



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:53 PM UTC

PDB ID : 3CHI / pdb_00003chi
Title : Crystal Structure of Di-iron AurF (Monoclinic form)
Authors : Zhang, H.; Brunzelle, J.S.; Nair, S.K.
Deposited on : 2008-03-09
Resolution : 2.10 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

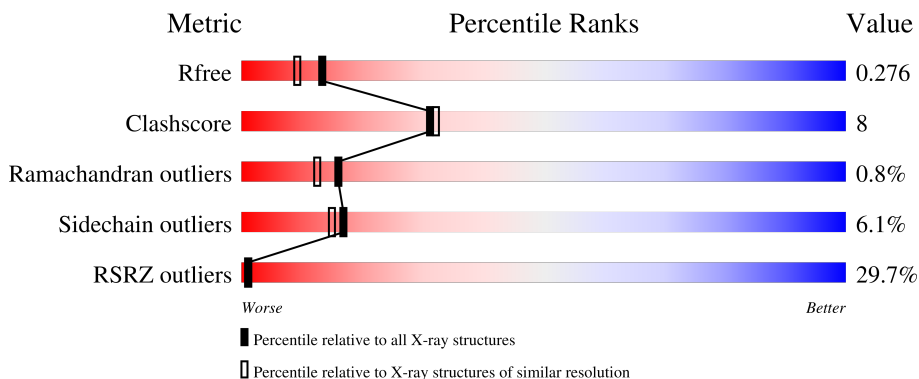
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	336	
1	B	336	

2 Entry composition [i](#)

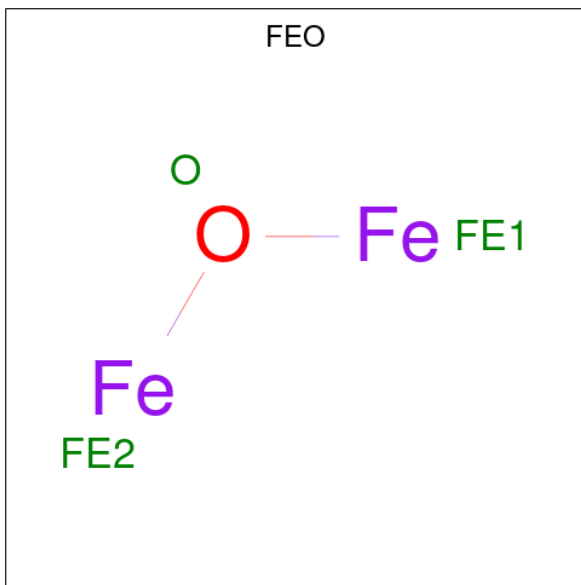
There are 3 unique types of molecules in this entry. The entry contains 5019 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 p-Aminobenzoate N-Oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	301	2404	1525	431	438	10	0	0	0
1	B	301	2404	1525	431	438	10	0	0	0

- Molecule 2 is MU-OXO-DIIRON (CCD ID: FEO) (formula: Fe₂O).



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

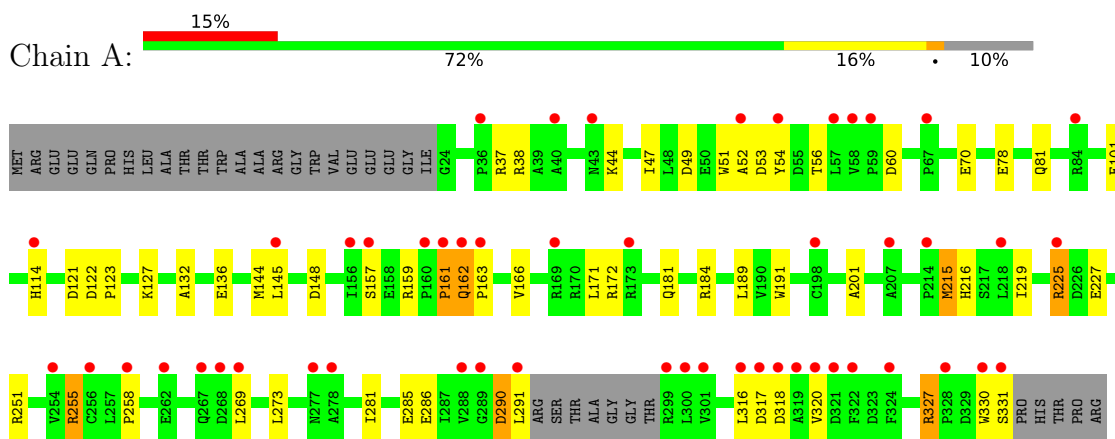
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	125	Total 125	O 125	0	0
3	B	80	Total 80	O 80	0	0

