



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 03:47 AM EDT

PDB ID : 2H9A
Title : Corrinoid Iron-Sulfur Protein
Authors : Dobbek, H.
Deposited on : 2006-06-09
Resolution : 1.90 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

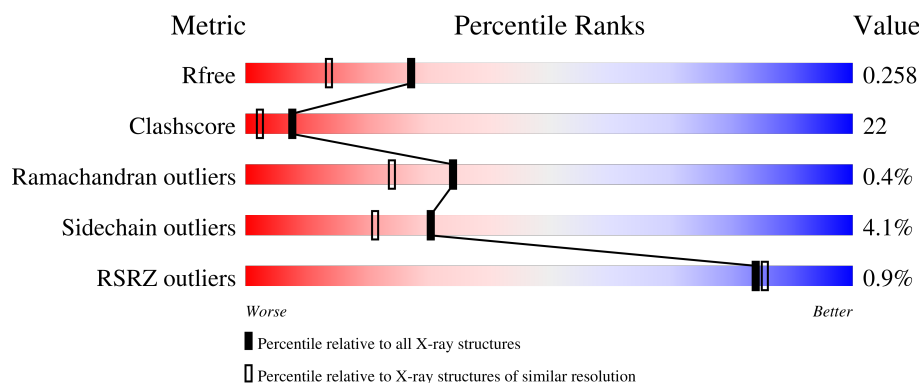
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	445	
2	B	310	

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
3	IOD	A	1450	-	-	X	-
3	IOD	B	1458	-	-	X	-
5	SF4	A	1443	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5968 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 Carbon monoxide dehydrogenase corrinoid/iron-sulfur protein, gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			2935	1899	482	549	5			

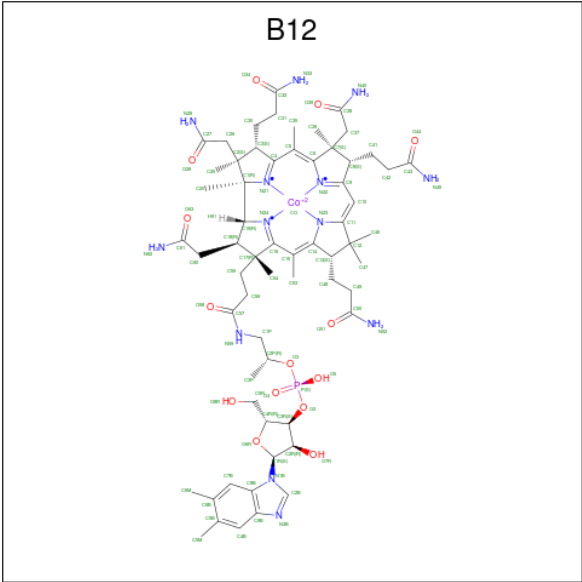
- Molecule 2 is a protein called CO dehydrogenase/acetyl-CoA synthase, iron-sulfur protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	307	Total	C	N	O	S	0	0	0
			2353	1509	390	438	16			

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

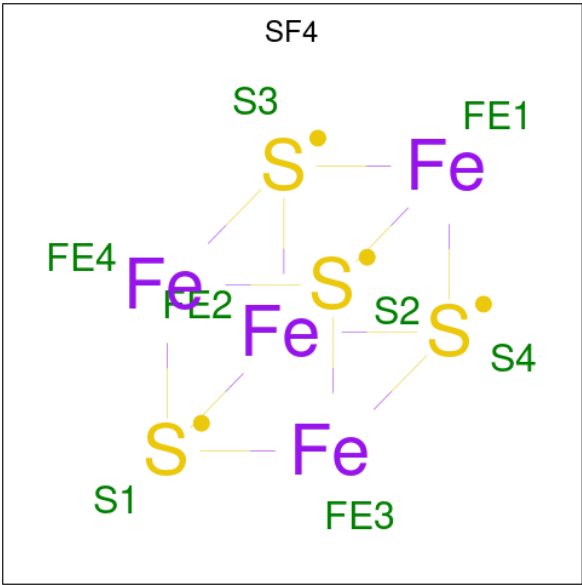
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	I	0	0
			11	11		
3	B	5	Total	I	0	0
			5	5		

- Molecule 4 is COBALAMIN (three-letter code: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

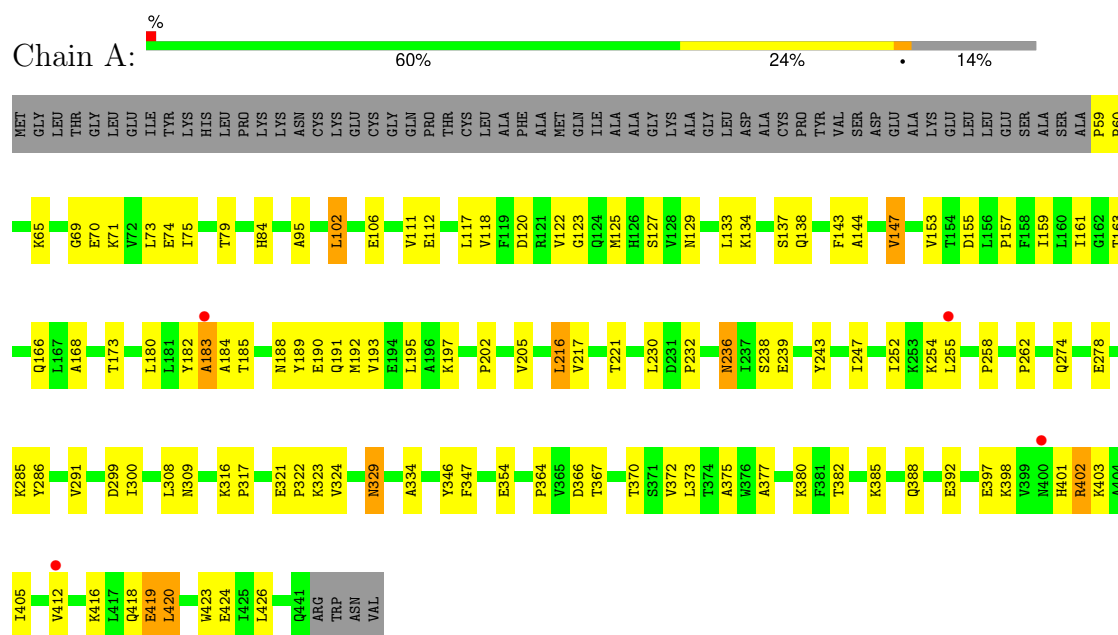
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	326	Total 326	O 326	0	0
6	B	239	Total 239	O 239	0	0

