



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:18 AM UTC

PDB ID : 1GAO / pdb_00001gao
Title : CRYSTAL STRUCTURE OF THE L44S MUTANT OF FERREDOXIN I
Authors : Stout, C.D.; Burgess, B.K.; Prasad, G.S.; Sridhar, V.; Jung, Y.S.
Deposited on : 2000-11-30
Resolution : 2.20 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

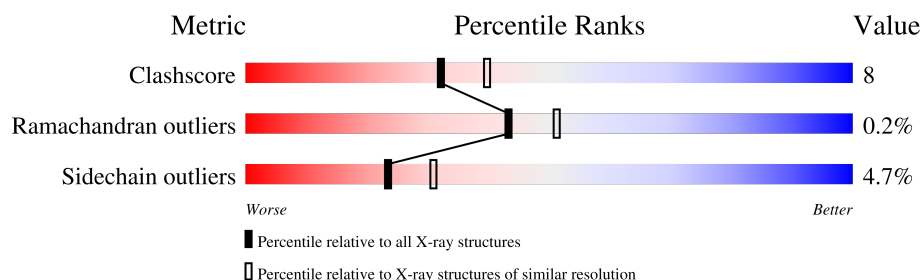
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$.

Note EDS was not executed.

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	A	107	-	-	X	-
2	SF4	D	707	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3673 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.

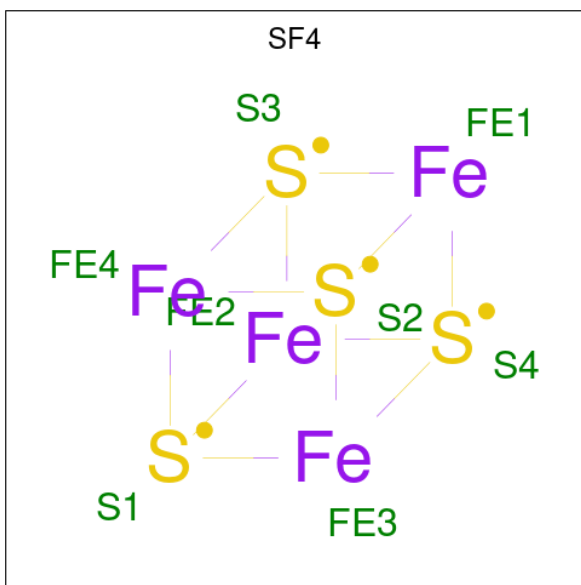
- Molecule 1 is a protein called FERREDOXIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	0	0	0
			839	528	129	172	10			
1	B	106	Total	C	N	O	S	0	0	0
			839	528	129	172	10			
1	C	106	Total	C	N	O	S	0	0	0
			839	528	129	172	10			
1	D	106	Total	C	N	O	S	0	0	0
			839	528	129	172	10			

There are 4 discrepancies between the modelled and reference sequences:

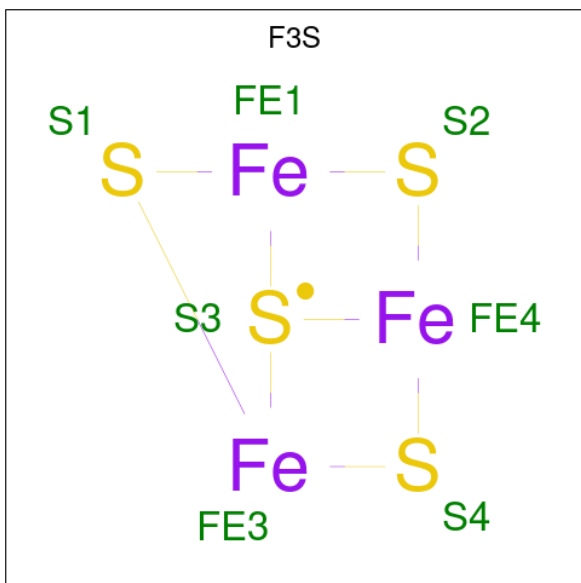
Chain	Residue	Modelled	Actual	Comment	Reference
A	44	SER	LEU	engineered mutation	UNP P00214
B	244	SER	LEU	engineered mutation	UNP P00214
C	444	SER	LEU	engineered mutation	UNP P00214
D	644	SER	LEU	engineered mutation	UNP P00214

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: 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 (CCD ID: 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

- Molecule 4 is water.

