



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:56 AM GMT

PDB ID : 1B0V
Title : I40N MUTANT OF AZOTOBACTER VINELANDII FDI
Authors : Sridhar, V.; Prasad, G.S.; Stout, C.D.; Chen, K.; Burgess, B.K.
Deposited on : 1998-11-12
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

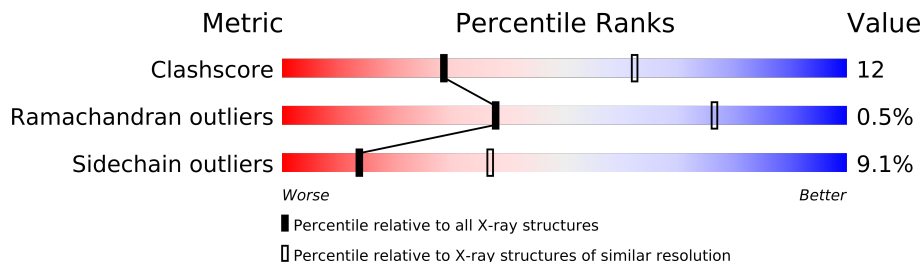
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	106	
1	B	106	
1	C	106	
1	D	106	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3424 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROTEIN (FERREDOXIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	0	0	0
			841	529	130	172	10			
1	B	106	Total	C	N	O	S	0	0	0
			841	529	130	172	10			
1	C	106	Total	C	N	O	S	0	0	0
			841	529	130	172	10			
1	D	106	Total	C	N	O	S	0	0	0
			841	529	130	172	10			

There are 4 discrepancies between the modelled and reference sequences:

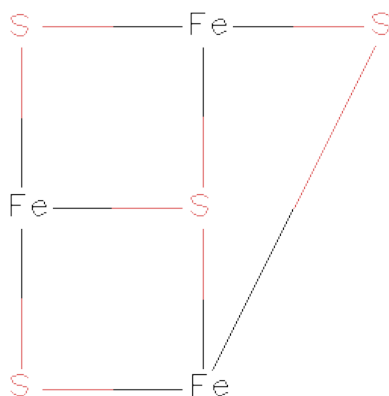
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ASN	ILE	ENGINEERED	UNP P00214
B	240	ASN	ILE	ENGINEERED	UNP P00214
C	440	ASN	ILE	ENGINEERED	UNP P00214
D	640	ASN	ILE	ENGINEERED	UNP P00214

- 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		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 7	Fe 3	S 4	0	0
3	B	1	Total 7	Fe 3	S 4	0	0
3	C	1	Total 7	Fe 3	S 4	0	0
3	D	1	Total 7	Fe 3	S 4	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: PROTEIN (FERREDOXIN)

Chain A: 



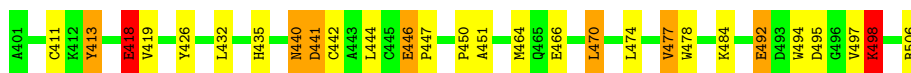
- Molecule 1: PROTEIN (FERREDOXIN)

Chain B: 



- Molecule 1: PROTEIN (FERREDOXIN)

Chain C: 



- Molecule 1: PROTEIN (FERREDOXIN)

Chain D: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.00Å 55.30Å 62.30Å 78.10° 85.20° 71.90°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	87.3 (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.209 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3424	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, F3S

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	1.00	1/862 (0.1%)	1.67	17/1175 (1.4%)
1	B	0.96	1/862 (0.1%)	1.71	22/1175 (1.9%)
1	C	1.03	2/862 (0.2%)	1.74	23/1175 (2.0%)
1	D	1.02	1/862 (0.1%)	1.73	19/1175 (1.6%)
All	All	1.00	5/3448 (0.1%)	1.71	81/4700 (1.7%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	698	LYS	CB-CG	6.17	1.69	1.52
1	B	298	LYS	CB-CG	5.47	1.67	1.52
1	A	98	LYS	CB-CG	5.47	1.67	1.52
1	C	498	LYS	CD-CE	5.30	1.64	1.51
1	C	498	LYS	CB-CG	5.11	1.66	1.52