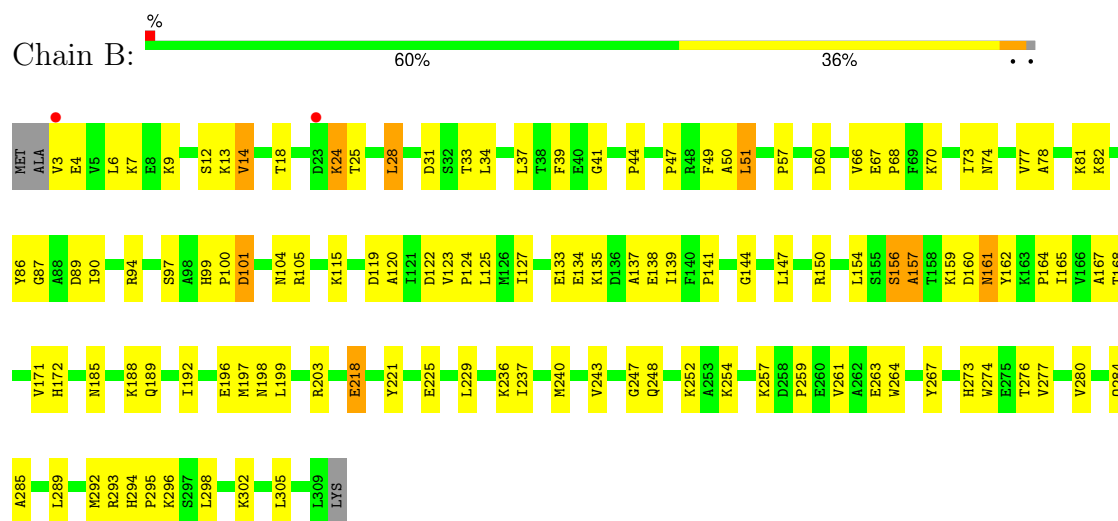
3 Residue-property plots [i](#)

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

- Molecule 1: Carbon monoxide dehydrogenase corrinoid/iron-sulfur protein, gamma subunit



- Molecule 2: CO dehydrogenase/acetyl-CoA synthase, iron-sulfur protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.03Å 44.27Å 100.66Å 90.00° 118.63° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.79 – 1.87	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.90) 100.0 (19.79-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 1.87Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.260 0.199 , 0.258	Depositor DCC
R_{free} test set	1530 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	10.0	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5968	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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: B12, IOD, 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	0.81	0/2996	0.92	5/4080 (0.1%)
2	B	0.80	0/2404	0.92	4/3271 (0.1%)
All	All	0.81	0/5400	0.92	9/7351 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	156	SER	N-CA-C	7.50	131.24	111.00
1	A	184	ALA	N-CA-C	-6.66	93.03	111.00
1	A	159	ILE	N-CA-C	-5.83	95.26	111.00
2	B	157	ALA	N-CA-C	-5.77	95.42	111.00
1	A	286	TYR	N-CA-C	5.65	126.26	111.00
2	B	203	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	A	419	GLU	N-CA-C	-5.39	96.43	111.00
2	B	199	LEU	N-CA-C	-5.27	96.77	111.00
1	A	71	LYS	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	346	TYR	Sidechain

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	2935	0	2997	100	2
2	B	2353	0	2384	130	0
3	A	11	0	0	4	0
3	B	5	0	0	4	0
4	A	91	0	87	13	0
5	A	8	0	0	0	0
6	A	326	0	0	19	2
6	B	239	0	0	19	1
All	All	5968	0	5468	238	3

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 22.

