



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2021 – 08:08 PM JST

PDB ID : 7DE4
Title : Hybrid cluster protein (HCP) from Escherichia coli
Authors : Fujishiro, T.; Ooi, M.; Takaoka, K.; Takahashi, Y.
Deposited on : 2020-11-02
Resolution : 3.61 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 : 2.25
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) : 2.25

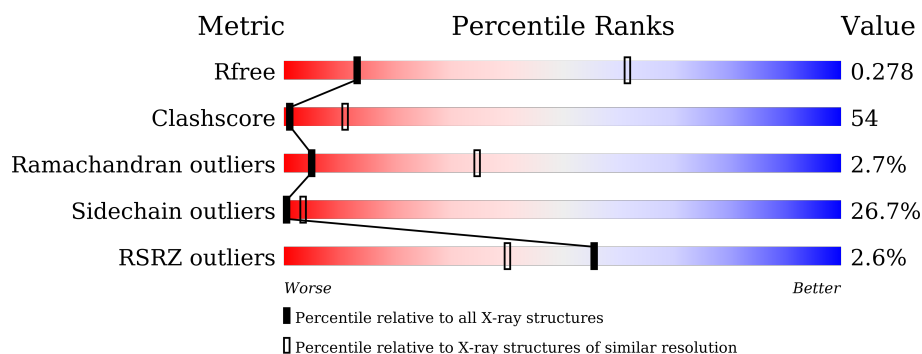
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.61 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	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

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	558	

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
1	CSS	A	405	-	-	X	-
3	FS2	A	602	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4237 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.

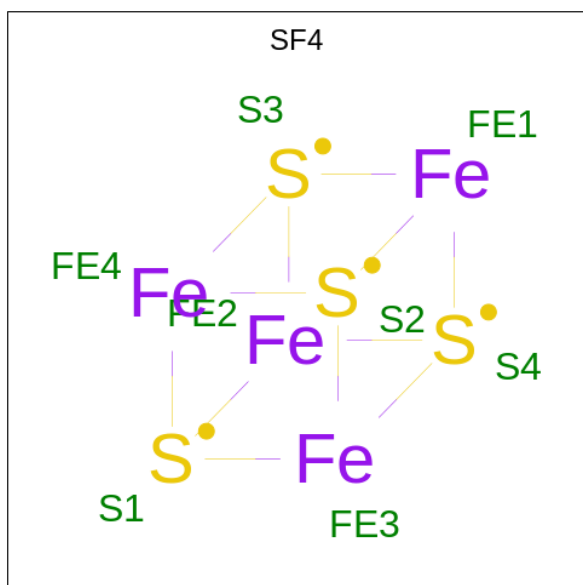
- Molecule 1 is a protein called Hydroxylamine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	550	4220	2682	717	793	28	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

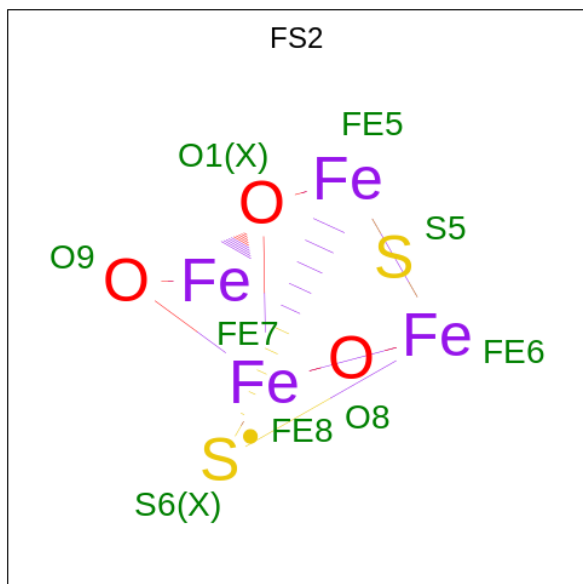
Chain	Residue	Modelled	Actual	Comment	Reference
A	551	LEU	-	expression tag	UNP P75825
A	552	GLU	-	expression tag	UNP P75825
A	553	HIS	-	expression tag	UNP P75825
A	554	HIS	-	expression tag	UNP P75825
A	555	HIS	-	expression tag	UNP P75825
A	556	HIS	-	expression tag	UNP P75825
A	557	HIS	-	expression tag	UNP P75825
A	558	HIS	-	expression tag	UNP P75825

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is FE-S-O HYBRID CLUSTER (three-letter code: FS2) (formula: $\text{Fe}_4\text{O}_3\text{S}_2$) (labeled as "Ligand of Interest" by depositor).