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	706	ARG	NE-CZ-NH2	-13.20	113.70	120.30
1	D	698	LYS	CA-CB-CG	12.87	141.71	113.40
1	C	498	LYS	CA-CB-CG	10.98	137.56	113.40
1	B	298	LYS	CA-CB-CG	10.31	136.08	113.40
1	A	98	LYS	CB-CG-CD	10.20	138.11	111.60
1	C	506	ARG	NE-CZ-NH2	-9.71	115.44	120.30
1	C	441	ASP	O-C-N	8.31	136.00	122.70
1	B	240	ASN	O-C-N	8.17	135.77	122.70
1	C	494	TRP	CD1-CG-CD2	8.13	112.80	106.30
1	B	306	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	106	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	D	698	LYS	CB-CG-CD	7.84	131.98	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	TRP	CD1-CG-CD2	7.48	112.29	106.30
1	A	106	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	C	478	TRP	CD1-CG-CD2	7.15	112.02	106.30
1	B	278	TRP	CD1-CG-CD2	7.14	112.01	106.30
1	D	706	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	C	441	ASP	CA-C-N	-6.96	101.90	117.20
1	D	678	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	B	306	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	B	298	LYS	CB-CG-CD	6.76	129.18	111.60
1	C	494	TRP	CG-CD1-NE1	-6.66	103.44	110.10
1	C	506	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	98	LYS	CG-CD-CE	6.62	131.77	111.90
1	D	678	TRP	CD1-CG-CD2	6.62	111.59	106.30
1	C	498	LYS	CB-CG-CD	6.55	128.62	111.60
1	A	94	TRP	CD1-CG-CD2	6.49	111.49	106.30
1	C	494	TRP	CE2-CD2-CG	-6.45	102.14	107.30
1	D	698	LYS	CG-CD-CE	6.43	131.20	111.90
1	B	278	TRP	CE2-CD2-CG	-6.43	102.16	107.30
1	C	464	MET	CA-CB-CG	-6.41	102.40	113.30
1	C	477	VAL	CG1-CB-CG2	-6.22	100.94	110.90
1	A	78	TRP	CE2-CD2-CG	-6.19	102.34	107.30
1	B	239	CYS	C-N-CA	6.17	137.13	121.70
1	A	94	TRP	CE2-CD2-CG	-6.16	102.37	107.30
1	A	98	LYS	CB-CA-C	-6.16	98.08	110.40
1	C	478	TRP	CE2-CD2-CG	-6.12	102.40	107.30
1	D	664	MET	CA-CB-CG	-6.12	102.90	113.30
1	A	98	LYS	CA-CB-CG	6.11	126.85	113.40
1	B	219	VAL	N-CA-CB	-6.07	98.14	111.50
1	C	418	GLU	CB-CA-C	-6.07	98.26	110.40
1	B	298	LYS	CB-CA-C	-6.07	98.27	110.40
1	C	498	LYS	CD-CE-NZ	6.05	125.62	111.70
1	B	218	GLU	CB-CA-C	-6.00	98.40	110.40
1	D	694	TRP	CD1-CG-CD2	5.97	111.08	106.30
1	B	294	TRP	CD1-CG-CD2	5.96	111.07	106.30
1	A	64	MET	CG-SD-CE	-5.89	90.77	100.20
1	D	694	TRP	CE2-CD2-CG	-5.88	102.60	107.30
1	B	266	GLU	CA-CB-CG	5.87	126.32	113.40
1	A	39	CYS	N-CA-CB	-5.84	100.09	110.60
1	C	419	VAL	N-CA-CB	-5.70	98.95	111.50
1	D	698	LYS	CB-CA-C	-5.57	99.25	110.40
1	B	222	VAL	CG1-CB-CG2	-5.56	102.00	110.90
1	D	706	ARG	CA-CB-CG	-5.55	101.18	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	LYS	CG-CD-CE	5.54	128.52	111.90
1	C	498	LYS	CA-C-N	-5.52	105.16	116.20
1	A	78	TRP	CG-CD1-NE1	-5.47	104.63	110.10