All (238) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:GLU:HG2	6:B:1554:HOH:O	1.57	1.01
2:B:298:LEU:HD11	2:B:302:LYS:HD2	1.52	0.91
3:B:1446:IOD:I	6:B:1597:HOH:O	2.57	0.91
4:A:1442:B12:H541	4:A:1442:B12:H621	1.40	0.87
1:A:419:GLU:O	1:A:420:LEU:HB2	1.73	0.86
2:B:294:HIS:HD2	2:B:296:LYS:H	1.21	0.86
2:B:125:LEU:CD2	2:B:127:ILE:HD11	2.07	0.85
3:B:1458:IOD:I	6:B:1551:HOH:O	2.64	0.84
1:A:254:LYS:O	1:A:255:LEU:HG	1.78	0.82
1:A:401:HIS:HD2	1:A:403:LYS:H	1.25	0.81
1:A:163:THR:H	1:A:166:GLN:HE21	1.28	0.79
1:A:274:GLN:O	1:A:278:GLU:HG3	1.82	0.79
1:A:309:ASN:HB3	2:B:218:GLU:HG3	1.64	0.79
1:A:419:GLU:O	1:A:420:LEU:CB	2.32	0.78
2:B:122:ASP:HB3	6:B:1671:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LEU:HD12	1:A:255:LEU:O	1.83	0.78
1:A:402:ARG:NH1	6:A:1782:HOH:O	2.18	0.77
1:A:418:GLN:HG3	1:A:423:TRP:O	1.86	0.76
4:A:1442:B12:H531	4:A:1442:B12:H552	1.67	0.75
2:B:254:LYS:HD3	3:B:1458:IOD:I	2.56	0.75
2:B:87:GLY:HA3	6:B:1676:HOH:O	1.84	0.75
2:B:97:SER:OG	2:B:105:ARG:HD3	1.86	0.74
1:A:236:ASN:HD22	1:A:238:SER:H	1.35	0.74
4:A:1442:B12:H252	4:A:1442:B12:H602	1.70	0.73
2:B:247:GLY:HA3	2:B:293:ARG:HG3	1.69	0.73
2:B:159:LYS:HE3	2:B:189:GLN:NE2	2.05	0.72
4:A:1442:B12:H362	4:A:1442:B12:H351	1.71	0.71
2:B:90:ILE:HD12	2:B:124:PRO:HG2	1.72	0.71
2:B:94:ARG:HH12	2:B:248:GLN:HE21	1.39	0.71
1:A:372:VAL:HG22	4:A:1442:B12:O5	1.91	0.70
2:B:33:THR:HB	2:B:41:GLY:HA3	1.74	0.70
1:A:236:ASN:HD21	1:A:238:SER:HB3	1.56	0.70
1:A:137:SER:O	1:A:138:GLN:HB2	1.91	0.70
2:B:99:HIS:CD2	2:B:101:ASP:HB2	2.27	0.70
1:A:367:THR:HA	1:A:385:LYS:HZ1	1.57	0.69
2:B:298:LEU:CD1	2:B:302:LYS:HD2	2.21	0.68
1:A:354:GLU:OE1	6:A:1780:HOH:O	2.09	0.68
1:A:323:LYS:HE3	6:A:1665:HOH:O	1.92	0.68
1:A:102:LEU:HG	1:A:106:GLU:HB3	1.75	0.68
1:A:173:THR:CB	6:A:1670:HOH:O	2.41	0.67
1:A:377:ALA:HB2	4:A:1442:B12:H331	1.59	0.67
1:A:243:TYR:O	1:A:247:ILE:HG12	1.95	0.67
1:A:403:LYS:HE2	1:A:424:GLU:OE2	1.94	0.67
1:A:129:ASN:O	1:A:157:PRO:HD2	1.94	0.67
1:A:95:ALA:HB3	1:A:291:VAL:HG22	1.75	0.66
1:A:236:ASN:ND2	1:A:238:SER:HB3	2.10	0.66
1:A:118:VAL:CG2	1:A:125:MET:HG2	2.26	0.66
2:B:167:ALA:O	2:B:171:VAL:HG12	1.96	0.65
2:B:252:LYS:HE3	6:B:1661:HOH:O	1.95	0.65
2:B:225:GLU:O	2:B:229:LEU:HD23	1.96	0.65
1:A:217:VAL:O	1:A:221:THR:HG23	1.97	0.65
1:A:405:ILE:CD1	1:A:426:LEU:HD12	2.27	0.64
2:B:66:VAL:HG13	2:B:73:ILE:HD12	1.80	0.64
2:B:147:LEU:HD22	2:B:150:ARG:HD3	1.79	0.64
1:A:309:ASN:O	2:B:218:GLU:HG2	1.98	0.64
2:B:125:LEU:HD21	2:B:127:ILE:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:ASN:C	2:B:161:ASN:ND2	2.51	0.64
2:B:263:GLU:HG2	6:B:1619:HOH:O	1.97	0.64
2:B:60:ASP:OD2	6:B:1514:HOH:O	2.15	0.63
2:B:165:ILE:HB	6:B:1622:HOH:O	1.98	0.63
2:B:120:ALA:HB2	6:B:1580:HOH:O	1.96	0.63
1:A:236:ASN:HD22	1:A:238:SER:N	1.96	0.63
2:B:87:GLY:CA	6:B:1676:HOH:O	2.46	0.63
2:B:294:HIS:CD2	2:B:296:LYS:H	2.10	0.62
2:B:3:VAL:CG1	2:B:4:GLU:N	2.63	0.62
2:B:133:GLU:OE2	2:B:160:ASP:HB2	1.99	0.62
1:A:412:VAL:HG23	6:A:1539:HOH:O	1.99	0.62
2:B:292:MET:CE	2:B:298:LEU:HA	2.31	0.61
1:A:188:ASN:OD1	1:A:188:ASN:C	2.37	0.60
2:B:119:ASP:OD1	2:B:150:ARG:NH1	2.22	0.60
2:B:159:LYS:HE3	2:B:189:GLN:HE22	1.65	0.60
1:A:125:MET:SD	1:A:125:MET:C	2.80	0.60
2:B:57:PRO:CG	2:B:74:ASN:HD22	2.15	0.60
2:B:94:ARG:NH1	2:B:248:GLN:HE21	2.00	0.59
2:B:159:LYS:CE	2:B:189:GLN:HE22	2.14	0.59
2:B:144:GLY:HA3	2:B:168:THR:HG21	1.85	0.59
1:A:143:PHE:O	1:A:147:VAL:HG12	2.02	0.59
2:B:97:SER:CB	2:B:105:ARG:HD3	2.33	0.59
2:B:115:LYS:HA	2:B:147:LEU:HD21	1.84	0.59
2:B:192:ILE:O	2:B:196:GLU:HG3	2.03	0.59
