



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:18 AM UTC

PDB ID : 4DIL / pdb_00004dil
Title : Flavo Di-iron protein H90N mutant from *Thermotoga maritima*
Authors : Fang, H.; Caranto, J.D.; Taylor, A.B.; Hart, P.J.; Kurtz, D.M.
Deposited on : 2012-01-31
Resolution : 2.00 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

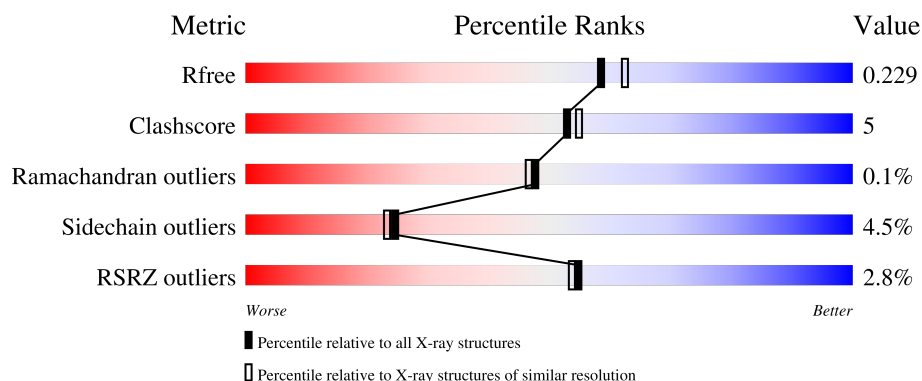
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	410	
1	B	410	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6608 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 FLAVOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	2	0
			3164	2059	507	590	8			
1	B	396	Total	C	N	O	S	0	8	0
			3250	2111	524	607	8			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9WZL4
A	-10	GLY	-	expression tag	UNP Q9WZL4
A	-9	SER	-	expression tag	UNP Q9WZL4
A	-8	ASP	-	expression tag	UNP Q9WZL4
A	-7	LYS	-	expression tag	UNP Q9WZL4
A	-6	ILE	-	expression tag	UNP Q9WZL4
A	-5	HIS	-	expression tag	UNP Q9WZL4
A	-4	HIS	-	expression tag	UNP Q9WZL4
A	-3	HIS	-	expression tag	UNP Q9WZL4
A	-2	HIS	-	expression tag	UNP Q9WZL4
A	-1	HIS	-	expression tag	UNP Q9WZL4
A	0	HIS	-	expression tag	UNP Q9WZL4
A	90	ASN	HIS	engineered mutation	UNP Q9WZL4
B	-11	MET	-	expression tag	UNP Q9WZL4
B	-10	GLY	-	expression tag	UNP Q9WZL4
B	-9	SER	-	expression tag	UNP Q9WZL4
B	-8	ASP	-	expression tag	UNP Q9WZL4
B	-7	LYS	-	expression tag	UNP Q9WZL4
B	-6	ILE	-	expression tag	UNP Q9WZL4
B	-5	HIS	-	expression tag	UNP Q9WZL4
B	-4	HIS	-	expression tag	UNP Q9WZL4
B	-3	HIS	-	expression tag	UNP Q9WZL4
B	-2	HIS	-	expression tag	UNP Q9WZL4
B	-1	HIS	-	expression tag	UNP Q9WZL4
B	0	HIS	-	expression tag	UNP Q9WZL4

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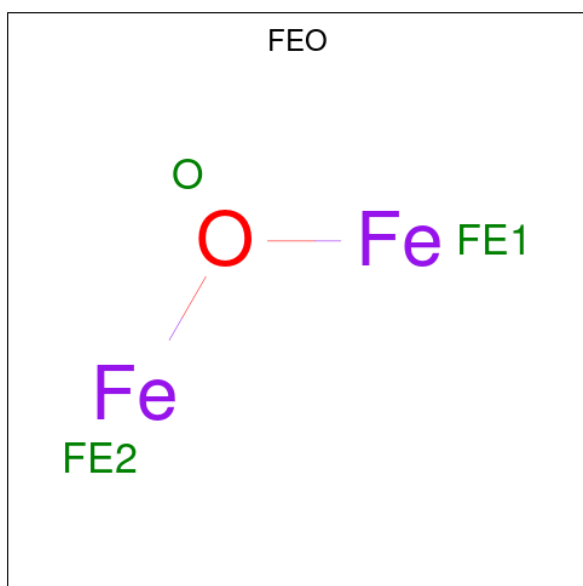
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Chain	Residue	Modelled	Actual	Comment	Reference
B	90	ASN	HIS	engineered mutation	UNP Q9WZL4