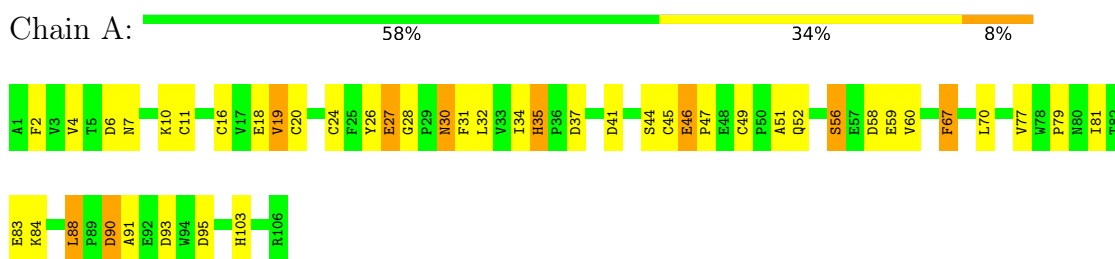
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total 63	O 63	0	0
4	B	69	Total 69	O 69	0	0
4	C	66	Total 66	O 66	0	0
4	D	59	Total 59	O 59	0	0

3 Residue-property plots

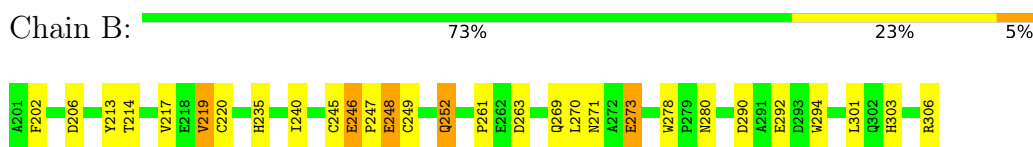
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

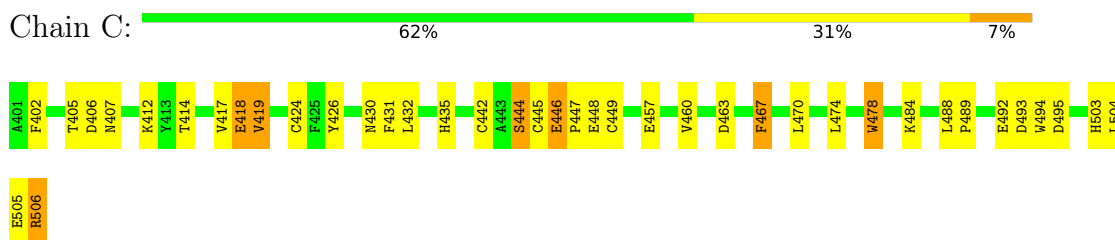
• Molecule 1: FERREDOXIN I



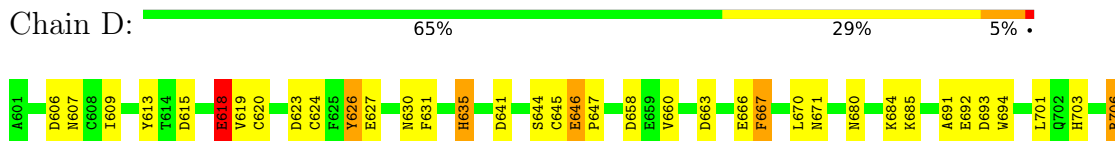
• Molecule 1: FERREDOXIN I



• Molecule 1: FERREDOXIN I



• Molecule 1: FERREDOXIN I



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.80Å 85.60Å 67.20Å 90.00° 117.90° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.20)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.243 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3673	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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: F3S, 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	0.98	2/860 (0.2%)	1.82	24/1172 (2.0%)
1	B	0.92	2/860 (0.2%)	1.75	16/1172 (1.4%)
1	C	0.93	2/860 (0.2%)	1.83	28/1172 (2.4%)
1	D	0.97	2/860 (0.2%)	1.81	23/1172 (2.0%)
All	All	0.95	8/3440 (0.2%)	1.80	91/4688 (1.9%)

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
1	D	0	2
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	HIS	CD2-NE2	-6.93	1.30	1.37
1	C	503	HIS	CD2-NE2	-6.91	1.30	1.37
1	D	635	HIS	CD2-NE2	-6.78	1.30	1.37
1	A	35	HIS	CD2-NE2	-6.27	1.30	1.37
1	D	703	HIS	CD2-NE2	-6.25	1.30	1.37
1	C	435	HIS	CD2-NE2	-6.18	1.31	1.37
1	B	303	HIS	CD2-NE2	-5.92	1.31	1.37
1	B	235	HIS	CD2-NE2	-5.59	1.31	1.37