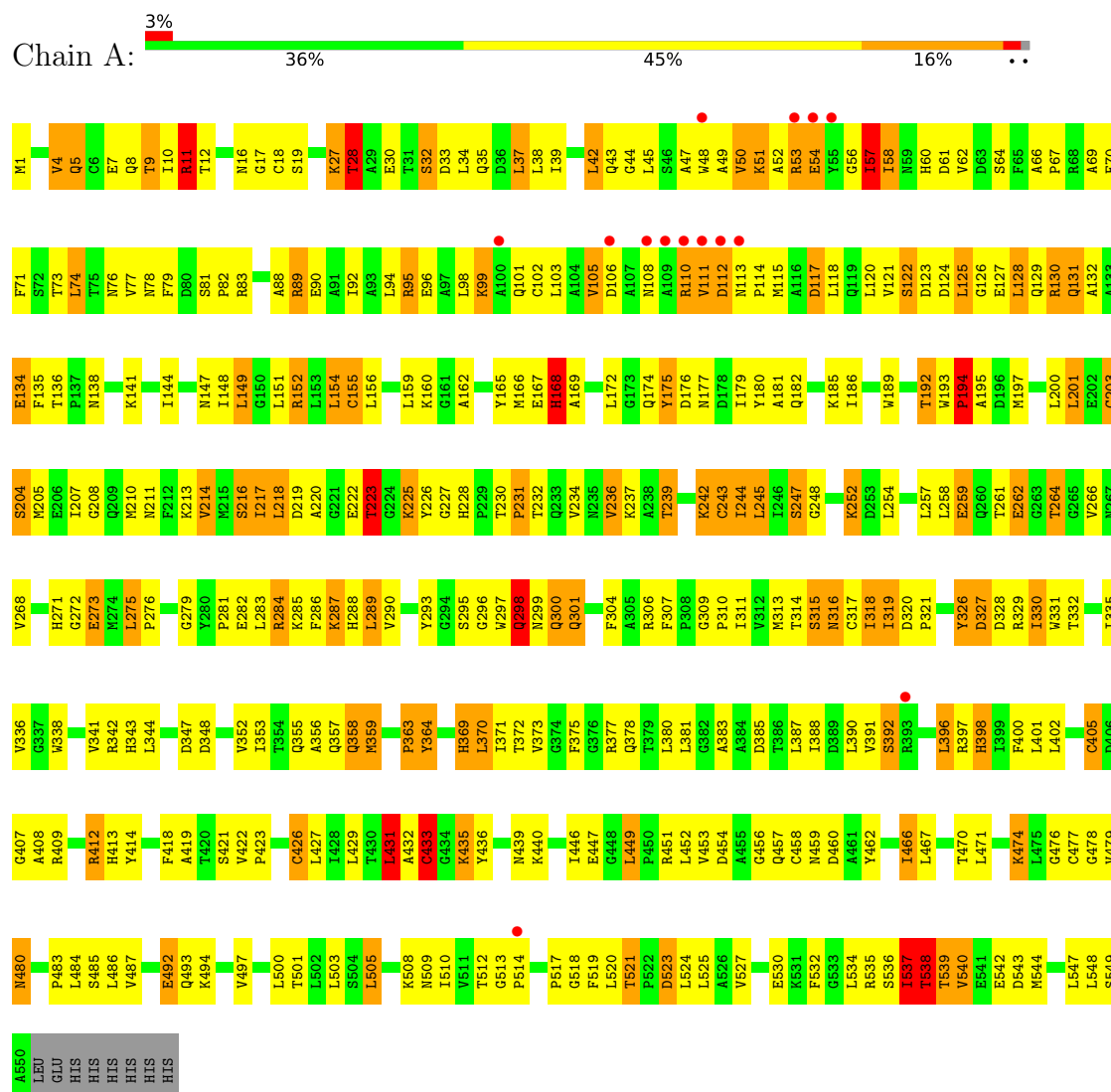


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	Fe	O	S	0	0
			9	4	3	2		

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: Hydroxylamine reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	142.54Å 142.54Å 117.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.29 – 3.61 46.29 – 3.61	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.29-3.61) 99.6 (46.29-3.61)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.203 , 0.278 0.203 , 0.278	Depositor DCC
R_{free} test set	717 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	116.3	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 144.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4237	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSS, FS2, 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	0.46	0/4299	1.17	24/5837 (0.4%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	ASN	CB-CA-C	-11.03	88.33	110.40
1	A	433	CYS	N-CA-CB	8.07	125.12	110.60
1	A	433	CYS	CB-CA-C	-7.72	94.96	110.40
1	A	168	HIS	CB-CA-C	7.37	125.14	110.40
1	A	298	GLN	CB-CA-C	6.87	124.14	110.40
1	A	347	ASP	CB-CA-C	6.63	123.67	110.40
1	A	512	THR	CB-CA-C	-6.32	94.55	111.60
1	A	117	ASP	CB-CA-C	6.16	122.73	110.40
1	A	231	PRO	N-CA-C	-6.16	96.09	112.10
1	A	385	ASP	CB-CA-C	6.13	122.66	110.40
1	A	358	GLN	CB-CA-C	6.13	122.65	110.40
1	A	523	ASP	CB-CA-C	-5.86	98.68	110.40
1	A	194	PRO	N-CA-C	5.81	127.21	112.10
1	A	259	GLU	CB-CA-C	-5.76	98.89	110.40
1	A	535	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	273	GLU	CB-CA-C	5.66	121.72	110.40
1	A	540	VAL	CB-CA-C	-5.48	100.99	111.40
1	A	223	THR	CB-CA-C	-5.21	97.54	111.60
1	A	264	THR	CA-CB-OG1	-5.20	98.07	109.00
1	A	122	SER	C-N-CA	5.20	134.70	121.70
1	A	194	PRO	N-CA-CB	-5.15	96.94	102.60
1	A	538	THR	C-N-CA	5.12	134.50	121.70
1	A	28	THR	CB-CA-C	-5.11	97.81	111.60
1	A	54	GLU	CB-CA-C	5.04	120.47	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4220	0	4179	458	0
2	A	8	0	0	0	0
3	A	9	0	0	3	0
All	All	4237	0	4179	458	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 54.