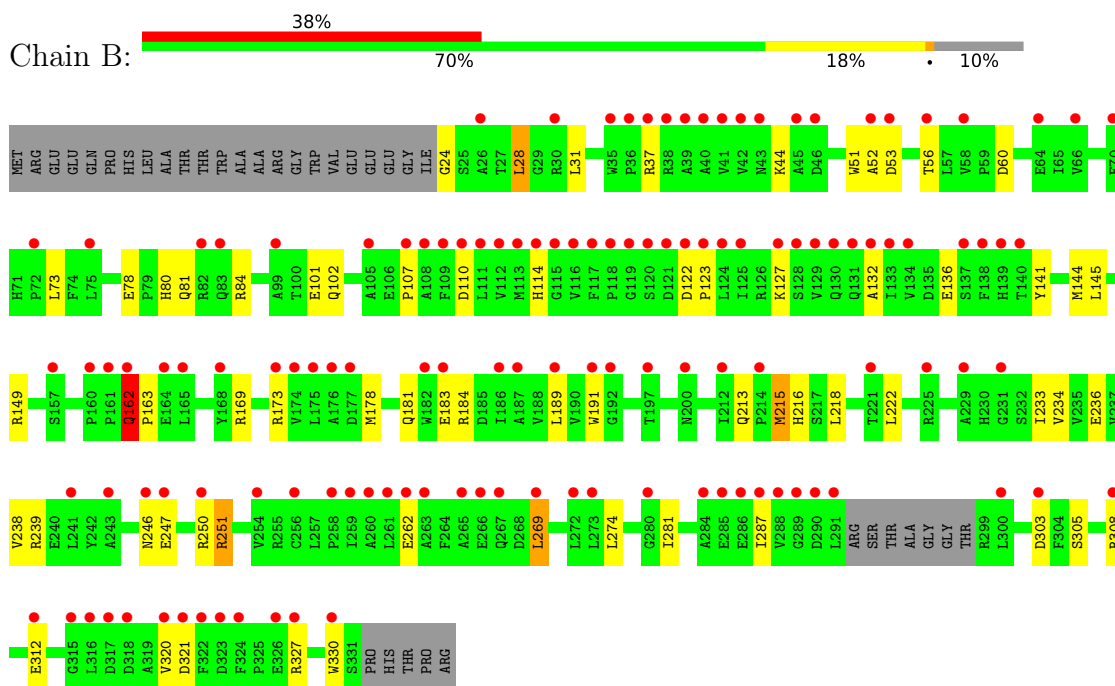
3 Residue-property plots [i](#)

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: p-Aminobenzoate N-Oxygenase



- Molecule 1: p-Aminobenzoate N-Oxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.42Å 73.32Å 74.69Å 90.00° 100.92° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 25.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.00-2.10) 99.5 (25.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.277 0.219 , 0.276	Depositor DCC
R_{free} test set	1802 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtrriage
Anisotropy	0.235	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5019	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4318e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.83	0/2454	0.98	1/3338 (0.0%)
1	B	0.82	4/2454 (0.2%)	1.03	4/3338 (0.1%)
All	All	0.82	4/4908 (0.1%)	1.00	5/6676 (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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	251	ARG	NE-CZ	7.17	1.41	1.33
1	B	321	ASP	C-N	6.85	1.42	1.33
1	B	251	ARG	CZ-NH2	6.50	1.42	1.33
1	B	321	ASP	CG-OD2	6.08	1.36	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	52	ALA	N-CA-C	6.57	119.00	111.11
1	A	162	GLN	N-CA-C	5.92	122.91	109.81
1	B	251	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	B	251	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	B	102	GLN	N-CA-C	5.05	117.68	111.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	162	GLN	Peptide