1:A:144:ALA:O	1:A:147:VAL:HG13	2.02	0.59
1:A:120:ASP:OD2	6:A:1772:HOH:O	2.16	0.58
1:A:185:THR:O	1:A:189:TYR:HB3	2.03	0.58
4:A:1442:B12:H301	4:A:1442:B12:H203	1.86	0.58
2:B:236:LYS:HG3	2:B:237:ILE:HD13	1.86	0.57
2:B:57:PRO:HG3	2:B:74:ASN:HD22	1.68	0.57
4:A:1442:B12:H291	4:A:1442:B12:H3	1.70	0.57
1:A:182:TYR:O	1:A:183:ALA:HB3	2.05	0.57
1:A:190:GLU:HG3	6:A:1554:HOH:O	2.04	0.57
1:A:183:ALA:O	1:A:192:MET:HE2	2.05	0.56
2:B:137:ALA:HB1	2:B:164:PRO:HG2	1.87	0.56
2:B:67:GLU:OE2	2:B:70:LYS:NZ	2.28	0.56
2:B:147:LEU:O	2:B:150:ARG:HG3	2.06	0.56
1:A:69:GLY:O	1:A:70:GLU:HB2	2.06	0.56
2:B:18:THR:HG23	2:B:25:THR:HG23	1.87	0.55
2:B:144:GLY:HA3	2:B:168:THR:CG2	2.37	0.55
2:B:77:VAL:HG12	2:B:81:LYS:HE2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:ASN:O	2:B:164:PRO:HD2	2.06	0.55
4:A:1442:B12:H3	4:A:1442:B12:N29	2.21	0.55
2:B:171:VAL:HG13	2:B:172:HIS:ND1	2.20	0.55
1:A:388:GLN:O	1:A:392:GLU:HB2	2.06	0.55
2:B:292:MET:HE3	2:B:298:LEU:HA	1.89	0.54
1:A:79:THR:C	1:A:252:ILE:HD13	2.28	0.54
2:B:172:HIS:HE1	6:B:1687:HOH:O	1.91	0.54
2:B:3:VAL:HG13	2:B:4:GLU:N	2.23	0.53
2:B:122:ASP:OD2	3:B:1459:IOD:I	2.97	0.53
2:B:298:LEU:O	2:B:302:LYS:HG3	2.07	0.53
2:B:44:PRO:HD2	6:B:1501:HOH:O	2.08	0.53
1:A:385:LYS:O	1:A:388:GLN:HG2	2.08	0.53
1:A:405:ILE:HD11	1:A:426:LEU:HD12	1.90	0.53
1:A:321:GLU:OE2	1:A:322:PRO:HD2	2.09	0.53
1:A:334:ALA:O	1:A:401:HIS:HE1	1.90	0.53
2:B:276:THR:O	2:B:280:VAL:HG22	2.09	0.53
2:B:298:LEU:O	2:B:298:LEU:HD12	2.08	0.52
1:A:112:GLU:HG2	6:A:1759:HOH:O	2.10	0.52
2:B:90:ILE:CD1	2:B:124:PRO:HG2	2.37	0.52
2:B:99:HIS:HD2	2:B:101:ASP:HB2	1.73	0.52
2:B:24:LYS:HB3	2:B:122:ASP:O	2.10	0.52
1:A:84:HIS:HD2	6:B:1475:HOH:O	1.92	0.52
1:A:367:THR:HA	1:A:385:LYS:NZ	2.25	0.51
1:A:192:MET:HE2	6:A:1559:HOH:O	2.11	0.51
2:B:99:HIS:CD2	2:B:101:ASP:H	2.28	0.51
2:B:157:ALA:HB2	2:B:165:ILE:HG21	1.93	0.51
1:A:236:ASN:ND2	1:A:239:GLU:H	2.09	0.51
2:B:302:LYS:HE2	6:B:1676:HOH:O	2.10	0.50
2:B:68:PRO:HB2	2:B:295:PRO:HG2	1.92	0.50
2:B:254:LYS:HG2	2:B:264:TRP:CH2	2.47	0.50
1:A:416:LYS:O	1:A:419:GLU:O	2.29	0.50
2:B:294:HIS:HD2	2:B:296:LYS:N	2.01	0.50
2:B:141:PRO:HA	2:B:168:THR:OG1	2.12	0.50
1:A:285:LYS:HE3	2:B:284:GLN:HE21	1.76	0.50
2:B:159:LYS:NZ	2:B:189:GLN:HE22	2.10	0.50
1:A:122:VAL:CG1	6:A:1642:HOH:O	2.59	0.49
1:A:382:THR:HG22	3:A:1453:IOD:I	2.82	0.49
1:A:323:LYS:O	1:A:364:PRO:HD2	2.12	0.49
2:B:78:ALA:HA	2:B:81:LYS:HE3	1.94	0.49
2:B:225:GLU:O	2:B:229:LEU:CD2	2.59	0.49
1:A:180:LEU:HA	1:A:202:PRO:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:LEU:HD13	2:B:298:LEU:HD22	1.94	0.49
2:B:125:LEU:HD23	2:B:127:ILE:HD11	1.89	0.49
2:B:185:ASN:O	6:B:1594:HOH:O	2.20	0.49
2:B:99:HIS:HD2	2:B:101:ASP:H	1.59	0.49
2:B:221:TYR:CD1	2:B:285:ALA:HB2	2.48	0.49
2:B:273:HIS:HD2	6:B:1525:HOH:O	1.94	0.49
2:B:254:LYS:HG2	2:B:264:TRP:HH2	1.78	0.49
2:B:259:PRO:HA	2:B:267:TYR:CD1	2.48	0.49
2:B:292:MET:HE3	2:B:298:LEU:HB2	1.94	0.48
1:A:118:VAL:CG2	1:A:125:MET:CG	2.92	0.48
1:A:155:ASP:OD2	6:A:1696:HOH:O	2.20	0.48
1:A:255:LEU:CB	6:A:1576:HOH:O	2.61	0.48
1:A:380:LYS:O	1:A:385:LYS:HD3	2.13	0.48
1:A:118:VAL:HA	1:A:127:SER:HB3	1.96	0.48
2:B:292:MET:HE1	2:B:298:LEU:HA	1.95	0.48
1:A:385:LYS:HA	1:A:388:GLN:HG2	1.95	0.48
2:B:14:VAL:HG22	2:B:31:ASP:H	1.79	0.48
2:B:134:GLU:O	2:B:138:GLU:HG3	2.14	0.47
2:B:34:LEU:HB2	2:B:37:LEU:HD12	1.97	0.47
2:B:243:VAL:CG2	2:B:289:LEU:HD23	2.44	0.47
2:B:3:VAL:HG13	2:B:4:GLU:H	1.79	0.47
2:B:147:LEU:CD2	2:B:150:ARG:HD3	2.44	0.47
2:B:50:ALA:HA	2:B:90:ILE:O	2.14	0.47