1	C	498	LYS	CG-CD-CE	5.47	128.31	111.90
1	B	213	TYR	CB-CG-CD1	-5.44	117.73	121.00
1	B	242	CYS	CA-CB-SG	5.42	123.76	114.00
1	C	470	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	D	694	TRP	CG-CD2-CE3	5.38	138.74	133.90
1	D	698	LYS	CD-CE-NZ	5.37	124.06	111.70
1	D	618	GLU	CB-CA-C	-5.34	99.73	110.40
1	C	413	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	A	94	TRP	CG-CD1-NE1	-5.26	104.83	110.10
1	B	292	GLU	CA-CB-CG	5.26	124.98	113.40
1	A	18	GLU	CB-CA-C	-5.25	99.90	110.40
1	C	441	ASP	C-N-CA	5.23	134.78	121.70
1	A	92	GLU	CA-CB-CG	5.23	124.90	113.40
1	B	306	ARG	CA-CB-CG	-5.20	101.97	113.40
1	D	692	GLU	CA-CB-CG	5.19	124.82	113.40
1	D	698	LYS	CA-C-N	-5.14	105.91	116.20
1	B	294	TRP	CE2-CD2-CG	-5.13	103.20	107.30
1	B	298	LYS	CA-C-N	-5.09	106.03	116.20
1	C	495	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	294	TRP	CD1-NE1-CE2	5.07	113.56	109.00
1	D	694	TRP	CB-CG-CD1	-5.06	120.42	127.00
1	C	492	GLU	CA-CB-CG	5.05	124.52	113.40
1	A	95	ASP	CB-CG-OD1	5.05	122.84	118.30
1	D	693	ASP	CB-CG-OD2	-5.04	113.77	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	841	0	773	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	841	0	770	27	0
1	C	841	0	770	29	0
1	D	841	0	770	25	0
2	A	8	0	0	2	0
2	B	8	0	0	3	0
2	C	8	0	0	1	0
2	D	8	0	0	0	0
3	A	7	0	0	1	0
3	B	7	0	0	2	0
3	C	7	0	0	4	0
3	D	7	0	0	2	0
All	All	3424	0	3083	81	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (81) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:498:LYS:HB2	1:D:698:LYS:HZ3	1.36	0.90
1:C:498:LYS:HB3	1:D:698:LYS:HB3	1.54	0.89
1:C:498:LYS:NZ	1:D:698:LYS:HB2	1.90	0.85
1:A:98:LYS:HB2	1:B:298:LYS:NZ	1.92	0.84
1:B:240:ASN:HB2	2:B:307:SF4:S3	2.17	0.83
1:A:98:LYS:NZ	1:B:298:LYS:HB2	1.97	0.79
1:C:497:VAL:HG13	1:D:697:VAL:HG13	1.68	0.74
1:C:498:LYS:HB2	1:D:698:LYS:NZ	2.00	0.74
1:C:413:TYR:HD1	3:C:508:F3S:S4	2.10	0.74
1:C:498:LYS:HZ3	1:D:698:LYS:HB2	1.52	0.71
1:A:98:LYS:HD3	1:B:298:LYS:HD3	1.75	0.67
1:C:440:ASN:HB3	1:C:442:CYS:HB3	1.76	0.67
1:C:440:ASN:HB2	2:C:507:SF4:S3	2.36	0.65
1:D:632:LEU:HD22	3:D:708:F3S:S2	2.38	0.64
1:D:618:GLU:OE1	1:D:684:LYS:HB2	1.98	0.62
1:A:46:GLU:HG3	1:A:47:PRO:HD3	1.82	0.62
1:A:18:GLU:OE1	1:A:84:LYS:HB2	2.02	0.60
1:B:218:GLU:OE1	1:B:284:LYS:HB2	2.01	0.60
1:A:98:LYS:HB2	1:B:298:LYS:HZ2	1.65	0.59
1:D:646:GLU:HG3	1:D:647:PRO:HD3	1.83	0.59
1:A:13:TYR:CE2	1:A:50:PRO:HB2	2.38	0.58
1:A:98:LYS:CG	1:B:298:LYS:HB3	2.34	0.58
1:A:98:LYS:HB3	1:B:298:LYS:HB3	1.85	0.57
1:B:232:LEU:HD22	3:B:308:F3S:S2	2.45	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:498:LYS:CB	1:D:698:LYS:HB3	2.33	0.56
1:C:446:GLU:HG3	1:C:447:PRO:HD3	1.88	0.56
1:B:220:CYS:HA	2:B:307:SF4:S1	2.45	0.56
1:A:98:LYS:HB2	1:B:298:LYS:HZ3	1.68	0.56