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cl 2 2	0	0
2	B	1	Total Cl 1 1	0	0

- Molecule 3 is MU-OXO-DIIRON (CCD ID: FEO) (formula: Fe₂O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe O 3 2 1	0	0
3	B	1	Total Fe O 3 2 1	0	0

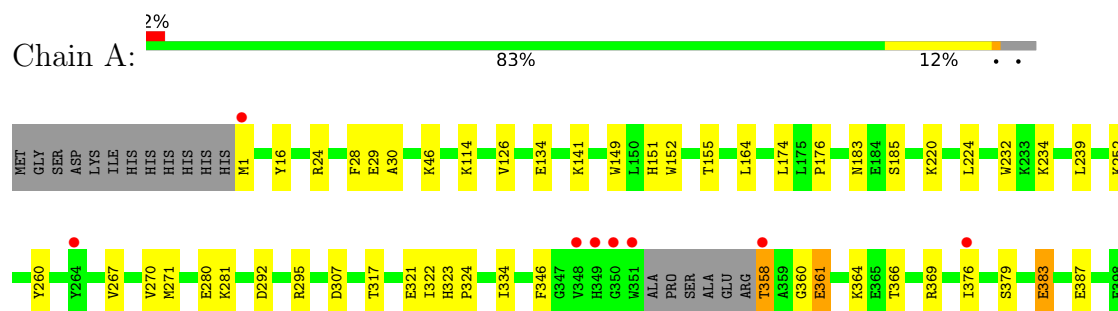
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	109	Total O 109 109	0	0
4	B	76	Total O 76 76	0	0

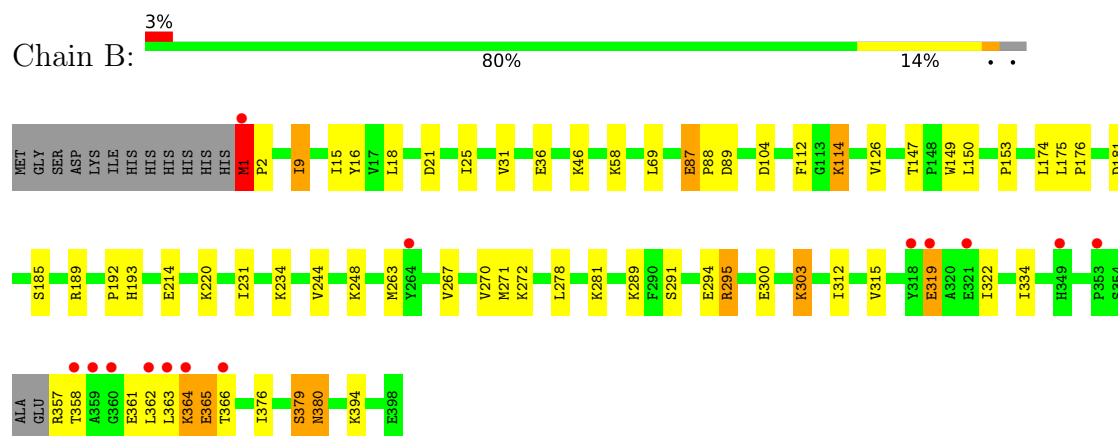
3 Residue-property plots [i](#)

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: FLAVOPROTEIN



• Molecule 1: FLAVOPROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.65Å 91.94Å 86.34Å 90.00° 96.79° 90.00°	Depositor
Resolution (Å)	28.86 – 2.00 28.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (28.86-2.00) 99.7 (28.86-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.198 , 0.235 0.195 , 0.229	Depositor DCC
R_{free} test set	2875 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6608	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.48	0/3244	0.80	2/4388 (0.0%)
1	B	0.46	0/3327	0.80	6/4502 (0.1%)
All	All	0.47	0/6571	0.80	8/8890 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	MET	CA-C-N	-7.78	111.99	119.85
1	A	1	MET	C-N-CA	-7.78	111.99	119.85
1	B	315	VAL	N-CA-C	5.41	115.65	107.75
1	B	379	SER	N-CA-C	-5.37	103.05	110.35
1	B	1	MET	CA-C-N	5.31	125.25	119.78
1	B	1	MET	C-N-CA	5.31	125.25	119.78
1	B	87	GLU	CA-C-N	5.03	124.69	119.56
1	B	87	GLU	C-N-CA	5.03	124.69	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3164	0	3201	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3250	0	3276	37	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	109	0	0	1	0
4	B	76	0	0	0	0
All	All	6608	0	6477	65	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 5.