1:A:255:LEU:HA	6:A:1576:HOH:O	2.15	0.47
2:B:261:VAL:HG12	2:B:263:GLU:HG3	1.97	0.47
2:B:277:VAL:HA	2:B:280:VAL:HG22	1.96	0.47
2:B:94:ARG:HH12	2:B:248:GLN:NE2	2.08	0.46
2:B:171:VAL:HG13	2:B:172:HIS:N	2.30	0.46
1:A:299:ASP:OD1	2:B:273:HIS:HE1	1.99	0.46
2:B:139:ILE:HG22	6:B:1591:HOH:O	2.15	0.46
2:B:89:ASP:O	2:B:90:ILE:HD13	2.15	0.46
2:B:97:SER:HB2	2:B:105:ARG:HD3	1.98	0.46
1:A:70:GLU:N	6:A:1514:HOH:O	2.44	0.46
2:B:159:LYS:CE	2:B:189:GLN:NE2	2.74	0.46
1:A:117:LEU:HD13	1:A:300:ILE:HG13	1.98	0.46
1:A:168:ALA:HB2	1:A:195:LEU:HD21	1.97	0.46
1:A:122:VAL:HG13	6:A:1642:HOH:O	2.14	0.46
1:A:401:HIS:CD2	1:A:403:LYS:H	2.17	0.46
2:B:162:TYR:O	2:B:165:ILE:HG22	2.16	0.46
2:B:161:ASN:C	2:B:161:ASN:HD22	2.18	0.46
1:A:329:ASN:ND2	6:A:1480:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:MET:O	2:B:198:ASN:HB2	2.16	0.45
2:B:298:LEU:HD12	2:B:302:LYS:HG3	1.98	0.45
1:A:163:THR:H	1:A:166:GLN:NE2	2.04	0.45
2:B:66:VAL:HG13	2:B:73:ILE:CD1	2.45	0.45
2:B:252:LYS:CE	6:B:1661:HOH:O	2.61	0.45
2:B:49:PHE:CD1	2:B:49:PHE:N	2.85	0.45
1:A:205:VAL:CG1	1:A:216:LEU:HD13	2.47	0.45
1:A:367:THR:HB	1:A:375:ALA:HB2	1.99	0.45
2:B:28:LEU:HD12	2:B:28:LEU:N	2.32	0.45
2:B:157:ALA:HA	2:B:161:ASN:HD21	1.82	0.45
1:A:366:ASP:O	1:A:385:LYS:HE2	2.18	0.44
1:A:134:LYS:HA	1:A:161:ILE:HB	2.00	0.44
3:A:1450:IOD:I	2:B:263:GLU:HB2	2.88	0.44
2:B:82:LYS:HE3	2:B:86:TYR:CE2	2.53	0.44
2:B:12:SER:OG	2:B:13:LYS:N	2.50	0.43
1:A:366:ASP:O	1:A:385:LYS:CE	2.66	0.43
1:A:65:LYS:HA	1:A:73:LEU:O	2.19	0.43
2:B:7:LYS:HG2	2:B:39:PHE:HD2	1.83	0.43
2:B:188:LYS:HE3	2:B:237:ILE:HB	2.01	0.43
1:A:316:LYS:HG2	1:A:317:PRO:O	2.19	0.43
2:B:57:PRO:CG	2:B:74:ASN:ND2	2.81	0.43
1:A:111:VAL:HG11	1:A:153:VAL:HG23	2.01	0.43
4:A:1442:B12:H533	4:A:1442:B12:H491	2.00	0.42
2:B:125:LEU:HG	2:B:127:ILE:CD1	2.49	0.42
1:A:398:LYS:HE2	6:A:1495:HOH:O	2.18	0.42
4:A:1442:B12:H363	4:A:1442:B12:H411	1.81	0.42
2:B:123:VAL:HB	2:B:124:PRO:HD2	2.01	0.42
1:A:75:ILE:HG13	1:A:262:PRO:HG2	2.02	0.42
1:A:182:TYR:O	1:A:183:ALA:CB	2.66	0.42
2:B:292:MET:HE3	2:B:298:LEU:CA	2.49	0.42
1:A:144:ALA:O	1:A:147:VAL:CG1	2.67	0.42
1:A:366:ASP:O	1:A:385:LYS:NZ	2.51	0.42
1:A:232:PRO:HG3	1:A:243:TYR:HB3	2.02	0.42
2:B:157:ALA:CB	2:B:165:ILE:HG21	2.50	0.42
1:A:193:VAL:HG12	1:A:197:LYS:HE2	2.02	0.42
2:B:252:LYS:O	2:B:257:LYS:HD3	2.20	0.42
2:B:261:VAL:HG12	2:B:263:GLU:CG	2.50	0.42
1:A:137:SER:O	1:A:138:GLN:CB	2.63	0.41
1:A:59:PRO:HA	1:A:60:PRO:HD3	1.94	0.41
4:A:1442:B12:H353	4:A:1442:B12:H302	2.02	0.41
3:A:1450:IOD:I	2:B:263:GLU:OE2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:PRO:HD2	2:B:305:LEU:HD11	2.02	0.41
1:A:205:VAL:HG13	1:A:216:LEU:HD13	2.02	0.41
1:A:372:VAL:HG23	1:A:373:LEU:N	2.36	0.41
1:A:377:ALA:HB2	4:A:1442:B12:N33	2.30	0.41
2:B:50:ALA:HB2	2:B:90:ILE:HB	2.02	0.41
1:A:111:VAL:CG1	1:A:153:VAL:HG23	2.51	0.41
1:A:123:GLY:HA3	1:A:347:PHE:CZ	2.56	0.41
2:B:294:HIS:HA	2:B:295:PRO:HD3	1.96	0.41
2:B:135:LYS:HA	2:B:135:LYS:HD2	1.84	0.41
2:B:162:TYR:HA	2:B:165:ILE:HG22	2.03	0.41
1:A:192:MET:CE	6:A:1559:HOH:O	2.66	0.41
2:B:125:LEU:CG	2:B:127:ILE:HD11	2.51	0.41
1:A:74:GLU:HB2	6:A:1747:HOH:O	2.20	0.41
1:A:163:THR:N	1:A:166:GLN:HE21	2.06	0.41
1:A:258:PRO:HG3	3:A:1448:IOD:I	2.91	0.41
2:B:257:LYS:O	2:B:259:PRO:HD3	2.21	0.40
2:B:100:PRO:HA	2:B:104:ASN:ND2	2.36	0.40
1:A:370:THR:OG1	1:A:375:ALA:HB2	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1688:HOH:O	6:B:1696:HOH:O[4_9510]	1.75	0.45
1:A:397:GLU:OE2	6:A:1587:HOH:O[2_949]	2.16	0.04
1:A:321:GLU:OE1	6:A:1541:HOH:O[2_949]	2.17	0.03