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	419	VAL	N-CA-CB	-13.64	94.66	112.26
1	A	90	ASP	CA-CB-CG	10.73	123.33	112.60
1	A	27	GLU	N-CA-C	8.80	122.57	108.41
1	A	58	ASP	CA-CB-CG	8.69	121.29	112.60
1	C	419	VAL	CB-CA-C	8.43	121.66	111.20
1	D	627	GLU	N-CA-C	8.37	122.89	109.24
1	A	41	ASP	N-CA-C	8.06	122.53	111.90
1	D	606	ASP	N-CA-C	7.66	120.30	111.11
1	B	202	PHE	CA-CB-CG	-7.62	106.18	113.80
1	A	19	VAL	N-CA-CB	-7.31	100.95	112.07
1	C	495	ASP	CA-CB-CG	7.06	119.66	112.60
1	D	693	ASP	CA-CB-CG	7.01	119.61	112.60
1	C	448	GLU	N-CA-C	6.91	118.89	111.36
1	D	607	ASN	OD1-CG-ND2	-6.84	115.76	122.60
1	D	663	ASP	CA-CB-CG	6.82	119.42	112.60
1	D	658	ASP	CA-CB-CG	6.79	119.39	112.60
1	D	630	ASN	CA-CB-CG	6.75	119.35	112.60
1	D	667	PHE	CA-CB-CG	-6.59	107.21	113.80
1	A	2	PHE	CA-CB-CG	-6.57	107.23	113.80
1	D	635	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	D	706	ARG	NE-CZ-NH1	-6.56	114.94	121.50
1	A	77	VAL	CB-CA-C	-6.56	104.22	110.65
1	C	445	CYS	N-CA-C	6.54	119.40	111.82
1	B	219	VAL	N-CA-CB	-6.53	101.11	112.08
1	D	671	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	C	402	PHE	CA-CB-CG	-6.37	107.43	113.80
1	B	206	ASP	N-CA-C	6.25	121.69	111.37
1	D	667	PHE	N-CA-C	6.25	118.89	111.71
1	A	103	HIS	CB-CG-CD2	-6.24	123.08	131.20
1	B	248	GLU	N-CA-C	6.17	119.28	111.69
1	A	11	CYS	N-CA-C	-6.11	103.77	112.13
1	D	641	ASP	N-CA-C	6.04	119.87	111.90
1	C	430	ASN	CA-CB-CG	6.03	118.63	112.60
1	C	467	PHE	N-CA-C	6.03	118.65	111.71
1	D	680	ASN	CA-CB-CG	6.02	118.62	112.60
1	C	505	GLU	CA-C-O	6.02	127.02	120.58
1	A	77	VAL	N-CA-C	6.02	119.43	113.53
1	A	67	PHE	N-CA-C	6.01	119.72	112.38
1	C	435	HIS	CB-CG-CD2	-5.99	123.41	131.20
1	C	435	HIS	CA-C-N	5.96	125.67	119.05
1	C	435	HIS	C-N-CA	5.96	125.67	119.05
1	C	449	CYS	CA-C-N	5.90	125.44	119.19
1	C	449	CYS	C-N-CA	5.90	125.44	119.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	D	691	ALA	N-CA-C	5.85	118.13	111.11
1	B	249	CYS	CA-C-N	5.83	125.53	119.64
1	B	249	CYS	C-N-CA	5.83	125.53	119.64
1	C	457	GLU	CA-CB-CG	-5.80	102.50	114.10
1	A	91	ALA	N-CA-C	5.68	118.21	111.33
1	B	235	HIS	CA-C-N	5.62	125.46	119.28
1	B	235	HIS	C-N-CA	5.62	125.46	119.28
1	D	607	ASN	CB-CG-ND2	5.58	124.77	116.40
1	D	631	PHE	CA-CB-CG	5.55	119.35	113.80
1	B	240	ILE	N-CA-C	5.53	117.49	112.29
1	C	463	ASP	CA-CB-CG	5.49	118.09	112.60
1	B	273	GLU	CB-CG-CD	5.48	121.92	112.60
1	A	88	LEU	CA-C-N	5.47	125.56	119.32
1	A	88	LEU	C-N-CA	5.47	125.56	119.32
1	B	263	ASP	CA-CB-CG	5.45	118.05	112.60
1	C	494	TRP	CG-CD2-CE3	5.45	139.34	133.90
1	A	60	VAL	CA-C-N	5.43	125.44	119.90
1	A	60	VAL	C-N-CA	5.43	125.44	119.90
1	D	666	GLU	CB-CA-C	-5.41	101.48	110.68
1	B	278	TRP	CA-C-N	5.41	125.17	119.76
1	B	278	TRP	C-N-CA	5.41	125.17	119.76
1	C	488	LEU	CA-C-N	5.38	125.02	119.05
1	C	488	LEU	C-N-CA	5.38	125.02	119.05
1	D	694	TRP	CG-CD2-CE3	5.34	139.24	133.90
1	C	478	TRP	CA-C-N	5.32	125.08	119.76
1	C	478	TRP	C-N-CA	5.32	125.08	119.76
1	A	30	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	93	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	95	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	28	GLY	CA-C-N	5.23	125.28	119.32
1	A	28	GLY	C-N-CA	5.23	125.28	119.32
1	B	280	ASN	CA-CB-CG	5.21	117.81	112.60
1	C	506	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	D	693	ASP	N-CA-C	-5.17	105.72	111.36
1	C	493	ASP	N-CA-C	-5.16	106.14	112.90
1	B	235	HIS	CB-CG-CD2	-5.14	124.51	131.20
1	D	660	VAL	CA-C-N	5.13	125.07	119.78
1	D	660	VAL	C-N-CA	5.13	125.07	119.78
1	A	31	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	6	ASP	N-CA-C	5.09	117.49	111.33
1	C	406	ASP	N-CA-C	5.08	121.63	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	618	GLU	CB-CA-C	-5.08	102.22	110.85
1	C	407	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	A	52	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	C	460	VAL	CA-C-N	5.04	125.04	119.90
1	C	460	VAL	C-N-CA	5.04	125.04	119.90
1	C	435	HIS	CB-CG-ND1	5.01	130.22	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	TYR	Sidechain
1	D	626	TYR	Sidechain
1	D	706	ARG	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	839	0	772	17	0
1	B	839	0	769	10	0
1	C	839	0	769	14	0
1	D	839	0	769	12	0
2	A	8	0	0	2	0
2	B	8	0	0	1	0
2	C	8	0	0	1	0
2	D	8	0	0	2	0
3	A	7	0	0	0	0
3	B	7	0	0	1	0
3	C	7	0	0	1	0
3	D	7	0	0	0	0
4	A	63	0	0	2	0
4	B	69	0	0	0	0
4	C	66	0	0	1	0
4	D	59	0	0	1	0
All	All	3673	0	3079	52	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 8.