All (458) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:CG2	1:A:195:ALA:HB1	1.67	1.24
1:A:232:THR:HG21	1:A:279:GLY:HA2	1.17	1.17
1:A:125:LEU:HB3	1:A:128:LEU:HD11	1.17	1.16
1:A:154:LEU:HB2	1:A:519:PHE:HE2	1.00	1.13
1:A:281:PRO:HA	1:A:284:ARG:HD3	1.25	1.13
1:A:401:LEU:HD12	1:A:429:LEU:O	1.49	1.10
1:A:48:TRP:CH2	1:A:112:ASP:HB3	1.85	1.10
1:A:189:TRP:HH2	1:A:200:LEU:HD23	1.10	1.09
1:A:148:ILE:HG22	1:A:195:ALA:HB1	1.33	1.06
1:A:48:TRP:HH2	1:A:112:ASP:HB3	1.12	1.05
1:A:51:LYS:HE3	1:A:51:LYS:HA	1.40	1.04
1:A:154:LEU:HB2	1:A:519:PHE:CE2	1.92	1.02
1:A:401:LEU:HD23	1:A:486:LEU:CD2	1.89	1.02
1:A:232:THR:HB	1:A:284:ARG:HH22	1.25	1.00
1:A:258:LEU:HD13	1:A:286:PHE:CD2	1.96	0.99
1:A:120:LEU:HD21	1:A:135:PHE:CZ	1.98	0.99
1:A:298:GLN:HG3	1:A:407:GLY:O	1.63	0.98
1:A:232:THR:CG2	1:A:279:GLY:HA2	1.94	0.98
1:A:125:LEU:HB3	1:A:128:LEU:CD1	1.93	0.98
1:A:176:ASP:HB3	1:A:179:ILE:HG13	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:HG21	1:A:195:ALA:HB1	1.47	0.97
1:A:120:LEU:HD21	1:A:135:PHE:HZ	1.28	0.97
1:A:203:CYS:O	1:A:203:CYS:SG	2.23	0.97
1:A:539:THR:CG2	1:A:542:GLU:HB2	1.95	0.97
1:A:5:GLN:HG3	1:A:493:GLN:NE2	1.81	0.96
1:A:223:THR:HG21	1:A:228:HIS:CE1	2.01	0.95
1:A:154:LEU:CB	1:A:519:PHE:HE2	1.79	0.94
1:A:189:TRP:CH2	1:A:200:LEU:HD23	2.01	0.94
1:A:151:LEU:CD1	1:A:524:LEU:HD22	1.98	0.93
1:A:239:THR:OG1	1:A:290:VAL:HG11	1.70	0.92
1:A:99:LYS:C	1:A:103:LEU:HD12	1.91	0.91
1:A:377:ARG:O	1:A:381:LEU:HD13	1.71	0.90
1:A:44:GLY:C	1:A:95:ARG:HH12	1.75	0.90
1:A:151:LEU:HD13	1:A:524:LEU:CD2	2.01	0.90
1:A:261:THR:O	1:A:264:THR:HG22	1.72	0.90
1:A:435:LYS:HD3	1:A:454:ASP:OD2	1.70	0.90
1:A:77:VAL:HG22	1:A:316:ASN:HD22	1.37	0.89
1:A:16:ASN:HB3	1:A:518:GLY:O	1.72	0.89
1:A:281:PRO:HA	1:A:284:ARG:CD	2.02	0.89
1:A:398:HIS:O	1:A:426:CYS:HB2	1.71	0.89
1:A:223:THR:CG2	1:A:228:HIS:CE1	2.57	0.88
1:A:258:LEU:HD13	1:A:286:PHE:HD2	1.34	0.88
1:A:45:LEU:HD21	1:A:62:VAL:HG13	1.56	0.88
1:A:151:LEU:CD1	1:A:524:LEU:CD2	2.52	0.88
1:A:125:LEU:CB	1:A:128:LEU:HD11	2.02	0.88
1:A:208:GLY:O	1:A:501:THR:HG22	1.73	0.88
1:A:213:LYS:O	1:A:216:SER:HB2	1.74	0.88
1:A:151:LEU:HD13	1:A:524:LEU:HD21	1.56	0.87
1:A:189:TRP:HH2	1:A:200:LEU:CD2	1.88	0.87
1:A:401:LEU:HD23	1:A:486:LEU:HD22	1.57	0.86
1:A:160:LYS:HD2	1:A:493:GLN:HG2	1.57	0.86
1:A:435:LYS:O	1:A:439:ASN:HB2	1.76	0.85
1:A:539:THR:HG21	1:A:542:GLU:HB2	1.60	0.84
1:A:264:THR:HG23	1:A:266:VAL:H	1.42	0.84
1:A:125:LEU:O	1:A:128:LEU:HD12	1.77	0.84
1:A:99:LYS:O	1:A:103:LEU:HD12	1.77	0.84
1:A:244:ILE:HG23	1:A:310:PRO:HG2	1.59	0.84
1:A:513:GLY:HA3	1:A:537:ILE:HG12	1.58	0.84
1:A:213:LYS:O	1:A:216:SER:CB	2.26	0.84
1:A:45:LEU:N	1:A:95:ARG:HH12	1.76	0.83
1:A:125:LEU:CB	1:A:128:LEU:CD1	2.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:O	1:A:261:THR:HG23	1.77	0.82
1:A:405:CSS:SD	1:A:492:GLU:HG3	2.18	0.82
1:A:48:TRP:CH2	1:A:112:ASP:CB	2.62	0.82
1:A:216:SER:HA	1:A:462:TYR:CE2	2.14	0.82
1:A:10:ILE:HG22	1:A:17:GLY:C	2.01	0.81
1:A:120:LEU:CD2	1:A:135:PHE:HZ	1.93	0.81
1:A:539:THR:HG23	1:A:542:GLU:HB2	1.60	0.81
1:A:423:PRO:HG2	1:A:426:CYS:SG	2.21	0.81
1:A:77:VAL:CG2	1:A:316:ASN:HD22	1.93	0.81
1:A:236:VAL:HG11	1:A:440:LYS:HE3	1.63	0.81
1:A:315:SER:HA	1:A:336:VAL:CG2	2.11	0.81
1:A:175:TYR:HD2	1:A:180:TYR:HE2	1.27	0.80
1:A:414:TYR:CE1	1:A:418:PHE:HD2	2.00	0.80
1:A:151:LEU:HD11	1:A:524:LEU:HD22	1.63	0.79
1:A:514:PRO:HA	1:A:537:ILE:HD11	1.65	0.79
1:A:189:TRP:CH2	1:A:200:LEU:CD2	2.65	0.79
1:A:47:ALA:O	1:A:50:VAL:HG12	1.83	0.79
1:A:77:VAL:CG2	1:A:316:ASN:ND2	2.46	0.78
1:A:281:PRO:CA	1:A:284:ARG:HD3	2.11	0.78
1:A:329:ARG:HD3	1:A:359:MET:CE	2.12	0.78
1:A:9:THR:HG21	1:A:17:GLY:HA2	1.65	0.78
1:A:264:THR:CG2	1:A:266:VAL:HG12	2.14	0.78
1:A:208:GLY:HA2	1:A:501:THR:HG22	1.66	0.77
1:A:211:ASN:HB3	1:A:501:THR:CG2	2.15	0.77
1:A:398:HIS:HB2	1:A:483:PRO:HB2	1.67	0.77
1:A:218:LEU:HD12	1:A:218:LEU:O	1.85	0.75
1:A:544:MET:HA	1:A:544:MET:HE3	1.66	0.75
1:A:81:SER:N	1:A:82:PRO:HD2	2.02	0.74
1:A:289:LEU:HD23	1:A:289:LEU:O	1.88	0.74
1:A:332:THR:HB	1:A:336:VAL:HG12	1.68	0.74
1:A:9:THR:CG2	1:A:17:GLY:HA2	2.18	0.73
1:A:108:ASN:HB3	1:A:112:ASP:HA	1.70	0.73
1:A:182:GLN:OE1	1:A:210:MET:HB2	1.88	0.73
1:A:258:LEU:CD1	1:A:286:PHE:CD2	2.69	0.73
1:A:539:THR:HG21	1:A:542:GLU:CD	2.09	0.73
1:A:539:THR:HG21	1:A:542:GLU:CB	2.18	0.73
1:A:48:TRP:CZ2	1:A:112:ASP:HB2	2.24	0.72
1:A:154:LEU:HG	1:A:154:LEU:O	1.89	0.72
1:A:297:TRP:HB2	1:A:317:CYS:HB3	1.72	0.72
1:A:254:LEU:O	1:A:258:LEU:HG	1.90	0.71
1:A:89:ARG:HH11	1:A:89:ARG:CG	2.02	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:MET:HA	1:A:544:MET:CE	2.18	0.71
1:A:51:LYS:HB2	1:A:51:LYS:NZ	2.05	0.71
1:A:232:THR:CB	1:A:284:ARG:HH22	2.01	0.71
1:A:234:VAL:HG21	1:A:373:VAL:HG11	1.72	0.71
1:A:5:GLN:HG3	1:A:493:GLN:CD	2.12	0.70
1:A:539:THR:HG21	1:A:542:GLU:CG	2.22	0.70
1:A:521:THR:OG1	1:A:523:ASP:HB2	1.90	0.70
1:A:175:TYR:CD2	1:A:180:TYR:HE2	2.09	0.70
1:A:259:GLU:O	1:A:262:GLU:HB2	1.91	0.70
1:A:16:ASN:CB	1:A:518:GLY:O	2.40	0.70
1:A:405:CSS:HB2	3:A:602:FS2:S6	2.31	0.70
1:A:401:LEU:CD1	1:A:429:LEU:O	2.36	0.70
1:A:58:ILE:HD12	1:A:58:ILE:H	1.57	0.69
1:A:45:LEU:HD21	1:A:62:VAL:CG1	2.22	0.69
1:A:48:TRP:O	1:A:51:LYS:HB3	1.92	0.69
1:A:155:CYS:SG	1:A:203:CYS:O	2.51	0.69
1:A:264:THR:HG21	1:A:266:VAL:HG12	1.74	0.69
1:A:48:TRP:CZ2	1:A:112:ASP:CB	2.76	0.68
1:A:76:ASN:O	1:A:318:ILE:HG22	1.94	0.68
1:A:401:LEU:CD2	1:A:486:LEU:CD2	2.68	0.68
1:A:273:GLU:OE1	1:A:458:CYS:N	2.26	0.68
1:A:315:SER:HA	1:A:336:VAL:HG23	1.75	0.68
1:A:234:VAL:HG23	1:A:373:VAL:HG12	1.76	0.67
1:A:165:TYR:CE1	1:A:459:ASN:HB3	2.30	0.67
1:A:243:CYS:O	1:A:309:GLY:HA3	1.93	0.67
1:A:398:HIS:O	1:A:426:CYS:CB	2.43	0.67
1:A:51:LYS:HE3	1:A:51:LYS:CA	2.18	0.67
1:A:234:VAL:HG23	1:A:373:VAL:CG1	2.24	0.67
1:A:89:ARG:NH1	1:A:89:ARG:HG3	2.09	0.67
1:A:126:GLY:O	1:A:129:GLN:HB3	1.95	0.67
1:A:175:TYR:HD2	1:A:180:TYR:CE2	2.13	0.67
1:A:492:GLU:OE1	1:A:494:LYS:N	2.28	0.67
1:A:11:ARG:HH21	1:A:11:ARG:HG2	1.59	0.66
1:A:297:TRP:CB	1:A:317:CYS:HB3	2.25	0.66
1:A:387:LEU:HD21	1:A:427:LEU:HD11	1.77	0.66
1:A:208:GLY:CA	1:A:501:THR:HG22	2.26	0.66
1:A:211:ASN:HB3	1:A:501:THR:HG21	1.77	0.66
1:A:77:VAL:HG11	1:A:335:ILE:HD12	1.78	0.66
1:A:10:ILE:CG2	1:A:17:GLY:O	2.44	0.66
1:A:234:VAL:CG2	1:A:373:VAL:CG1	2.75	0.65
1:A:168:HIS:O	1:A:172:LEU:HD12	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:CB	1:A:112:ASP:HA	2.26	0.64
1:A:239:THR:CB	1:A:290:VAL:HG11	2.27	0.64
1:A:115:MET:HG3	1:A:118:LEU:H	1.63	0.64
1:A:310:PRO:HD3	1:A:356:ALA:HA	1.79	0.64
1:A:151:LEU:HD22	1:A:197:MET:HG3	1.79	0.63
1:A:258:LEU:CD1	1:A:286:PHE:HD2	2.07	0.63
1:A:48:TRP:HZ2	1:A:112:ASP:HB2	1.62	0.63
1:A:272:GLY:HA2	1:A:436:TYR:HE2	1.63	0.63