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	381/445 (86%)	364 (96%)	15 (4%)	2 (0%)	29 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	305/310 (98%)	289 (95%)	15 (5%)	1 (0%)	41	31
All	All	686/755 (91%)	653 (95%)	30 (4%)	3 (0%)	34	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	ALA
1	A	420	LEU
2	B	156	SER

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	312/364 (86%)	301 (96%)	11 (4%)	36	27
2	B	255/257 (99%)	243 (95%)	12 (5%)	26	16
All	All	567/621 (91%)	544 (96%)	23 (4%)	30	21

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	133	LEU
1	A	147	VAL
1	A	191	GLN
1	A	216	LEU
1	A	230	LEU
1	A	236	ASN
1	A	308	LEU
1	A	324	VAL
1	A	329	ASN
1	A	402	ARG
2	B	6	LEU
2	B	9	LYS

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Mol	Chain	Res	Type
2	B	14	VAL
2	B	24	LYS
2	B	28	LEU
2	B	51	LEU
2	B	101	ASP
2	B	154	LEU
2	B	161	ASN
2	B	218	GLU
2	B	240	MET
2	B	274	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	115	ASN
1	A	166	GLN
1	A	200	ASN
1	A	218	GLN
1	A	233	GLN
1	A	236	ASN
1	A	244	GLN
1	A	315	GLN
1	A	329	ASN
1	A	401	HIS
1	A	436	ASN
2	B	45	ASN
2	B	74	ASN
2	B	99	HIS
2	B	104	ASN
2	B	161	ASN
2	B	172	HIS
2	B	185	ASN
2	B	189	GLN
2	B	191	ASN
2	B	248	GLN
2	B	273	HIS
2	B	284	GLN
2	B	294	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 16 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	B12	A	1442	6	91,101,101	1.47	14 (15%)	140,166,166	2.17	38 (27%)
5	SF4	A	1443	-	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	B12	A	1442	6	-	9/52/223/223	0/3/11/11
5	SF4	A	1443	-	-	-	0/6/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1442	B12	C41-C8	4.26	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1442	B12	C14-N23	4.02	1.40	1.35
4	A	1442	B12	C6B-C5B	3.62	1.49	1.40
4	A	1442	B12	C7B-C6B	3.44	1.46	1.37
4	A	1442	B12	C55-C56	2.98	1.59	1.53
4	A	1442	B12	C1P-C2P	2.75	1.58	1.51
4	A	1442	B12	C35-C5	2.52	1.55	1.50
4	A	1442	B12	C54-C17	2.51	1.58	1.54
4	A	1442	B12	C60-C18	-2.46	1.48	1.54
4	A	1442	B12	O58-C57	2.43	1.28	1.23
4	A	1442	B12	C11-N23	2.22	1.41	1.36
4	A	1442	B12	O6R-C1R	2.11	1.43	1.40
4	A	1442	B12	C3P-C2P	-2.08	1.43	1.51
4	A	1442	B12	C25-C2	-2.07	1.50	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1442	B12	O2-P-O3	8.22	125.83	102.87
4	A	1442	B12	C18-C60-C61	7.54	133.21	114.04
4	A	1442	B12	O2-P-O4	-5.69	91.63	109.81
4	A	1442	B12	C20-C1-N21	-5.59	101.02	110.26
4	A	1442	B12	O7R-C2R-C3R	5.38	126.24	111.19
4	A	1442	B12	O6R-C1R-N1B	-5.19	101.86	108.75
4	A	1442	B12	C60-C61-N62	5.04	128.27	116.19
4	A	1442	B12	C60-C18-C17	4.73	128.77	115.82
4	A	1442	B12	C48-C13-C12	-4.52	103.59	116.52
4	A	1442	B12	C3R-C2R-C1R	4.08	108.87	99.89
4	A	1442	B12	C41-C8-C9	-3.81	104.55	111.19
4	A	1442	B12	C55-C17-C18	-3.53	104.38	111.12
4	A	1442	B12	C20-C1-C19	-3.49	105.99	109.35
4	A	1442	B12	O63-C61-C60	-3.30	113.96	120.87
4	A	1442	B12	C9-N22-C6	3.21	109.14	105.28
4	A	1442	B12	C2-C1-C19	3.20	123.58	118.61
4	A	1442	B12	O58-C57-C56	-3.09	116.42	122.02
4	A	1442	B12	C47-C12-C46	-2.99	104.45	109.41
4	A	1442	B12	O8R-C5R-C4R	2.90	121.20	111.33
4	A	1442	B12	O58-C57-N59	2.76	128.45	123.03
4	A	1442	B12	C47-C12-C13	2.73	123.79	112.74
4	A	1442	B12	C37-C7-C8	-2.70	101.24	108.37
4	A	1442	B12	O6R-C4R-C3R	2.66	110.53	104.92
4	A	1442	B12	C7-C8-C9	2.66	104.26	100.89
4	A	1442	B12	C8-C9-C10	-2.59	117.82	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1442	B12	C2P-C1P-N59	2.55	116.67	112.92
4	A	1442	B12	C46-C12-C11	-2.53	101.03	110.08
4	A	1442	B12	C1-C2-C3	-2.48	98.47	101.60
4	A	1442	B12	C49-C48-C13	2.45	121.60	114.65
4	A	1442	B12	C19-C1-N21	2.44	104.65	102.14
4	A	1442	B12	C25-C2-C1	-2.43	110.12	113.75
4	A	1442	B12	C4B-C9B-C8B	-2.30	118.75	121.10
4	A	1442	B12	C12-C13-C14	2.27	105.98	102.26
4	A	1442	B12	C25-C2-C3	2.18	118.45	112.91
4	A	1442	B12	C26-C2-C1	2.10	113.25	110.00
4	A	1442	B12	P-O3-C2P	2.10	128.26	121.10
4	A	1442	B12	C54-C17-C18	2.05	115.93	112.99
4	A	1442	B12	C47-C12-C11	2.04	117.35	110.08

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1442	B12	C17-C18-C60-C61
4	A	1442	B12	C18-C60-C61-O63
4	A	1442	B12	C18-C60-C61-N62
4	A	1442	B12	C1P-C2P-O3-P
4	A	1442	B12	C3P-C2P-O3-P
4	A	1442	B12	C41-C42-C43-O44
4	A	1442	B12	C41-C42-C43-N45
4	A	1442	B12	C3-C30-C31-C32
4	A	1442	B12	C19-C18-C60-C61

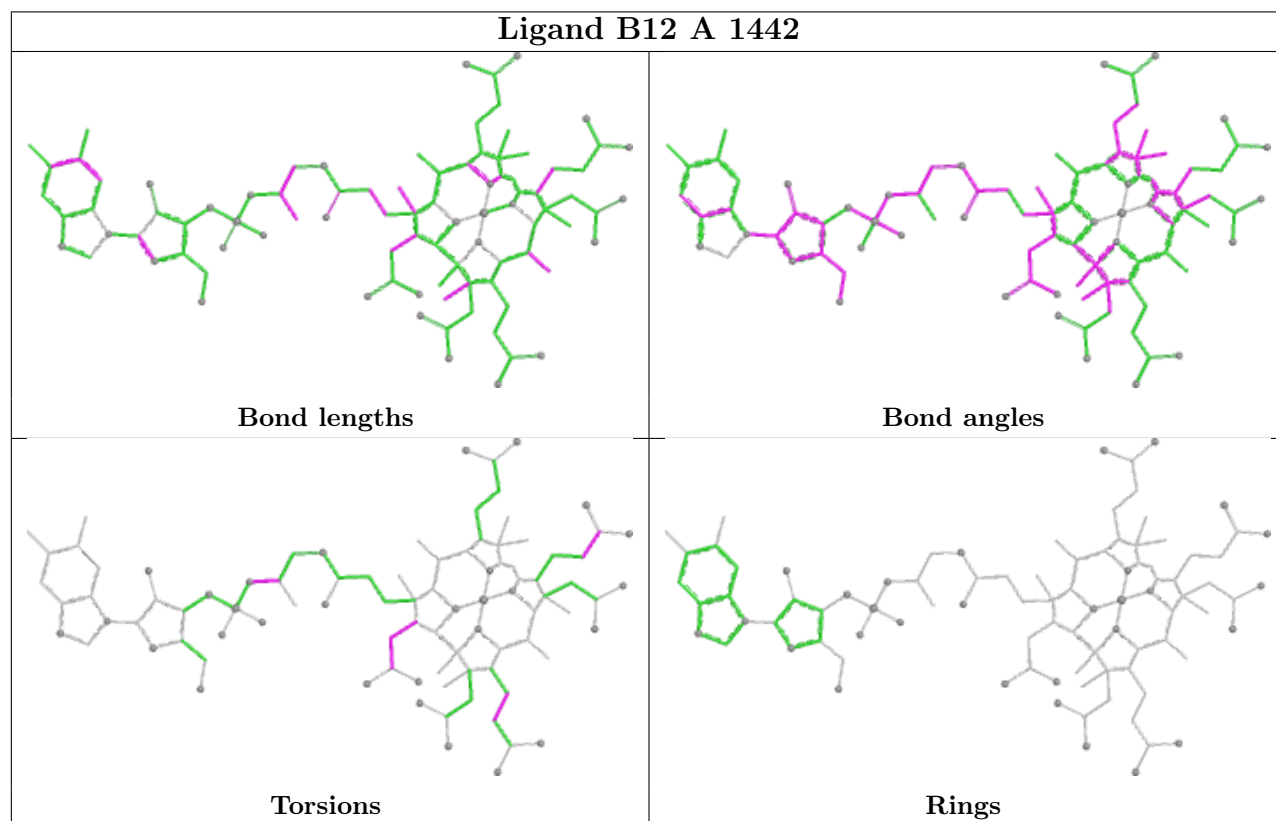
There are no ring outliers.

