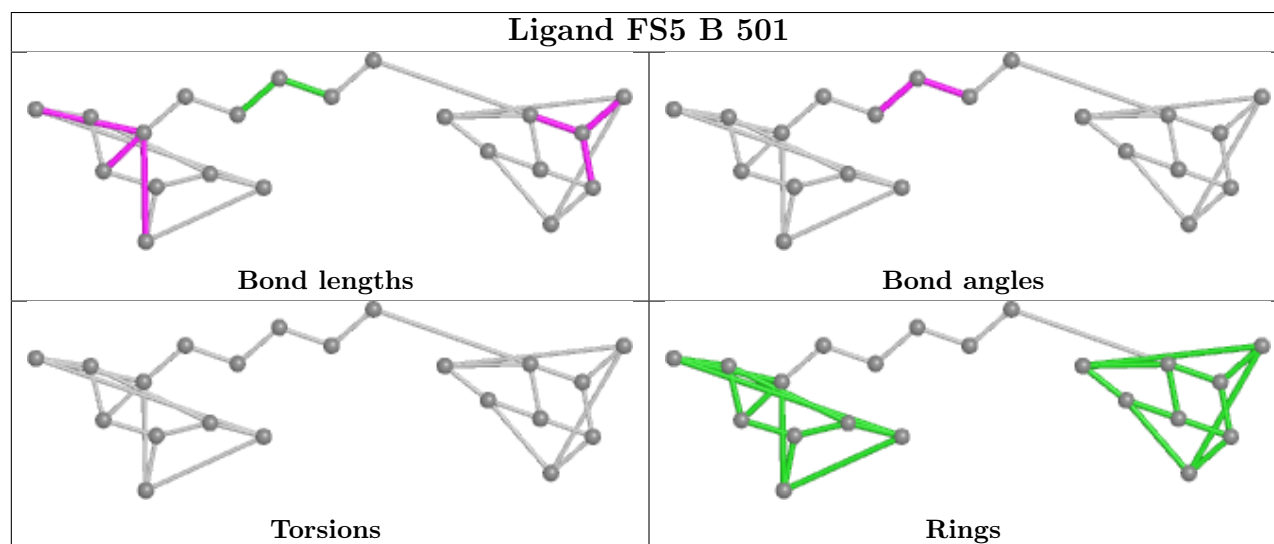
There are no torsion outliers.

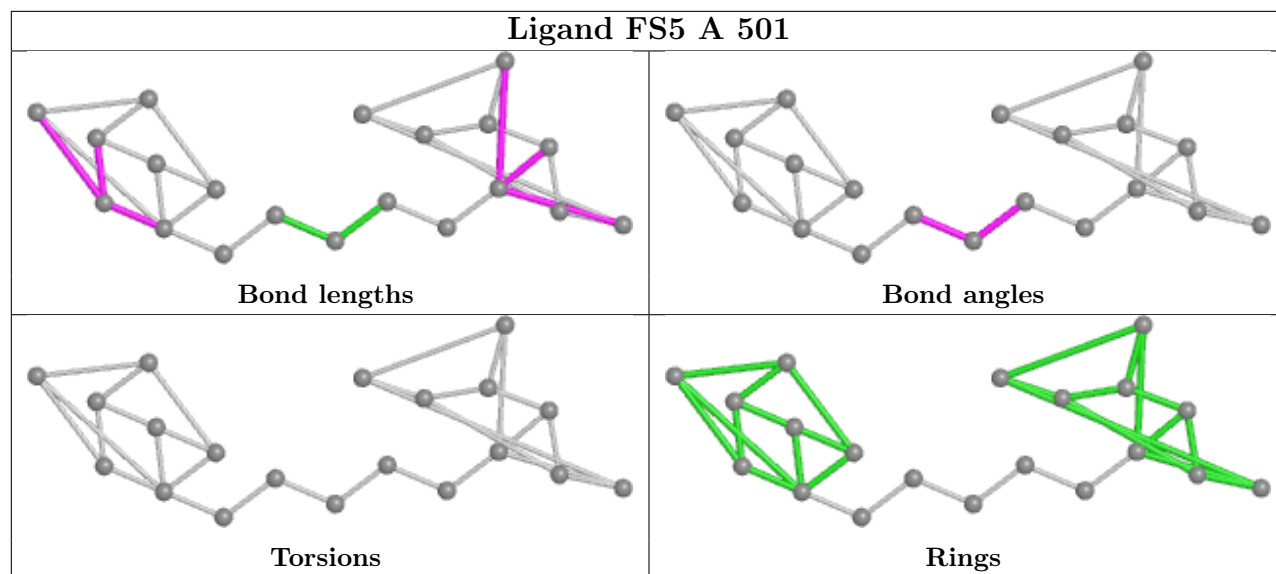
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FS5	5	0
2	A	501	FS5	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	424/438 (96%)	-0.12	3 (0%) 84 70	37, 94, 140, 201	0
1	B	421/438 (96%)	-0.13	3 (0%) 84 70	45, 95, 140, 201	0
All	All	845/876 (96%)	-0.12	6 (0%) 84 70	37, 94, 140, 201	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	410	GLY	3.2
1	A	243	GLU	2.9
1	B	99	ILE	2.6
1	A	159	SER	2.2
1	B	32	VAL	2.1
1	B	107	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