All (65) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:SER:O	1:B:380:ASN:ND2	2.11	0.82
1:B:357:ARG:HH21	1:B:361:GLU:HG2	1.51	0.76
1:B:295:ARG:HG3	1:B:295:ARG:HH11	1.56	0.71
1:B:114:LYS:HD3	1:B:126:VAL:HB	1.72	0.71
1:A:358:THR:HG22	1:A:361:GLU:HG2	1.74	0.69
1:B:334:ILE:HG12	1:B:366:THR:HG21	1.74	0.68
1:B:21:ASP:HB3	1:B:175:LEU:HD13	1.78	0.64
1:B:295:ARG:HG3	1:B:295:ARG:NH1	2.16	0.60
1:A:281:LYS:NZ	1:A:387:GLU:OE2	2.35	0.59
1:A:114:LYS:HG3	1:A:126:VAL:HB	1.85	0.58
1:A:334:ILE:HG12	1:A:366:THR:HG21	1.84	0.58
1:B:300:GLU:OE1	1:B:303:LYS:NZ	2.32	0.57
1:B:278:LEU:HD11	1:B:312:ILE:HD12	1.87	0.56
1:A:29:GLU:O	1:A:30:ALA:HB3	2.07	0.54
1:A:152:TRP:HE1	1:B:319[A]:GLU:CD	2.15	0.54
1:B:9:ILE:HD11	1:B:15:ILE:HG22	1.91	0.53
1:B:281:LYS:HB3	1:B:394:LYS:HD2	1.90	0.53
1:A:369:ARG:O	1:A:369:ARG:HG3	2.12	0.48
1:B:114:LYS:CD	1:B:126:VAL:HB	2.42	0.48
1:A:252:LYS:HG2	1:A:307:ASP:HB2	1.96	0.48
1:A:361:GLU:HG2	1:A:361:GLU:H	1.53	0.48
1:B:361:GLU:O	1:B:364:LYS:HD2	2.14	0.48
1:A:16:TYR:CE1	1:A:46:LYS:HD3	2.49	0.47
1:A:267:VAL:HG22	1:A:376:ILE:HD13	1.97	0.47
1:B:289:LYS:HE2	1:B:291:SER:HB3	1.96	0.47
1:A:174:LEU:O	1:A:176:PRO:HD3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:TYR:HE1	1:A:46:LYS:HD3	1.80	0.46
1:A:28:PHE:O	1:A:29:GLU:HB2	2.16	0.46
1:B:147:THR:HB	1:B:150:LEU:HD12	1.98	0.46
1:B:270:VAL:HG21	1:B:376:ILE:HG23	1.98	0.46
1:B:87:GLU:HA	1:B:88:PRO:HD3	1.82	0.46
1:B:379:SER:C	1:B:380:ASN:HD22	2.23	0.46
1:B:174:LEU:O	1:B:176:PRO:HD3	2.15	0.45
1:A:358:THR:HG23	1:A:360:GLY:N	2.31	0.45
1:A:270:VAL:HG12	1:A:271:MET:HE2	1.97	0.45
1:B:291:SER:OG	1:B:294:GLU:HG2	2.16	0.45
1:B:189:ARG:O	1:B:192:PRO:HD2	2.16	0.45
1:A:292:ASP:HB2	1:B:25:ILE:HG13	1.97	0.45
1:B:267:VAL:O	1:B:271:MET:HG2	2.18	0.44
1:A:232:TRP:CD1	1:A:239:LEU:HD22	2.52	0.44
1:A:360:GLY:O	1:A:364:LYS:HG3	2.18	0.44
1:B:16:TYR:HE1	1:B:46:LYS:HD3	1.82	0.44
1:B:357:ARG:NH2	1:B:361:GLU:HG2	2.26	0.44
1:B:364:LYS:HG2	1:B:365:GLU:N	2.33	0.44
1:B:181:ASP:O	1:B:234:LYS:NZ	2.37	0.43
1:B:319[A]:GLU:H	1:B:319[A]:GLU:HG2	1.58	0.43
1:B:18:LEU:HD21	1:B:69:LEU:HA	2.01	0.43
1:B:1:MET:HE3	1:B:1:MET:HB2	1.73	0.42
1:A:134:GLU:OE2	1:A:141:LYS:HD3	2.19	0.42
1:A:260:TYR:CG	1:A:271:MET:HG3	2.54	0.42
1:B:362:LEU:HA	1:B:362:LEU:HD12	1.76	0.42
1:B:1:MET:HA	1:B:2:PRO:HD3	1.78	0.42
1:A:183:ASN:OD1	1:A:185:SER:HB3	2.20	0.42
1:B:36:GLU:OE2	1:B:193:HIS:ND1	2.49	0.42
1:A:321:GLU:HB3	1:A:322:ILE:H	1.51	0.41
1:A:383:GLU:O	1:A:383:GLU:HG2	2.21	0.41
1:B:149:TRP:CZ3	1:B:153:PRO:HD3	2.56	0.41
1:A:149:TRP:C	1:A:151:HIS:HA	2.46	0.41
1:B:58:LYS:HG3	1:B:89:ASP:HA	2.03	0.41
1:B:244:VAL:HG12	1:B:248:LYS:HE2	2.03	0.41
1:A:134:GLU:CD	1:A:141:LYS:HD3	2.45	0.40
1:A:155[B]:THR:HG23	4:A:528:HOH:O	2.21	0.40
1:A:271:MET:HE1	1:A:346:PHE:CB	2.51	0.40
1:A:224:LEU:HD22	1:A:239:LEU:HD23	2.03	0.40
1:A:323:HIS:HA	1:A:324:PRO:HD3	1.95	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	390/410 (95%)	377 (97%)	13 (3%)	0	100	100
1	B	400/410 (98%)	384 (96%)	15 (4%)	1 (0%)	36	35
All	All	790/820 (96%)	761 (96%)	28 (4%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	31	VAL