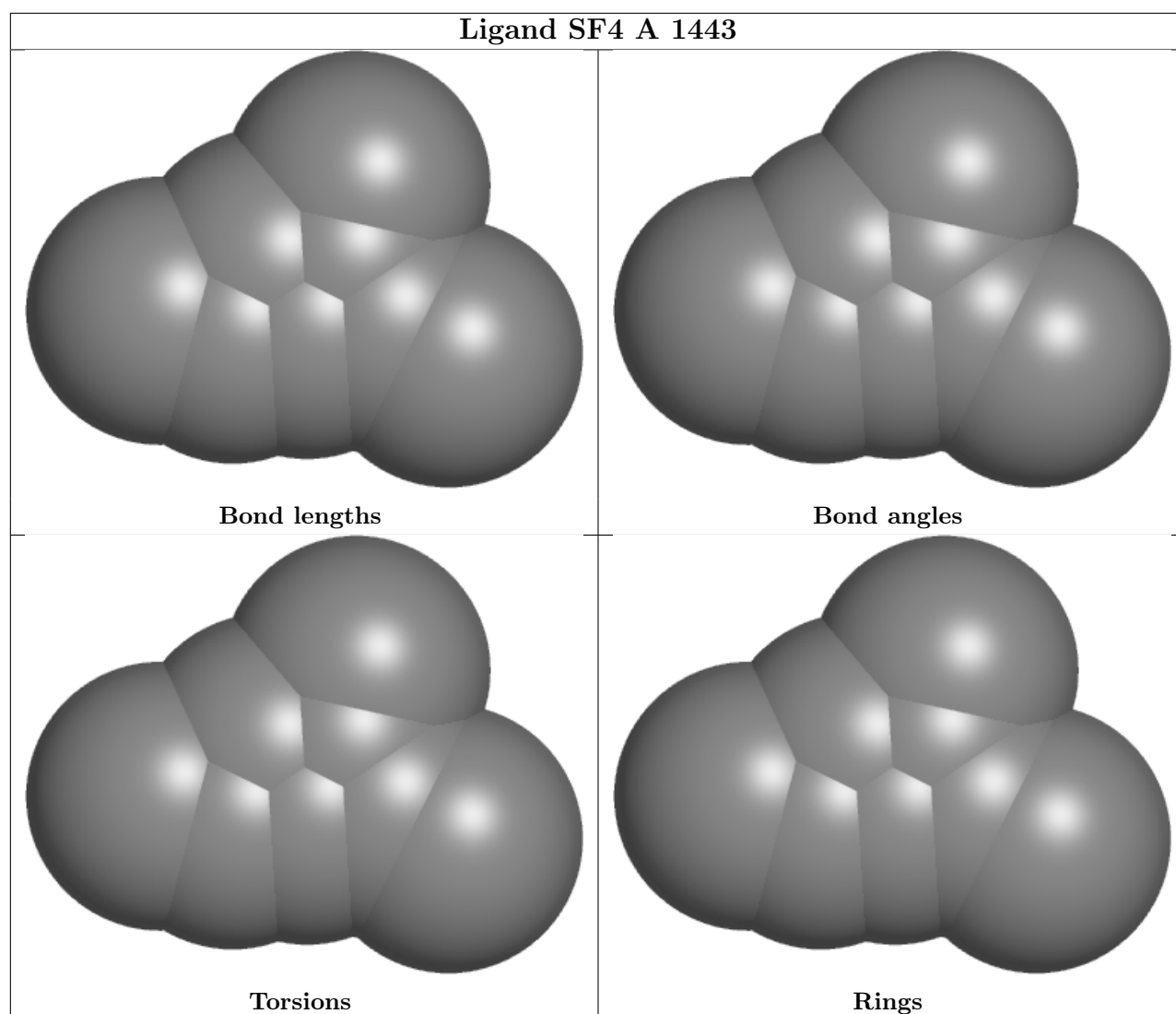
1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1442	B12	13	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	383/445 (86%)	-0.18	4 (1%) 82 84	4, 13, 30, 44	0
2	B	307/310 (99%)	-0.24	2 (0%) 87 88	4, 11, 30, 46	0
All	All	690/755 (91%)	-0.21	6 (0%) 84 85	4, 13, 30, 46	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3	VAL	4.5
1	A	400	ASN	2.6
1	A	183	ALA	2.5
1	A	255	LEU	2.2
2	B	23	ASP	2.2
1	A	412	VAL	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

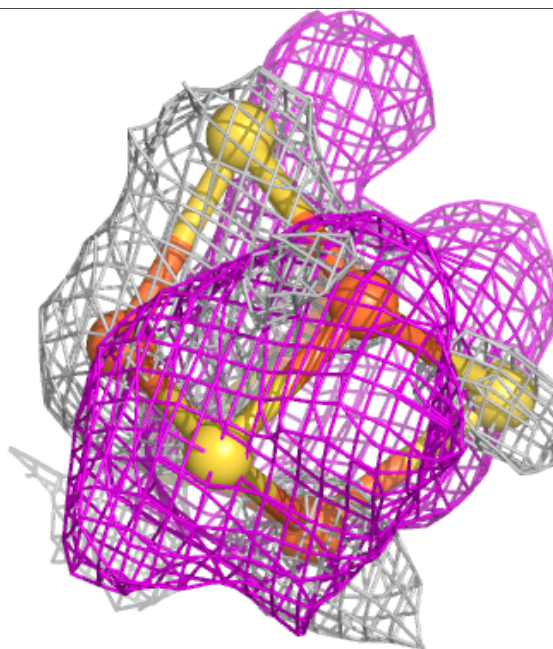
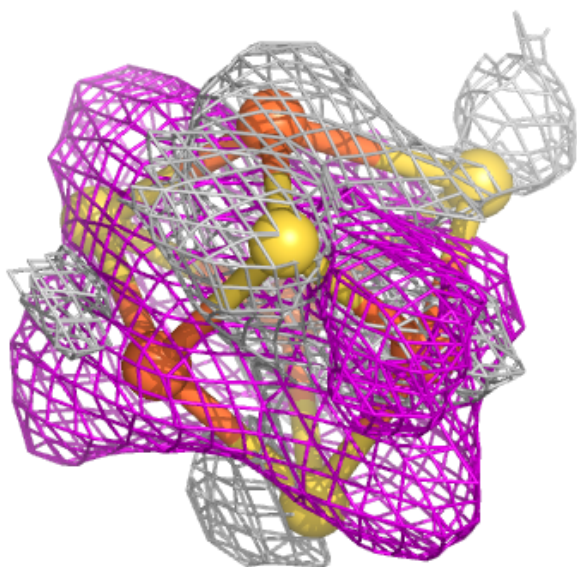
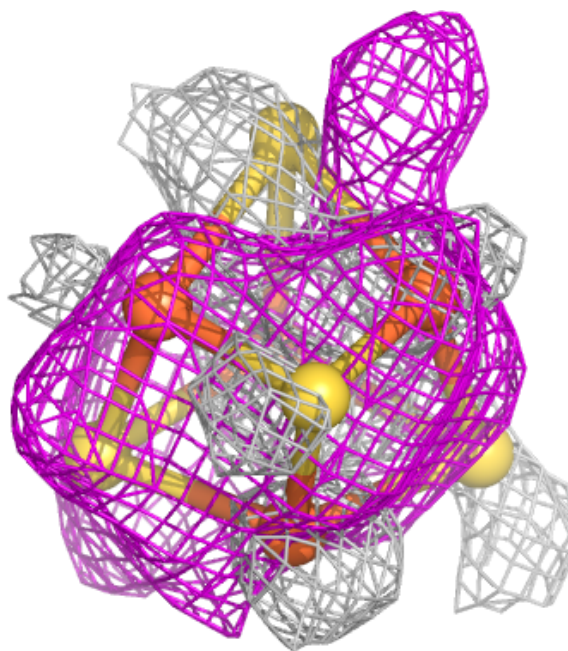
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