All (52) 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:D:620:CYS:HA	2:D:707:SF4:S1	2.37	0.64
1:D:624:CYS:SG	2:D:707:SF4:S2	2.95	0.64
1:D:619:VAL:HG22	1:D:644:SER:HB3	1.81	0.63
1:D:646:GLU:HG3	1:D:647:PRO:HD3	1.79	0.63
1:A:20:CYS:HA	2:A:107:SF4:S1	2.39	0.62
1:C:424:CYS:SG	2:C:507:SF4:S2	3.01	0.58
1:A:56:SER:HB3	1:A:59:GLU:HG2	1.85	0.58
1:C:446:GLU:HG3	1:C:447:PRO:HD3	1.85	0.58
1:A:27:GLU:HB2	1:A:81:ILE:HB	1.87	0.56
1:A:7:ASN:HB2	4:A:836:HOH:O	2.06	0.56
1:B:219:VAL:HG11	1:B:248:GLU:HG3	1.86	0.55
1:A:49:CYS:SG	1:A:51:ALA:HB3	2.47	0.55
1:B:214:THR:O	1:B:217:VAL:HG22	2.07	0.55
1:B:246:GLU:HG3	1:B:247:PRO:HD3	1.89	0.54
1:C:489:PRO:HD2	4:C:842:HOH:O	2.08	0.54
1:A:30:ASN:HA	1:A:88:LEU:HD11	1.90	0.54
1:A:79:PRO:HB2	1:B:306:ARG:NH1	2.22	0.53
1:D:619:VAL:HG11	1:D:645:CYS:HA	1.91	0.52
1:C:442:CYS:SG	1:C:444:SER:HB2	2.51	0.51
1:A:46:GLU:HB3	1:A:47:PRO:HD3	1.94	0.50
1:C:412:LYS:HA	3:C:508:F3S:S1	2.51	0.50
1:A:10:LYS:HE3	4:A:829:HOH:O	2.11	0.50
1:D:626:TYR:CE2	1:D:635:HIS:HB2	2.47	0.50
1:C:431:PHE:CD2	1:C:504:LEU:HD11	2.47	0.49
1:B:213:TYR:HD2	3:B:308:F3S:S4	2.36	0.49
1:D:609:ILE:HD13	1:D:701:LEU:HA	1.94	0.49
1:C:474:LEU:HD13	1:C:478:TRP:CH2	2.48	0.49
1:A:19:VAL:HG11	1:A:45:CYS:HA	1.95	0.48
1:D:667:PHE:HA	1:D:670:LEU:HB2	1.94	0.48
1:A:19:VAL:HG22	1:A:44:SER:HB3	1.96	0.47
1:D:613:TYR:HB3	1:D:615:ASP:OD1	2.14	0.47
1:D:618:GLU:OE1	1:D:684:LYS:HB2	2.15	0.47
1:A:24:CYS:SG	2:A:107:SF4:S2	3.14	0.46
1:C:506:ARG:HH21	1:C:506:ARG:HG3	1.81	0.46
1:B:270:LEU:HD11	1:B:301:LEU:HD11	1.98	0.45
1:A:18:GLU:HG2	1:A:84:LYS:HB2	1.98	0.45
1:A:4:VAL:HG23	1:A:34:ILE:HG13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:THR:HA	1:C:467:PHE:CD1	2.52	0.45
1:D:623:ASP:HA	4:D:991:HOH:O	2.16	0.45
1:C:426:TYR:CD2	1:C:426:TYR:N	2.85	0.44
1:C:414:THR:O	1:C:417:VAL:HG22	2.18	0.44
1:D:684:LYS:HG2	1:D:685:LYS:N	2.33	0.43
1:C:467:PHE:HA	1:C:470:LEU:HB2	2.01	0.43
1:B:245:CYS:O	1:B:248:GLU:HB2	2.18	0.42
1:C:418:GLU:OE1	1:C:484:LYS:HB2	2.19	0.42
1:B:290:ASP:O	1:B:294:TRP:HD1	2.03	0.42
1:B:220:CYS:HA	2:B:307:SF4:S1	2.60	0.42
1:A:67:PHE:HA	1:A:70:LEU:HB2	2.02	0.41
1:C:470:LEU:HD23	1:C:470:LEU:HA	1.79	0.41
1:A:16:CYS:O	1:A:19:VAL:HG12	2.21	0.41
1:B:269:GLN:O	1:B:273:GLU:HG2	2.21	0.41
1:A:35:HIS:CE1	1:A:37:ASP:HB2	2.56	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%)	102 (98%)	2 (2%)	0	100	100
1	B	104/106 (98%)	92 (88%)	11 (11%)	1 (1%)	12	11
1	C	104/106 (98%)	96 (92%)	8 (8%)	0	100	100
1	D	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
All	All	416/424 (98%)	391 (94%)	24 (6%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	252	GLN