1:C:413:TYR:HB2	3:C:508:F3S:S1	2.46	0.55
1:C:418:GLU:OE1	1:C:484:LYS:HB2	2.06	0.55
1:C:498:LYS:HB3	1:D:698:LYS:CB	2.34	0.54
1:A:98:LYS:HZ3	1:B:298:LYS:HB2	1.71	0.54
1:C:426:TYR:CE1	1:C:435:HIS:HB2	2.43	0.53
1:C:413:TYR:CE2	1:C:450:PRO:HB2	2.43	0.53
1:C:498:LYS:CD	1:D:698:LYS:HB3	2.40	0.52
1:C:498:LYS:HZ2	1:D:698:LYS:HB2	1.72	0.52
1:C:498:LYS:HG3	1:D:698:LYS:HZ2	1.74	0.52
1:A:13:TYR:CD2	1:A:50:PRO:HB2	2.45	0.52
1:D:626:TYR:CE1	1:D:635:HIS:HB2	2.46	0.51
1:A:98:LYS:HZ2	1:B:298:LYS:HB2	1.74	0.51
1:C:413:TYR:HE1	1:C:451:ALA:HB2	1.75	0.51
1:D:613:TYR:HD2	3:D:708:F3S:S4	2.34	0.50
1:A:98:LYS:CG	1:A:99:GLY:N	2.73	0.50
1:A:24:CYS:SG	2:A:107:SF4:S2	3.10	0.49
1:C:498:LYS:HD2	1:D:698:LYS:HB3	1.94	0.49
1:B:224:CYS:SG	2:B:307:SF4:S2	3.11	0.48
1:A:20:CYS:HA	2:A:107:SF4:S1	2.54	0.47
1:C:411:CYS:HB3	1:C:413:TYR:CE1	2.50	0.47
1:C:413:TYR:CE1	1:C:451:ALA:HB2	2.50	0.47
1:B:246:GLU:HG3	1:B:247:PRO:HD3	1.96	0.47
1:C:498:LYS:HZ2	1:D:698:LYS:HG3	1.79	0.46
1:C:432:LEU:HD22	3:C:508:F3S:S2	2.55	0.46
1:B:219:VAL:HG23	1:D:669:GLN:NE2	2.31	0.46
1:B:298:LYS:CG	1:B:299:GLY:N	2.79	0.45
1:A:32:LEU:HD22	3:A:108:F3S:S2	2.56	0.45
1:A:26:TYR:CE1	1:A:35:HIS:HB2	2.52	0.45
1:C:498:LYS:HG3	1:D:698:LYS:NZ	2.32	0.45
1:B:213:TYR:HE2	1:B:251:ALA:HB2	1.81	0.45
1:C:498:LYS:CG	1:D:698:LYS:HB3	2.48	0.44
1:A:98:LYS:CB	1:B:298:LYS:HB3	2.47	0.44
1:D:674:LEU:HA	1:D:677:VAL:HG22	1.99	0.44
1:B:216:CYS:O	1:B:219:VAL:HG12	2.18	0.43
1:A:94:TRP:O	1:A:97:VAL:HB	2.18	0.43
1:B:221:PRO:HB2	1:D:701:LEU:HD21	2.00	0.43
1:B:226:TYR:CE1	1:B:235:HIS:HB2	2.54	0.43
1:A:19:VAL:HG11	1:A:45:CYS:HA	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:98:LYS:HB3	1:B:298:LYS:CB	2.49	0.42
1:A:97:VAL:HG13	1:B:297:VAL:HG13	2.02	0.42
1:A:42:CYS:SG	1:A:44:LEU:HB2	2.60	0.42
1:A:27:GLU:HB2	1:A:81:ILE:HB	2.01	0.42
1:C:474:LEU:HA	1:C:477:VAL:HG22	2.02	0.42
1:D:684:LYS:HG2	1:D:685:LYS:N	2.35	0.42
1:A:40:ASN:OD1	1:A:42:CYS:HB3	2.20	0.41
1:A:33:VAL:HG11	1:A:71:ASN:HA	2.02	0.41
1:B:213:TYR:HD2	3:B:308:F3S:S4	2.42	0.41
1:B:297:VAL:HG12	1:B:300:LYS:CG	2.50	0.41
1:C:413:TYR:CD1	3:C:508:F3S:S4	3.01	0.41
1:A:33:VAL:CG1	1:A:71:ASN:HA	2.50	0.41
1:A:97:VAL:HG12	1:A:100:LYS:CG	2.51	0.40
1:D:627:GLU:O	1:D:678:TRP:HB3	2.22	0.40
1:B:267:PHE:HA	1:B:270:LEU:HB2	2.02	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	104/106 (98%)	96 (92%)	8 (8%)	0	100	100
1	B	104/106 (98%)	98 (94%)	5 (5%)	1 (1%)	22	60
1	C	104/106 (98%)	99 (95%)	4 (4%)	1 (1%)	22	60
1	D	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
All	All	416/424 (98%)	390 (94%)	24 (6%)	2 (0%)	38	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	441	ASP
1	B	241	ASP