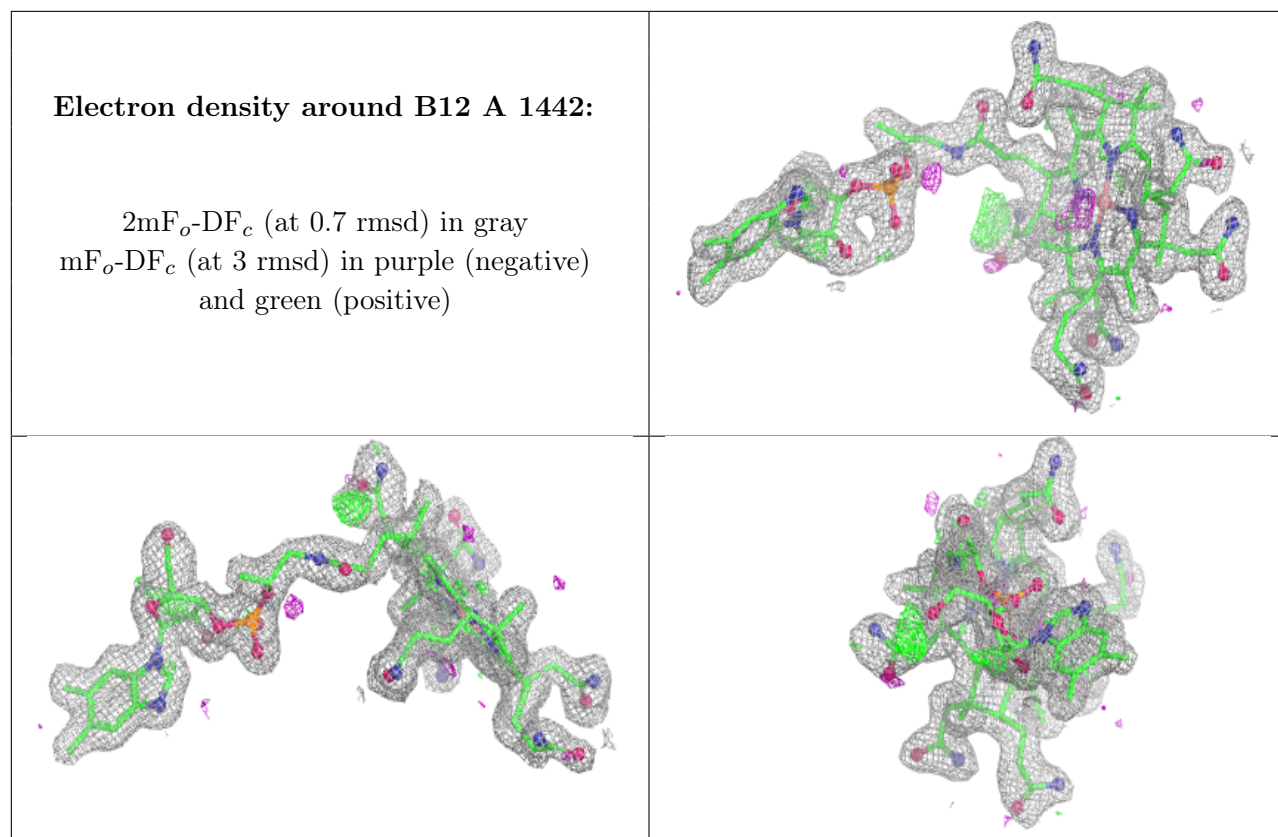
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SF4	A	1443	8/8	0.44	0.66	71,71,73,78	0
4	B12	A	1442	91/91	0.94	0.11	6,13,23,28	0
3	IOD	A	1453	1/1	0.98	0.04	20,20,20,20	1
3	IOD	A	1455	1/1	0.98	0.06	22,22,22,22	1
3	IOD	A	1454	1/1	0.99	0.09	13,13,13,13	1
3	IOD	A	1450	1/1	0.99	0.04	17,17,17,17	1
3	IOD	A	1456	1/1	0.99	0.03	16,16,16,16	1
3	IOD	A	1457	1/1	0.99	0.03	21,21,21,21	1
3	IOD	B	1444	1/1	0.99	0.07	17,17,17,17	1
3	IOD	B	1446	1/1	0.99	0.02	20,20,20,20	1
3	IOD	B	1458	1/1	0.99	0.03	21,21,21,21	1
3	IOD	B	1459	1/1	0.99	0.04	17,17,17,17	1
3	IOD	A	1452	1/1	0.99	0.08	21,21,21,21	1
3	IOD	A	1448	1/1	0.99	0.11	24,24,24,24	1
3	IOD	A	1451	1/1	1.00	0.04	11,11,11,11	1
3	IOD	A	1449	1/1	1.00	0.02	16,16,16,16	0
3	IOD	A	1445	1/1	1.00	0.06	13,13,13,13	1
3	IOD	B	1447	1/1	1.00	0.03	11,11,11,11	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 A 1443:

$2mF_o-DF_c$ (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.