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	2404	0	2403	36	1
1	B	2404	0	2403	45	0
2	A	3	0	0	0	0
2	B	3	0	0	1	0
3	A	125	0	0	9	0
3	B	80	0	0	7	0
All	All	5019	0	4806	79	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ARG:HD3	3:A:719:HOH:O	1.70	0.89
1:B:78:GLU:H	1:B:81:GLN:HE21	1.20	0.85
1:A:148:ASP:OD2	3:A:721:HOH:O	1.95	0.83
1:A:38:ARG:O	1:A:225:ARG:NH2	2.12	0.83
1:B:181:GLN:NE2	1:B:184:ARG:HH11	1.76	0.82
1:A:49:ASP:HB3	3:A:708:HOH:O	1.80	0.80
1:B:169:ARG:O	1:B:173:ARG:HG3	1.82	0.80
1:A:101:GLU:OE2	1:A:136:GLU:OE1	2.04	0.74
1:A:78:GLU:H	1:A:81:GLN:HE21	1.32	0.74
1:B:78:GLU:H	1:B:81:GLN:NE2	1.85	0.73
1:B:101:GLU:OE2	2:B:501:FEO:FE2	1.41	0.73
1:A:144:MET:SD	3:B:672:HOH:O	2.48	0.72
1:A:37:ARG:HG2	3:A:716:HOH:O	1.92	0.69
1:B:262:GLU:HB3	3:B:656:HOH:O	1.93	0.68
1:B:162:GLN:HB3	1:B:163:PRO:HD3	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ARG:CD	3:A:719:HOH:O	2.32	0.64
1:A:37:ARG:NE	3:A:716:HOH:O	2.31	0.64
1:B:162:GLN:HB3	1:B:163:PRO:CD	2.27	0.62
1:A:145:LEU:HD22	1:B:127:LYS:HE3	1.80	0.62
1:B:73:LEU:HB3	3:B:614:HOH:O	2.01	0.61
1:B:31:LEU:HD13	1:B:233:ILE:HG13	1.83	0.61
1:B:81:GLN:HG2	1:B:84:ARG:HH11	1.66	0.61
1:A:51:TRP:CD1	1:A:215:MET:HE3	2.37	0.59
1:A:78:GLU:H	1:A:81:GLN:NE2	2.00	0.59
1:A:181:GLN:NE2	1:A:184:ARG:HH11	2.01	0.58
1:B:132:ALA:O	1:B:136:GLU:HG2	2.03	0.57
1:B:101:GLU:OE2	1:B:136:GLU:OE1	2.22	0.56
1:B:107:PRO:O	3:B:680:HOH:O	2.18	0.56
1:B:24:GLY:N	3:B:671:HOH:O	2.39	0.55
1:B:216:HIS:HE1	3:B:609:HOH:O	1.89	0.54
1:A:127:LYS:HE3	1:B:145:LEU:HD22	1.91	0.53
1:B:162:GLN:CB	1:B:163:PRO:HD3	2.38	0.53
1:B:181:GLN:HE21	1:B:184:ARG:HH11	1.53	0.53
1:B:269:LEU:H	1:B:269:LEU:CD2	2.22	0.53
1:A:38:ARG:HA	1:A:225:ARG:HH22	1.75	0.52
1:A:290:ASP:C	1:A:290:ASP:OD2	2.53	0.51
1:A:316:LEU:C	1:A:318:ASP:H	2.20	0.49