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	96/96 (100%)	86 (90%)	10 (10%)	10	28
1	B	96/96 (100%)	86 (90%)	10 (10%)	10	28
1	C	96/96 (100%)	88 (92%)	8 (8%)	16	42
1	D	96/96 (100%)	89 (93%)	7 (7%)	20	49
All	All	384/384 (100%)	349 (91%)	35 (9%)	14	37

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	41	ASP
1	A	44	LEU
1	A	46	GLU
1	A	66	GLU
1	A	70	LEU
1	A	90	ASP
1	A	92	GLU
1	A	97	VAL
1	A	98	LYS
1	B	218	GLU
1	B	240	ASN
1	B	244	LEU
1	B	246	GLU
1	B	266	GLU
1	B	270	LEU
1	B	280	ASN
1	B	292	GLU
1	B	297	VAL
1	B	298	LYS
1	C	418	GLU
1	C	440	ASN
1	C	444	LEU
1	C	446	GLU
1	C	466	GLU
1	C	470	LEU

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Mol	Chain	Res	Type
1	C	492	GLU
1	C	498	LYS
1	D	618	GLU
1	D	644	LEU
1	D	646	GLU
1	D	666	GLU
1	D	670	LEU
1	D	692	GLU
1	D	698	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	502	GLN
1	D	669	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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	SF4	A	107	1	12,12,12	8.97	12 (100%)	0,24,24	0.00	-
3	F3S	A	108	1	3,9,9	8.10	3 (100%)	0,15,15	0.00	-
2	SF4	B	307	1	12,12,12	7.22	11 (91%)	0,24,24	0.00	-
3	F3S	B	308	1	3,9,9	8.22	3 (100%)	0,15,15	0.00	-
2	SF4	C	507	1	12,12,12	6.18	10 (83%)	0,24,24	0.00	-
3	F3S	C	508	1	3,9,9	6.65	3 (100%)	0,15,15	0.00	-
2	SF4	D	707	1	12,12,12	13.18	12 (100%)	0,24,24	0.00	-
3	F3S	D	708	1	3,9,9	15.89	3 (100%)	0,15,15	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	A	107	1	-	0/0/48/48	0/0/5/5
3	F3S	A	108	1	-	0/0/24/24	0/0/3/3
2	SF4	B	307	1	-	0/0/48/48	0/0/5/5
3	F3S	B	308	1	-	0/0/24/24	0/0/3/3
2	SF4	C	507	1	-	0/0/48/48	0/0/5/5
3	F3S	C	508	1	-	0/0/24/24	0/0/3/3
2	SF4	D	707	1	-	0/0/48/48	0/0/5/5
3	F3S	D	708	1	-	0/0/24/24	0/0/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	707	SF4	S3-FE4	-22.30	2.18	2.33
2	D	707	SF4	S2-FE1	-20.02	2.19	2.33
3	D	708	F3S	S3-FE3	-18.11	2.21	2.33
2	A	107	SF4	S2-FE1	-15.86	2.22	2.33
3	D	708	F3S	S3-FE4	-15.52	2.22	2.33
2	D	707	SF4	S3-FE1	-14.57	2.23	2.33