1:A:223:THR:HG22	1:A:228:HIS:CE1	2.32	0.63
1:A:162:ALA:HB2	1:A:497:VAL:HG21	1.81	0.63
1:A:159:LEU:C	1:A:159:LEU:HD23	2.18	0.63
1:A:9:THR:HG22	1:A:18:CYS:N	2.15	0.62
1:A:230:THR:HB	1:A:231:PRO:CD	2.29	0.62
1:A:94:LEU:O	1:A:98:LEU:HB2	1.99	0.62
1:A:182:GLN:O	1:A:186:ILE:HG13	2.00	0.62
1:A:264:THR:HG23	1:A:266:VAL:HG12	1.82	0.61
1:A:275:LEU:N	1:A:276:PRO:CD	2.62	0.61
1:A:169:ALA:HB2	1:A:218:LEU:HB2	1.82	0.61
1:A:151:LEU:HD11	1:A:524:LEU:CD2	2.25	0.61
1:A:480:ASN:OD1	1:A:480:ASN:N	2.32	0.61
1:A:204:SER:O	1:A:500:LEU:HD13	2.01	0.61
1:A:381:LEU:N	1:A:381:LEU:HD12	2.14	0.61
1:A:151:LEU:CD1	1:A:524:LEU:HD21	2.25	0.61
1:A:120:LEU:CD2	1:A:135:PHE:CZ	2.73	0.61
1:A:432:ALA:O	1:A:435:LYS:HB3	2.01	0.61
1:A:89:ARG:CG	1:A:89:ARG:NH1	2.60	0.60
1:A:223:THR:HG22	1:A:228:HIS:ND1	2.16	0.60
1:A:470:THR:O	1:A:474:LYS:HG3	2.00	0.60
1:A:152:ARG:NH2	1:A:193:TRP:HB3	2.16	0.60
1:A:414:TYR:HE1	1:A:418:PHE:CD2	2.20	0.59
1:A:401:LEU:HB3	1:A:486:LEU:HD23	1.85	0.59
1:A:275:LEU:N	1:A:276:PRO:HD3	2.17	0.59
1:A:304:PHE:HB2	1:A:326:TYR:CE2	2.36	0.59
1:A:9:THR:HG21	1:A:17:GLY:CA	2.32	0.59
1:A:248:GLY:HA3	1:A:314:THR:OG1	2.02	0.59
1:A:329:ARG:HD3	1:A:359:MET:HE1	1.84	0.59
1:A:16:ASN:CG	1:A:518:GLY:O	2.41	0.59
1:A:10:ILE:HG22	1:A:18:CYS:N	2.18	0.59
1:A:5:GLN:CG	1:A:493:GLN:NE2	2.60	0.59
1:A:148:ILE:HG21	1:A:195:ALA:CB	2.28	0.58
1:A:186:ILE:HG21	1:A:207:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:TYR:CE1	1:A:418:PHE:CD2	2.87	0.58
1:A:321:PRO:HG3	1:A:341:VAL:HG21	1.85	0.58
1:A:39:ILE:O	1:A:43:GLN:HG3	2.03	0.58
1:A:525:LEU:HD12	1:A:525:LEU:C	2.24	0.57
1:A:331:TRP:CZ3	1:A:342:ARG:HD2	2.38	0.57
1:A:38:LEU:CD1	1:A:42:LEU:HD23	2.35	0.57
1:A:60:HIS:CE1	1:A:175:TYR:CE2	2.92	0.57
1:A:217:ILE:O	1:A:220:ALA:HB3	2.04	0.57
1:A:315:SER:HA	1:A:336:VAL:HG21	1.86	0.57
1:A:5:GLN:O	1:A:493:GLN:NE2	2.37	0.57
1:A:234:VAL:CG2	1:A:373:VAL:HG11	2.33	0.57
1:A:38:LEU:HD11	1:A:42:LEU:HD23	1.85	0.56
1:A:77:VAL:HG23	1:A:316:ASN:ND2	2.19	0.56
1:A:208:GLY:C	1:A:501:THR:HG22	2.24	0.56
1:A:4:VAL:HG22	1:A:4:VAL:O	2.05	0.56
1:A:148:ILE:HG22	1:A:195:ALA:CB	2.23	0.56
1:A:208:GLY:O	1:A:501:THR:CG2	2.52	0.56
1:A:338:TRP:HD1	1:A:341:VAL:HG23	1.70	0.56
1:A:405:CSS:CB	3:A:602:FS2:S6	2.92	0.56
1:A:47:ALA:HB1	1:A:113:ASN:HD21	1.71	0.56
1:A:329:ARG:HD3	1:A:359:MET:HE2	1.86	0.56
1:A:226:TYR:OH	1:A:252:LYS:HA	2.05	0.56
1:A:480:ASN:ND2	1:A:508:LYS:H	2.03	0.56
1:A:381:LEU:H	1:A:381:LEU:CD1	2.18	0.56
1:A:176:ASP:OD1	1:A:177:ASN:N	2.39	0.56
1:A:76:ASN:HA	1:A:79:PHE:CZ	2.41	0.55
1:A:321:PRO:HB3	1:A:326:TYR:HE1	1.71	0.55
1:A:134:GLU:O	1:A:134:GLU:HG3	2.05	0.55
1:A:148:ILE:CD1	1:A:197:MET:HB2	2.37	0.55
1:A:401:LEU:CB	1:A:486:LEU:HD23	2.36	0.55
1:A:405:CSS:SD	1:A:492:GLU:CD	2.84	0.55
1:A:77:VAL:CG1	1:A:335:ILE:HD12	2.36	0.55
1:A:400:PHE:CZ	1:A:544:MET:HE1	2.42	0.55
1:A:239:THR:OG1	1:A:290:VAL:CG1	2.51	0.55
1:A:60:HIS:O	1:A:64:SER:HB3	2.06	0.55
1:A:51:LYS:CA	1:A:51:LYS:CE	2.85	0.54
1:A:414:TYR:HE1	1:A:418:PHE:HD2	1.47	0.54
1:A:92:ILE:HG23	1:A:95:ARG:HE	1.72	0.54
1:A:125:LEU:C	1:A:128:LEU:HD12	2.27	0.54
1:A:42:LEU:HD21	1:A:69:ALA:HB3	1.90	0.54
1:A:193:TRP:N	1:A:194:PRO:HD2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:HD12	1:A:218:LEU:C	2.28	0.54
1:A:8:GLN:OE1	1:A:408:ALA:N	2.40	0.54
1:A:147:ASN:O	1:A:524:LEU:HD11	2.08	0.54
1:A:81:SER:N	1:A:82:PRO:CD	2.71	0.54
1:A:363:PRO:HD2	1:A:364:TYR:H	1.73	0.54
1:A:517:PRO:HB2	1:A:520:LEU:HD23	1.89	0.54
1:A:9:THR:CG2	1:A:18:CYS:H	2.21	0.54
1:A:9:THR:HG22	1:A:10:ILE:H	1.73	0.54
1:A:45:LEU:N	1:A:95:ARG:NH1	2.53	0.54
1:A:95:ARG:HG3	1:A:95:ARG:HH11	1.72	0.54
1:A:154:LEU:CB	1:A:519:PHE:CE2	2.69	0.54
1:A:7:GLU:OE2	1:A:409:ARG:NH1	2.41	0.54
1:A:418:PHE:CZ	1:A:487:VAL:HG21	2.43	0.53
1:A:51:LYS:HE2	1:A:53:ARG:HG3	1.89	0.53
1:A:213:LYS:O	1:A:216:SER:HB3	2.05	0.53
1:A:402:LEU:CD1	1:A:419:ALA:HB2	2.37	0.53
1:A:245:LEU:H	1:A:307:PHE:HE2	1.56	0.53
1:A:296:GLY:N	1:A:436:TYR:CD2	2.76	0.53
1:A:320:ASP:HA	1:A:338:TRP:CZ2	2.44	0.53
1:A:295:SER:OG	1:A:295:SER:O	2.24	0.53
1:A:103:LEU:CD2	1:A:108:ASN:OD1	2.57	0.53
1:A:245:LEU:O	1:A:311:ILE:HA	2.09	0.53
1:A:76:ASN:HA	1:A:79:PHE:HZ	1.74	0.53
1:A:297:TRP:O	1:A:300:GLN:HG2	2.09	0.53
1:A:51:LYS:HB2	1:A:51:LYS:HZ2	1.74	0.52
1:A:230:THR:HB	1:A:231:PRO:HD3	1.91	0.52
1:A:370:LEU:HD12	1:A:370:LEU:H	1.73	0.52
1:A:381:LEU:N	1:A:381:LEU:CD1	2.71	0.52
1:A:175:TYR:HB2	1:A:180:TYR:CE2	2.44	0.52
1:A:405:CSS:SG	3:A:602:FS2:S6	3.07	0.52
1:A:508:LYS:HG2	1:A:532:PHE:HA	1.92	0.52
1:A:88:ALA:O	1:A:92:ILE:HG13	2.09	0.52
1:A:391:VAL:CG2	1:A:396:LEU:HB3	2.39	0.52
1:A:513:GLY:HA3	1:A:537:ILE:CG1	2.34	0.52
1:A:10:ILE:CG2	1:A:17:GLY:C	2.73	0.52
1:A:60:HIS:ND1	1:A:175:TYR:CE2	2.78	0.52
1:A:321:PRO:CB	1:A:326:TYR:HE1	2.22	0.52
1:A:398:HIS:H	1:A:426:CYS:HB3	1.74	0.52
1:A:49:ALA:C	1:A:51:LYS:H	2.13	0.52
1:A:375:PHE:HB2	1:A:454:ASP:O	2.10	0.52
1:A:503:LEU:HD22	1:A:532:PHE:CG	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:HB3	1:A:226:TYR:CD2	2.45	0.51
1:A:9:THR:HG22	1:A:18:CYS:H	1.75	0.51
1:A:147:ASN:ND2	1:A:523:ASP:CB	2.72	0.51
1:A:42:LEU:HD21	1:A:69:ALA:CB	2.41	0.51
1:A:453:VAL:HG12	1:A:453:VAL:O	2.10	0.51
1:A:537:ILE:HD12	1:A:538:THR:H	1.76	0.51
1:A:391:VAL:HG23	1:A:396:LEU:HB3	1.92	0.51
1:A:110:ARG:HD2	1:A:111:VAL:H	1.75	0.51
1:A:245:LEU:N	1:A:307:PHE:HE2	2.07	0.51
1:A:77:VAL:HG22	1:A:316:ASN:ND2	2.13	0.50
1:A:539:THR:HG23	1:A:539:THR:O	2.09	0.50
1:A:45:LEU:CD2	1:A:62:VAL:HG13	2.36	0.50
1:A:327:ASP:O	1:A:341:VAL:HG13	2.10	0.50
1:A:405:CSS:SD	1:A:492:GLU:CG	2.90	0.50
1:A:396:LEU:HD23	1:A:426:CYS:HA	1.92	0.50
1:A:462:TYR:CE1	1:A:466:ILE:HD13	2.47	0.50
1:A:544:MET:HG3	1:A:548:LEU:CD2	2.41	0.50
1:A:321:PRO:CG	1:A:341:VAL:HG21	2.42	0.50
1:A:514:PRO:HA	1:A:537:ILE:CD1	2.41	0.50
1:A:245:LEU:N	1:A:307:PHE:CE2	2.80	0.50
1:A:44:GLY:C	1:A:95:ARG:NH1	2.57	0.49
1:A:147:ASN:ND2	1:A:523:ASP:HB2	2.27	0.49
1:A:52:ALA:HA	1:A:56:GLY:HA3	1.95	0.49
1:A:70:PHE:CE2	1:A:160:LYS:HA	2.48	0.49
1:A:147:ASN:HD21	1:A:523:ASP:CB	2.26	0.49
1:A:247:SER:HB2	1:A:271:HIS:ND1	2.28	0.49
1:A:181:ALA:O	1:A:185:LYS:HG3	2.12	0.49
1:A:192:THR:O	1:A:192:THR:OG1	2.30	0.49
1:A:166:MET:O	1:A:169:ALA:HB3	2.13	0.49
1:A:297:TRP:CG	1:A:317:CYS:HB3	2.47	0.49
1:A:505:LEU:O	1:A:505:LEU:HD22	2.13	0.48
1:A:34:LEU:HD12	1:A:81:SER:HB3	1.95	0.48
1:A:412:ARG:O	1:A:413:HIS:C	2.52	0.48
1:A:45:LEU:O	1:A:45:LEU:HD23	2.13	0.48
1:A:166:MET:CG	1:A:214:VAL:HG21	2.44	0.48
1:A:33:ASP:HB3	1:A:130:ARG:HG3	1.96	0.48
1:A:538:THR:O	1:A:539:THR:HG22	2.14	0.48
1:A:103:LEU:HD21	1:A:112:ASP:OD2	2.13	0.48
1:A:258:LEU:HD23	1:A:268:VAL:HG21	1.96	0.48
1:A:321:PRO:HD2	1:A:338:TRP:CE2	2.49	0.48