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	348/361 (96%)	337 (97%)	11 (3%)	34	35
1	B	356/361 (99%)	334 (94%)	22 (6%)	16	13
All	All	704/722 (98%)	671 (95%)	33 (5%)	24	22

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	164	LEU
1	A	220	LYS
1	A	234	LYS
1	A	280	GLU

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Mol	Chain	Res	Type
1	A	295	ARG
1	A	317	THR
1	A	358	THR
1	A	361	GLU
1	A	379	SER
1	A	383	GLU
1	B	1	MET
1	B	9	ILE
1	B	104	ASP
1	B	112	PHE
1	B	114	LYS
1	B	185	SER
1	B	214	GLU
1	B	220	LYS
1	B	231	ILE
1	B	263	MET
1	B	272	LYS
1	B	295	ARG
1	B	303	LYS
1	B	319[A]	GLU
1	B	319[B]	GLU
1	B	322[A]	ILE
1	B	322[B]	ILE
1	B	358	THR
1	B	363	LEU
1	B	364	LYS
1	B	365	GLU
1	B	380	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 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	$\# Z > 2$
3	FEO	A	402	4,1	0,2,2	-	-	-		
3	FEO	B	402	4,1	0,2,2	-	-	-		

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.

No monomer is involved in short contacts.

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	392/410 (95%)	-0.16	8 (2%) 65 64	18, 32, 53, 65	2 (0%)
1	B	396/410 (96%)	0.17	14 (3%) 47 46	16, 38, 58, 77	8 (2%)
All	All	788/820 (96%)	0.00	22 (2%) 55 54	16, 35, 56, 77	10 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	318[A]	TYR	5.4
1	B	319[A]	GLU	5.1
1	B	363	LEU	4.5
1	B	362	LEU	4.2
1	B	321[A]	GLU	4.1
1	A	264	TYR	4.1
1	B	359	ALA	3.5
1	B	353	PRO	3.2
1	B	360	GLY	3.0
1	B	364	LYS	2.8
1	B	358	THR	2.8
1	A	351	TRP	2.8
1	B	349	HIS	2.7
1	A	358	THR	2.6
1	B	1	MET	2.5
1	B	264	TYR	2.5
1	A	348	VAL	2.4
1	A	1	MET	2.4
1	A	350	GLY	2.4
1	A	349	HIS	2.1
1	A	376	ILE	2.1
1	B	366	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	A	401	1/1	0.98	0.07	50,50,50,50	0
3	FEO	A	402	3/3	0.98	0.06	29,29,30,30	0
3	FEO	B	402	3/3	0.98	0.05	29,29,36,37	0
2	CL	A	403	1/1	0.99	0.06	26,26,26,26	0
2	CL	B	401	1/1	0.99	0.04	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.