1:A:225:ARG:CZ	1:A:225:ARG:HB3	2.43	0.48
1:B:178:MET:SD	1:B:183:GLU:HG2	2.53	0.48
1:A:286:GLU:O	1:A:290:ASP:HB3	2.13	0.48
1:B:51:TRP:CD1	1:B:215:MET:HE3	2.49	0.48
1:A:227:GLU:HA	1:A:227:GLU:OE2	2.14	0.47
1:B:308:ARG:O	1:B:312:GLU:HG3	2.13	0.47
3:A:622:HOH:O	1:B:144:MET:HG3	2.14	0.47
1:B:80:HIS:O	1:B:84:ARG:HG3	2.16	0.46
1:B:246:ASN:O	1:B:250:ARG:HG2	2.16	0.46
1:B:234:VAL:O	1:B:238:VAL:HG23	2.14	0.46
1:B:269:LEU:H	1:B:269:LEU:HD23	1.81	0.46
1:B:44:LYS:HE3	1:B:218:LEU:HD21	1.98	0.45
1:B:303:ASP:HB2	1:B:330:TRP:CH2	2.51	0.45
1:B:51:TRP:CE2	1:B:215:MET:HG3	2.51	0.45
1:B:305:SER:OG	1:B:327:ARG:NE	2.49	0.45
1:A:78:GLU:N	1:A:81:GLN:HE21	2.09	0.44
1:B:149:ARG:HA	1:B:149:ARG:HD2	1.83	0.44
1:B:141:TYR:CZ	1:B:145:LEU:HD11	2.52	0.43
1:A:51:TRP:NE1	1:A:215:MET:HE3	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:TYR:HE1	1:A:56:THR:HG22	1.83	0.43
1:A:255:ARG:O	1:A:258:PRO:HD2	2.18	0.43
1:B:122:ASP:HA	1:B:123:PRO:HD3	1.87	0.43
1:B:287:ILE:HD11	3:B:614:HOH:O	2.16	0.43
1:A:201:ALA:HA	1:A:330:TRP:CZ2	2.54	0.43
1:B:236:GLU:CD	1:B:239:ARG:HH12	2.27	0.43
1:B:44:LYS:HG2	1:B:222:LEU:HD11	2.00	0.43
1:B:114:HIS:HD1	1:B:114:HIS:N	2.17	0.42
1:A:54:TYR:HD2	1:A:215:MET:HE1	1.84	0.42
1:B:110:ASP:O	1:B:114:HIS:ND1	2.51	0.42
1:B:213:GLN:NE2	1:B:215:MET:HE1	2.34	0.42
1:A:161:PRO:O	1:A:163:PRO:CD	2.67	0.42
1:B:247:GLU:HB3	1:B:251:ARG:NH2	2.34	0.42
1:A:60:ASP:O	1:A:216:HIS:HD2	2.03	0.42
1:A:285:GLU:H	1:A:285:GLU:CD	2.27	0.41
1:A:132:ALA:O	1:A:136:GLU:HG2	2.20	0.41
1:B:60:ASP:O	1:B:216:HIS:HD2	2.03	0.41
1:A:166:VAL:HG12	3:A:678:HOH:O	2.20	0.41
1:B:28:LEU:HD12	1:B:28:LEU:HA	1.97	0.41
1:A:47:ILE:HD11	1:A:219:ILE:HG13	2.04	0.40
1:A:121:ASP:CG	3:A:715:HOH:O	2.63	0.40
1:A:122:ASP:HA	1:A:123:PRO:HD3	1.94	0.40
1:A:327:ARG:HD3	1:A:331:SER:HB3	2.03	0.40