1:A:387:LEU:HD21	1:A:427:LEU:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:CYS:O	1:A:105:VAL:HG23	2.13	0.48
1:A:409:ARG:HD2	1:A:514:PRO:HG2	1.96	0.48
1:A:115:MET:CE	1:A:117:ASP:H	2.26	0.48
1:A:208:GLY:HA2	1:A:501:THR:CG2	2.40	0.48
1:A:1:MET:O	1:A:19:SER:HA	2.14	0.48
1:A:527:VAL:O	1:A:530:GLU:HB3	2.13	0.48
1:A:454:ASP:OD1	1:A:456:GLY:N	2.40	0.47
1:A:108:ASN:OD1	1:A:112:ASP:OD2	2.32	0.47
1:A:186:ILE:HD13	1:A:207:ILE:HG13	1.95	0.47
1:A:225:LYS:HB3	1:A:226:TYR:CE2	2.49	0.47
1:A:400:PHE:CZ	1:A:544:MET:CE	2.97	0.47
1:A:166:MET:HG3	1:A:214:VAL:HG21	1.96	0.47
1:A:321:PRO:HA	1:A:326:TYR:CE1	2.48	0.47
1:A:407:GLY:H	1:A:412:ARG:HD3	1.79	0.47
1:A:422:VAL:HG12	1:A:451:ARG:HH21	1.80	0.47
1:A:540:VAL:HG12	1:A:540:VAL:O	2.14	0.47
1:A:9:THR:CG2	1:A:17:GLY:CA	2.92	0.47
1:A:363:PRO:CD	1:A:364:TYR:H	2.28	0.47
1:A:120:LEU:HD21	1:A:135:PHE:CE2	2.49	0.47
1:A:407:GLY:HA3	1:A:412:ARG:CZ	2.43	0.47
1:A:446:ILE:O	1:A:447:GLU:HB2	2.15	0.47
1:A:48:TRP:O	1:A:51:LYS:CB	2.62	0.47
1:A:232:THR:CG2	1:A:279:GLY:CA	2.82	0.47
1:A:369:HIS:C	1:A:369:HIS:CD2	2.88	0.47
1:A:248:GLY:HA3	1:A:314:THR:HG1	1.78	0.47
1:A:285:LYS:HE3	1:A:286:PHE:CZ	2.50	0.47
1:A:380:LEU:O	1:A:383:ALA:HB3	2.15	0.47
1:A:381:LEU:HD12	1:A:381:LEU:H	1.79	0.47
1:A:129:GLN:O	1:A:131:GLN:N	2.48	0.46
1:A:261:THR:HB	1:A:264:THR:HG21	1.96	0.46
1:A:457:GLN:O	1:A:458:CYS:C	2.53	0.46
1:A:99:LYS:O	1:A:103:LEU:CD1	2.55	0.46
1:A:4:VAL:HB	1:A:17:GLY:HA3	1.96	0.46
1:A:114:PRO:O	1:A:114:PRO:HG2	2.15	0.46
1:A:261:THR:C	1:A:264:THR:HG22	2.35	0.46
1:A:480:ASN:HD22	1:A:508:LYS:H	1.63	0.46
1:A:10:ILE:CG2	1:A:18:CYS:HA	2.45	0.46
1:A:152:ARG:HH21	1:A:193:TRP:HE3	1.64	0.46
1:A:268:VAL:HG12	1:A:289:LEU:HB2	1.98	0.46
1:A:4:VAL:CG2	1:A:518:GLY:HA3	2.46	0.46
1:A:300:GLN:HG2	1:A:300:GLN:H	1.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:GLN:CD	1:A:493:GLN:N	2.69	0.46
1:A:103:LEU:HD23	1:A:108:ASN:OD1	2.16	0.45
1:A:275:LEU:HD22	1:A:373:VAL:HG21	1.98	0.45
1:A:388:ILE:O	1:A:392:SER:HB2	2.16	0.45
1:A:99:LYS:CG	1:A:103:LEU:HD11	2.45	0.45
1:A:245:LEU:HB3	1:A:307:PHE:CZ	2.52	0.45
1:A:380:LEU:HD23	1:A:380:LEU:HA	1.78	0.45
1:A:432:ALA:O	1:A:435:LYS:HE2	2.16	0.45
1:A:321:PRO:HD2	1:A:338:TRP:NE1	2.32	0.45
1:A:218:LEU:O	1:A:222:GLU:HG3	2.16	0.45
1:A:283:LEU:HD12	1:A:283:LEU:HA	1.79	0.45
1:A:92:ILE:O	1:A:96:GLU:HG2	2.17	0.45
1:A:521:THR:HG23	1:A:524:LEU:HD12	1.98	0.45
1:A:125:LEU:HB2	1:A:128:LEU:CD1	2.44	0.45
1:A:326:TYR:HD1	1:A:326:TYR:C	2.20	0.45
1:A:412:ARG:HG3	1:A:514:PRO:HG3	1.99	0.45
1:A:301:GLN:OE1	1:A:319:ILE:HD12	2.16	0.44
1:A:433:CYS:C	1:A:435:LYS:N	2.70	0.44
1:A:477:CYS:SG	1:A:478:GLY:N	2.90	0.44
1:A:38:LEU:O	1:A:42:LEU:HB2	2.17	0.44
1:A:49:ALA:C	1:A:51:LYS:N	2.71	0.44
1:A:154:LEU:CA	1:A:519:PHE:CE2	3.01	0.44
1:A:77:VAL:HG12	1:A:78:ASN:HB2	1.98	0.44
1:A:151:LEU:HD21	1:A:201:LEU:HD23	2.00	0.44
1:A:414:TYR:CD1	1:A:414:TYR:C	2.90	0.44
1:A:27:LYS:HE2	1:A:35:GLN:OE1	2.17	0.44
1:A:44:GLY:O	1:A:45:LEU:C	2.55	0.44
1:A:95:ARG:HH11	1:A:95:ARG:CG	2.30	0.44
1:A:226:TYR:HA	1:A:282:GLU:HB3	2.00	0.44
1:A:66:ALA:N	1:A:67:PRO:HD2	2.33	0.44
1:A:113:ASN:OD1	1:A:114:PRO:HD2	2.18	0.44
1:A:254:LEU:HD11	1:A:268:VAL:HG11	2.00	0.44
1:A:38:LEU:HD11	1:A:42:LEU:CD2	2.48	0.44
1:A:227:GLY:HA3	1:A:281:PRO:HG2	1.99	0.44
1:A:282:GLU:O	1:A:282:GLU:HG3	2.17	0.44
1:A:427:LEU:HD21	1:A:449:LEU:HD13	1.99	0.44
1:A:431:LEU:HD13	1:A:431:LEU:O	2.17	0.44
1:A:519:PHE:CD1	1:A:519:PHE:N	2.84	0.44
1:A:74:LEU:HD12	1:A:160:LYS:HG2	1.99	0.43
1:A:175:TYR:CD1	1:A:175:TYR:N	2.86	0.43
1:A:4:VAL:O	1:A:4:VAL:CG2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:HE2	1:A:252:LYS:HB2	1.52	0.43
1:A:266:VAL:HG11	1:A:353:ILE:HG23	2.00	0.43
1:A:298:GLN:CG	1:A:407:GLY:O	2.51	0.43
1:A:300:GLN:HG3	1:A:319:ILE:CG1	2.48	0.43
1:A:321:PRO:CB	1:A:326:TYR:CE1	3.01	0.43
1:A:11:ARG:HG2	1:A:11:ARG:NH2	2.30	0.43
1:A:90:GLU:O	1:A:94:LEU:HD12	2.17	0.43
1:A:243:CYS:HB2	1:A:307:PHE:CZ	2.53	0.43
1:A:83:ARG:NH2	1:A:343:HIS:HD2	2.17	0.43
1:A:103:LEU:C	1:A:105:VAL:H	2.21	0.43
1:A:115:MET:HE2	1:A:117:ASP:H	1.82	0.43
1:A:56:GLY:O	1:A:57:ILE:O	2.37	0.43
1:A:122:SER:OG	1:A:131:GLN:NE2	2.52	0.43
1:A:431:LEU:O	1:A:432:ALA:HB2	2.19	0.43
1:A:57:ILE:HG23	1:A:58:ILE:N	2.33	0.43
1:A:326:TYR:C	1:A:326:TYR:CD1	2.92	0.43
1:A:471:LEU:HD23	1:A:471:LEU:HA	1.89	0.43
1:A:245:LEU:CD2	1:A:293:TYR:CD1	3.02	0.42
1:A:457:GLN:O	1:A:460:ASP:HB2	2.19	0.42
1:A:39:ILE:HG13	1:A:73:THR:HG21	2.01	0.42
1:A:152:ARG:CA	1:A:200:LEU:HD13	2.49	0.42
1:A:462:TYR:CE1	1:A:466:ILE:CD1	3.01	0.42
1:A:37:LEU:HD21	1:A:120:LEU:HD11	2.01	0.42
1:A:242:LYS:C	1:A:266:VAL:HG23	2.40	0.42
1:A:244:ILE:HD12	1:A:257:LEU:HD11	2.02	0.42
1:A:275:LEU:HB3	1:A:276:PRO:HD3	2.02	0.42
1:A:27:LYS:HD3	1:A:32:SER:OG	2.19	0.42
1:A:48:TRP:HZ2	1:A:99:LYS:HZ3	1.62	0.42
1:A:234:VAL:O	1:A:370:LEU:HA	2.20	0.42
1:A:81:SER:H	1:A:82:PRO:HD2	1.79	0.42
1:A:435:LYS:HB3	1:A:435:LYS:HE2	1.67	0.42
1:A:175:TYR:N	1:A:175:TYR:HD1	2.18	0.42
1:A:211:ASN:HD22	1:A:501:THR:CG2	2.33	0.42
1:A:236:VAL:HG23	1:A:369:HIS:O	2.19	0.42
1:A:402:LEU:HD23	1:A:402:LEU:HA	1.92	0.42
1:A:103:LEU:C	1:A:105:VAL:N	2.72	0.41
1:A:167:GLU:C	1:A:169:ALA:H	2.22	0.41
1:A:344:LEU:HD21	1:A:348:ASP:O	2.20	0.41
1:A:313:MET:HE3	1:A:318:ILE:HG13	2.02	0.41
1:A:28:THR:HB	1:A:30:GLU:H	1.85	0.41
1:A:117:ASP:O	1:A:120:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:THR:CB	1:A:231:PRO:HD3	2.50	0.41
1:A:311:ILE:HB	1:A:330:ILE:HG12	2.03	0.41
1:A:355:GLN:O	1:A:355:GLN:HG2	2.20	0.41
1:A:136:THR:O	1:A:193:TRP:CH2	2.73	0.41
1:A:201:LEU:HD22	1:A:201:LEU:HA	1.92	0.41
1:A:293:TYR:CD1	1:A:293:TYR:C	2.94	0.41
1:A:449:LEU:HD23	1:A:449:LEU:HA	1.74	0.41
1:A:136:THR:O	1:A:193:TRP:HH2	2.03	0.41
1:A:264:THR:HG23	1:A:266:VAL:N	2.22	0.41
1:A:287:LYS:HE2	1:A:287:LYS:HB3	1.56	0.41
1:A:414:TYR:CZ	1:A:537:ILE:HG22	2.56	0.41
1:A:517:PRO:HB3	1:A:519:PHE:CE1	2.55	0.41
1:A:390:LEU:HB3	1:A:396:LEU:HB2	2.02	0.41
1:A:37:LEU:HB2	1:A:132:ALA:HB2	2.03	0.41
1:A:45:LEU:HD23	1:A:45:LEU:C	2.41	0.41
1:A:387:LEU:HD22	1:A:396:LEU:CD1	2.51	0.41
1:A:321:PRO:CA	1:A:326:TYR:CE1	3.04	0.41
1:A:537:ILE:H	1:A:537:ILE:HG13	1.58	0.40
1:A:232:THR:HB	1:A:284:ARG:NH2	2.09	0.40
1:A:258:LEU:HB3	1:A:286:PHE:CD2	2.57	0.40
1:A:138:ASN:HB3	1:A:149:LEU:HD11	2.04	0.40
1:A:159:LEU:HD23	1:A:159:LEU:O	2.21	0.40
1:A:226:TYR:O	1:A:281:PRO:HD2	2.22	0.40
1:A:245:LEU:HB3	1:A:307:PHE:CE2	2.56	0.40
1:A:261:THR:OG1	1:A:288:HIS:CD2	2.74	0.40
1:A:543:ASP:O	1:A:547:LEU:HG	2.21	0.40
1:A:151:LEU:HD22	1:A:197:MET:CG	2.47	0.40
1:A:433:CYS:C	1:A:435:LYS:H	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	547/558 (98%)	479 (88%)	53 (10%)	15 (3%)	5 35