2	A	107	SF4	S3-FE4	-14.29	2.23	2.33
3	D	708	F3S	S3-FE1	-13.75	2.24	2.33
2	D	707	SF4	S1-FE4	-13.11	2.24	2.33
2	D	707	SF4	S1-FE3	-13.00	2.24	2.33
2	D	707	SF4	S2-FE3	-12.83	2.24	2.33
2	D	707	SF4	S1-FE2	-12.60	2.24	2.33
2	B	307	SF4	S3-FE4	-12.50	2.24	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	108	F3S	S3-FE4	-12.25	2.25	2.33
2	A	107	SF4	S3-FE1	-12.07	2.25	2.33
3	B	308	F3S	S3-FE4	-10.64	2.26	2.33
2	B	307	SF4	S1-FE3	-10.50	2.26	2.33
2	B	307	SF4	S2-FE4	-10.36	2.26	2.33
2	C	507	SF4	S3-FE1	-10.33	2.26	2.33
2	D	707	SF4	S2-FE4	-9.45	2.26	2.33
2	B	307	SF4	S2-FE1	-9.00	2.27	2.33
2	A	107	SF4	S2-FE4	-8.73	2.27	2.33
3	C	508	F3S	S3-FE4	-8.67	2.27	2.33
2	D	707	SF4	S4-FE1	-8.43	2.27	2.33
2	C	507	SF4	S2-FE4	-8.28	2.27	2.33
2	A	107	SF4	S4-FE3	-8.20	2.27	2.33
3	B	308	F3S	S3-FE3	-7.83	2.28	2.33
2	D	707	SF4	S4-FE3	-7.74	2.28	2.33
2	C	507	SF4	S3-FE4	-7.64	2.28	2.33
2	B	307	SF4	S4-FE1	-7.47	2.28	2.33
2	C	507	SF4	S4-FE1	-7.25	2.28	2.33
2	D	707	SF4	S4-FE2	-7.08	2.28	2.33
2	A	107	SF4	S2-FE3	-7.02	2.28	2.33
2	A	107	SF4	S1-FE3	-6.64	2.28	2.33
2	C	507	SF4	S2-FE1	-6.49	2.28	2.33
2	C	507	SF4	S4-FE3	-6.44	2.28	2.33
2	D	707	SF4	S3-FE2	-6.35	2.29	2.33
2	A	107	SF4	S3-FE2	-6.27	2.29	2.33
2	C	507	SF4	S3-FE2	-6.25	2.29	2.33
2	B	307	SF4	S4-FE2	-6.13	2.29	2.33
2	B	307	SF4	S1-FE2	-5.89	2.29	2.33
3	A	108	F3S	S3-FE1	-5.82	2.29	2.33
2	A	107	SF4	S4-FE1	-5.77	2.29	2.33
3	C	508	F3S	S3-FE1	-5.52	2.29	2.33
3	B	308	F3S	S3-FE1	-5.32	2.29	2.33
3	C	508	F3S	S3-FE3	-5.20	2.29	2.33
2	C	507	SF4	S1-FE3	-5.09	2.29	2.33
2	A	107	SF4	S1-FE4	-4.88	2.30	2.33
2	A	107	SF4	S1-FE2	-4.79	2.30	2.33
2	B	307	SF4	S4-FE3	-4.56	2.30	2.33
3	A	108	F3S	S3-FE3	-3.62	2.30	2.33
2	C	507	SF4	S1-FE4	-3.44	2.30	2.33
2	B	307	SF4	S2-FE3	-3.26	2.31	2.33
2	C	507	SF4	S2-FE3	-3.04	2.31	2.33
2	A	107	SF4	S4-FE2	-2.81	2.31	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	307	SF4	S1-FE4	-2.60	2.31	2.33
2	B	307	SF4	S3-FE1	-2.03	2.31	2.33

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.