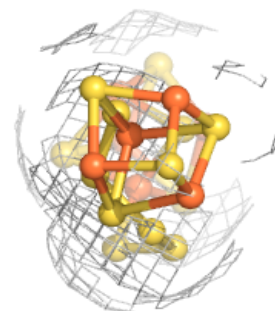
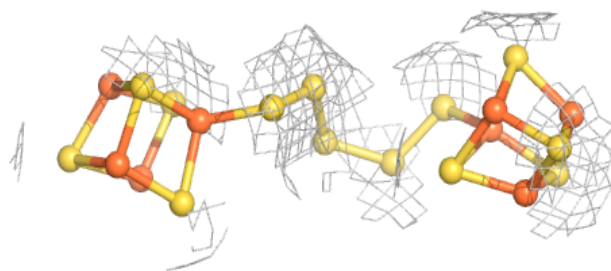
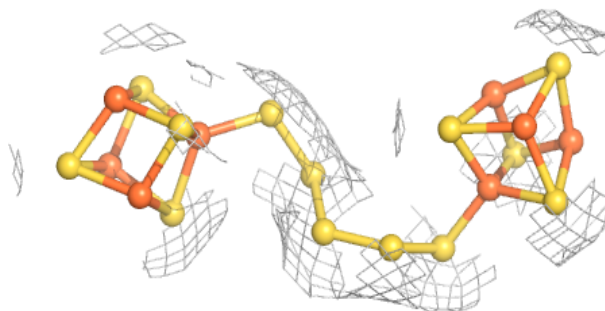
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FS5	A	501	21/21	0.98	0.04	2,56,90,101	5
2	FS5	B	501	21/21	0.99	0.03	51,68,84,93	5

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.

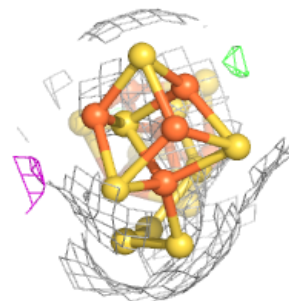
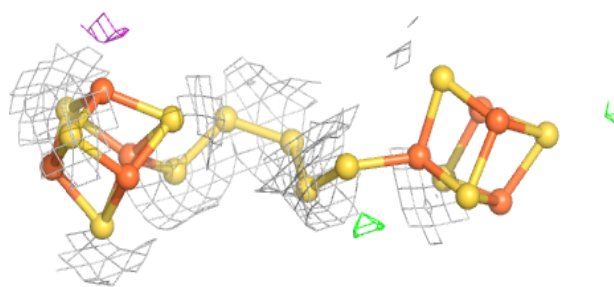
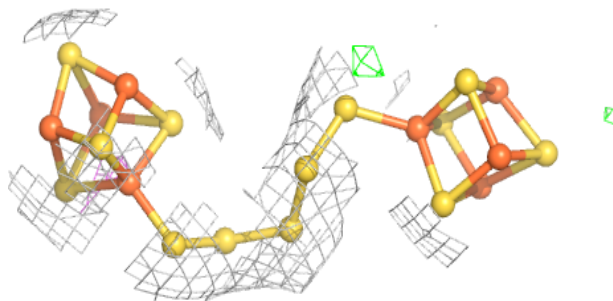
Electron density around FS5 A 501:

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 FS5 B 501:

$2mF_o - DF_c$ (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.