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	124	ASP
1	A	130	ARG
1	A	194	PRO
1	A	539	THR
1	A	315	SER
1	A	509	ASN
1	A	537	ILE
1	A	11	ARG
1	A	125	LEU
1	A	4	VAL
1	A	431	LEU
1	A	538	THR
1	A	363	PRO
1	A	476	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	445/453 (98%)	326 (73%)	119 (27%)	0 3

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	9	THR
1	A	11	ARG
1	A	12	THR
1	A	27	LYS
1	A	28	THR

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Mol	Chain	Res	Type
1	A	32	SER
1	A	37	LEU
1	A	42	LEU
1	A	50	VAL
1	A	51	LYS
1	A	53	ARG
1	A	54	GLU
1	A	57	ILE
1	A	58	ILE
1	A	61	ASP
1	A	71	PHE
1	A	74	LEU
1	A	89	ARG
1	A	95	ARG
1	A	99	LYS
1	A	101	GLN
1	A	105	VAL
1	A	106	ASP
1	A	110	ARG
1	A	111	VAL
1	A	112	ASP
1	A	121	VAL
1	A	123	ASP
1	A	127	GLU
1	A	128	LEU
1	A	131	GLN
1	A	134	GLU
1	A	141	LYS
1	A	144	ILE
1	A	149	LEU
1	A	152	ARG
1	A	154	LEU
1	A	155	CYS
1	A	156	LEU
1	A	168	HIS
1	A	174	GLN
1	A	175	TYR
1	A	192	THR
1	A	194	PRO
1	A	201	LEU
1	A	203	CYS
1	A	204	SER