5.3.2 Protein sidechains [i](#)

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%)	91 (95%)	5 (5%)	21	26
1	B	96/96 (100%)	92 (96%)	4 (4%)	26	36
1	C	96/96 (100%)	90 (94%)	6 (6%)	16	19
1	D	96/96 (100%)	93 (97%)	3 (3%)	35	48
All	All	384/384 (100%)	366 (95%)	18 (5%)	23	31

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	46	GLU
1	A	56	SER
1	A	83	GLU
1	A	90	ASP
1	B	246	GLU
1	B	252	GLN
1	B	261	PRO
1	B	292	GLU
1	C	418	GLU
1	C	419	VAL
1	C	432	LEU
1	C	444	SER
1	C	446	GLU
1	C	492	GLU
1	D	618	GLU
1	D	646	GLU
1	D	692	GLU

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

Mol	Chain	Res	Type
1	B	252	GLN
1	B	303	HIS
1	C	503	HIS
1	D	665	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	307	1	0,12,12	-	-	-		
3	F3S	A	108	1	0,9,9	-	-	-		
2	SF4	C	507	1	0,12,12	-	-	-		
2	SF4	D	707	1	0,12,12	-	-	-		
3	F3S	C	508	1	0,9,9	-	-	-		
3	F3S	D	708	1	0,9,9	-	-	-		
2	SF4	A	107	1	0,12,12	-	-	-		
3	F3S	B	308	1	0,9,9	-	-	-		

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	B	307	1	-	-	0/6/5/5
3	F3S	A	108	1	-	-	0/3/3/3
2	SF4	C	507	1	-	-	0/6/5/5
2	SF4	D	707	1	-	-	0/6/5/5
3	F3S	C	508	1	-	-	0/3/3/3
3	F3S	D	708	1	-	-	0/3/3/3
2	SF4	A	107	1	-	-	0/6/5/5
3	F3S	B	308	1	-	-	0/3/3/3

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.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	307	SF4	1	0
2	C	507	SF4	1	0
2	D	707	SF4	2	0
3	C	508	F3S	1	0
2	A	107	SF4	2	0
3	B	308	F3S	1	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.