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Mol	Chain	Res	Type
1	A	205	MET
1	A	214	VAL
1	A	216	SER
1	A	217	ILE
1	A	218	LEU
1	A	219	ASP
1	A	223	THR
1	A	225	LYS
1	A	236	VAL
1	A	237	LYS
1	A	239	THR
1	A	242	LYS
1	A	243	CYS
1	A	244	ILE
1	A	245	LEU
1	A	247	SER
1	A	252	LYS
1	A	262	GLU
1	A	275	LEU
1	A	284	ARG
1	A	287	LYS
1	A	289	LEU
1	A	298	GLN
1	A	300	GLN
1	A	301	GLN
1	A	306	ARG
1	A	316	ASN
1	A	318	ILE
1	A	319	ILE
1	A	326	TYR
1	A	327	ASP
1	A	328	ASP
1	A	330	ILE
1	A	352	VAL
1	A	357	GLN
1	A	358	GLN
1	A	359	MET
1	A	364	TYR
1	A	369	HIS
1	A	370	LEU
1	A	371	ILE
1	A	372	THR

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Mol	Chain	Res	Type
1	A	378	GLN
1	A	392	SER
1	A	396	LEU
1	A	397	ARG
1	A	398	HIS
1	A	412	ARG
1	A	421	SER
1	A	426	CYS
1	A	431	LEU
1	A	433	CYS
1	A	435	LYS
1	A	449	LEU
1	A	452	LEU
1	A	466	ILE
1	A	467	LEU
1	A	474	LYS
1	A	479	VAL
1	A	480	ASN
1	A	484	LEU
1	A	485	SER
1	A	492	GLU
1	A	505	LEU
1	A	510	ILE
1	A	521	THR
1	A	534	LEU
1	A	536	SER
1	A	537	ILE
1	A	538	THR
1	A	549	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	131	GLN
1	A	147	ASN
1	A	174	GLN
1	A	211	ASN
1	A	278	HIS
1	A	299	ASN
1	A	316	ASN
1	A	343	HIS

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Mol	Chain	Res	Type
1	A	369	HIS
1	A	493	GLN
1	A	509	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	CSS	A	405	3,1	4,6,7	1.41	1 (25%)	1,6,8	1.73	0

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
1	CSS	A	405	3,1	-	1/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	405	CSS	CB-CA	-2.66	1.46	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	405	CSS	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	405	CSS	6	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	FS2	A	602	1	0,14,14	-	-	-		
2	SF4	A	601	1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	A	601	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

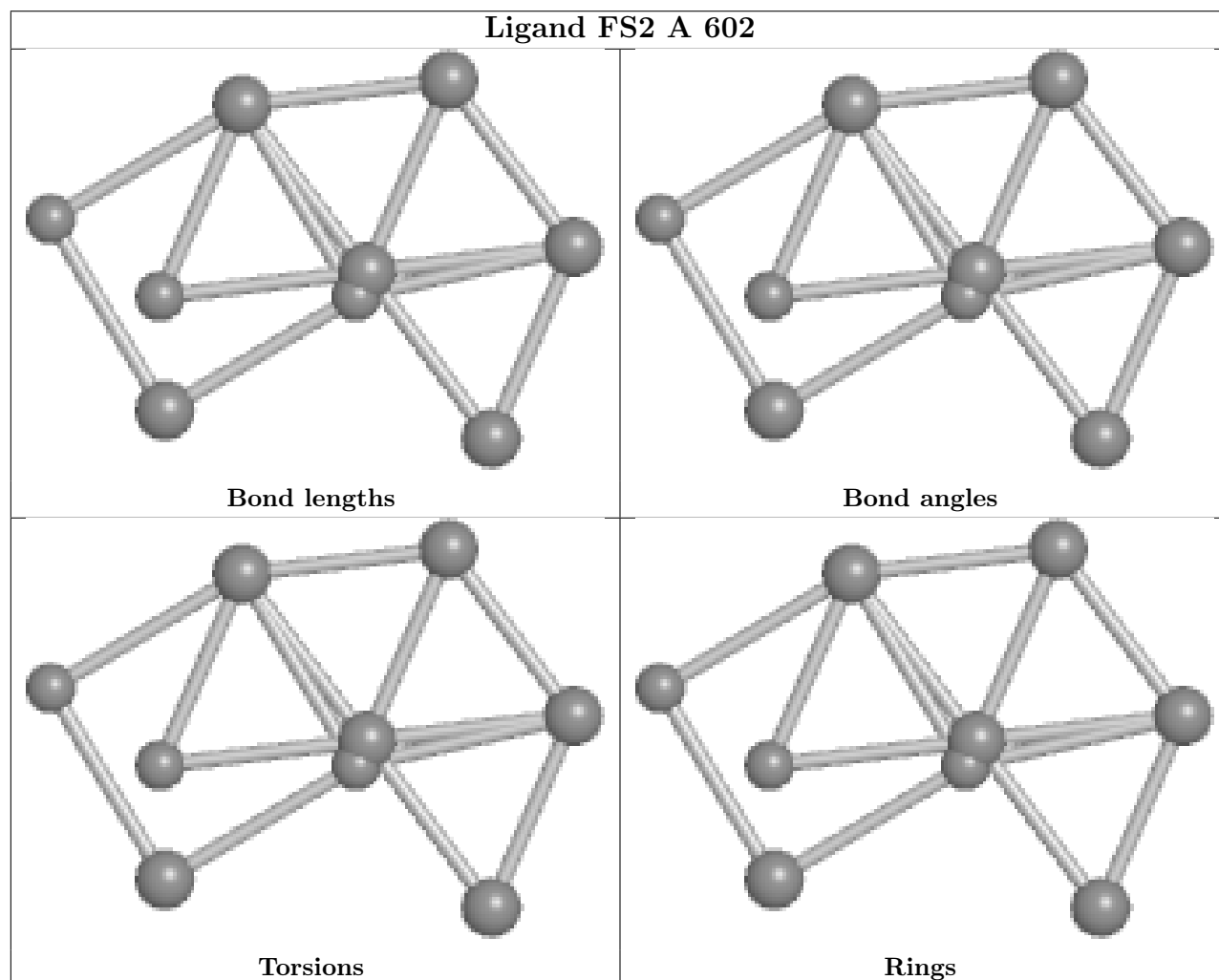
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	FS2	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	549/558 (98%)	0.01	14 (2%) 56 40	77, 121, 185, 306	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	ARG	6.0
1	A	112	ASP	4.1
1	A	106	ASP	3.4
1	A	111	VAL	3.3
1	A	113	ASN	2.8
1	A	108	ASN	2.5
1	A	109	ALA	2.5
1	A	48	TRP	2.5
1	A	393	ARG	2.4
1	A	54	GLU	2.3
1	A	100	ALA	2.2
1	A	514	PRO	2.2
1	A	55	TYR	2.1
1	A	53	ARG	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSS	A	405	7/8	0.97	0.21	109,117,153,182	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

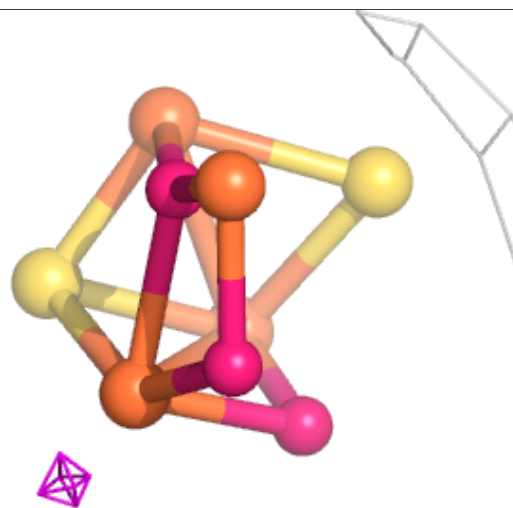
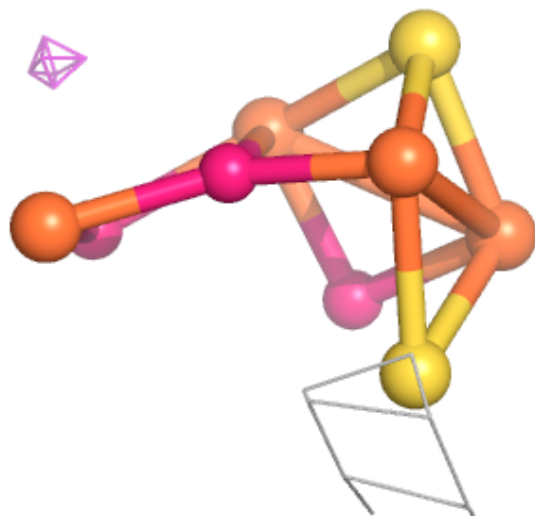
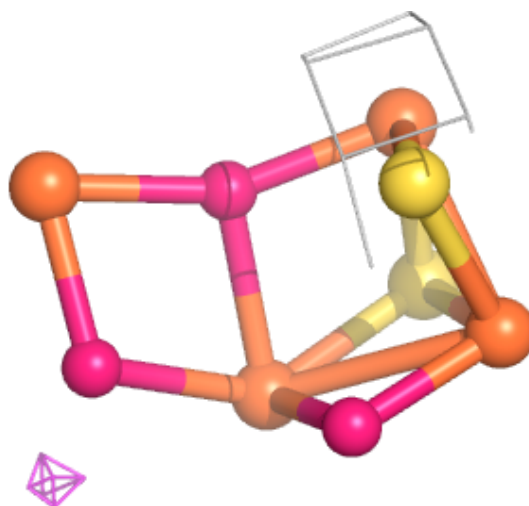
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FS2	A	602	9/9	0.98	0.21	123,136,155,164	0
2	SF4	A	601	8/8	0.99	0.15	100,114,136,148	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 FS2 A 602:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.