All (1) 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)
1:A:225:ARG:NH1	1:A:251:ARG:NH2[2_646]	1.90	0.30

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/336 (88%)	282 (95%)	11 (4%)	4 (1%)	9	6
1	B	297/336 (88%)	290 (98%)	6 (2%)	1 (0%)	36	36
All	All	594/672 (88%)	572 (96%)	17 (3%)	5 (1%)	16	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	B	162	GLN
1	A	52	ALA
1	A	317	ASP
1	A	161	PRO

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	253/281 (90%)	233 (92%)	20 (8%)	11	9
1	B	253/281 (90%)	242 (96%)	11 (4%)	26	27
All	All	506/562 (90%)	475 (94%)	31 (6%)	17	15

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LYS
1	A	53	ASP
1	A	70	GLU
1	A	114	HIS
1	A	157	SER
1	A	159	ARG
1	A	171	LEU
1	A	172	ARG
1	A	189	LEU
1	A	191	TRP
1	A	215	MET

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Mol	Chain	Res	Type
1	A	225	ARG
1	A	255	ARG
1	A	269	LEU
1	A	273	LEU
1	A	281	ILE
1	A	290	ASP
1	A	291	LEU
1	A	320	VAL
1	A	327	ARG
1	B	28	LEU
1	B	37	ARG
1	B	53	ASP
1	B	56	THR
1	B	189	LEU
1	B	191	TRP
1	B	215	MET
1	B	269	LEU
1	B	274	LEU
1	B	281	ILE
1	B	320	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	83	GLN
1	A	181	GLN
1	A	213	GLN
1	A	216	HIS
1	A	267	GLN
1	A	277	ASN
1	B	81	GLN
1	B	162	GLN
1	B	181	GLN
1	B	213	GLN
1	B	216	HIS
1	B	248	GLN
1	B	277	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FEO	A	501	1,3	0,2,2	-	-	-		
2	FEO	B	501	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FEO	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

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	301/336 (89%)	1.24	51 (16%) 4 4	19, 34, 55, 62	0
1	B	301/336 (89%)	1.93	128 (42%) 0 1	17, 34, 52, 59	0
All	All	602/672 (89%)	1.58	179 (29%) 1 1	17, 34, 53, 62	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	PRO	6.0
1	B	254	VAL	5.5
1	B	291	LEU	5.3
1	A	319	ALA	5.0
1	B	288	VAL	5.0
1	B	330	TRP	4.7
1	A	160	PRO	4.7
1	B	160	PRO	4.6
1	A	330	TRP	4.5
1	A	162	GLN	4.3
1	B	191	TRP	4.1
1	A	256	CYS	4.1
1	B	289	GLY	4.1
1	B	133	ILE	3.9
1	B	260	ALA	3.8
1	B	258	PRO	3.8
1	B	290	ASP	3.8
1	B	267	GLN	3.8
1	B	320	VAL	3.8
1	B	256	CYS	3.7
1	B	161	PRO	3.7
1	B	287	ILE	3.7
1	A	321	ASP	3.7
1	B	37	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	317	ASP	3.7
1	A	225	ARG	3.6
1	B	176	ALA	3.6
1	B	134	VAL	3.5
1	B	107	PRO	3.5
1	B	197	THR	3.4
1	A	318	ASP	3.4
1	B	265	ALA	3.4
1	B	56	THR	3.4
1	B	116	VAL	3.4
1	B	243	ALA	3.4
1	B	322	PHE	3.4
1	A	317	ASP	3.3
1	B	115	GLY	3.3
1	A	52	ALA	3.3
1	A	173	ARG	3.3
1	B	124	LEU	3.3
1	B	39	ALA	3.2
1	B	45	ALA	3.2
1	A	289	GLY	3.2
1	B	162	GLN	3.2
1	B	128	SER	3.2
1	B	129	VAL	3.1
1	A	328	PRO	3.1
1	B	285	GLU	3.1
1	B	139	HIS	3.1
1	B	120	SER	3.1
1	B	122	ASP	3.1
1	B	272	LEU	3.1
1	B	138	PHE	3.0
1	B	247	GLU	3.0
1	A	58	VAL	3.0
1	A	301	VAL	3.0
1	B	327	ARG	3.0
1	B	36	PRO	3.0
1	B	53	ASP	3.0
1	B	70	GLU	2.9
1	B	137	SER	2.9
1	B	246	ASN	2.9
1	A	291	LEU	2.9
1	B	83	GLN	2.9
1	B	99	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	263	ALA	2.9
1	B	318	ASP	2.9
1	B	324	PHE	2.9
1	B	262	GLU	2.8
1	A	300	LEU	2.8
1	B	269	LEU	2.8
1	A	288	VAL	2.8
1	B	58	VAL	2.8
1	B	127	LYS	2.8
1	B	119	GLY	2.8
1	B	26	ALA	2.8
1	B	132	ALA	2.8
1	B	118	PRO	2.8
1	A	169	ARG	2.8
1	B	41	VAL	2.8
1	B	114	HIS	2.7
1	B	165	LEU	2.7
1	B	300	LEU	2.7
1	B	130	GLN	2.7
1	B	43	ASN	2.7
1	A	145	LEU	2.7
1	B	174	VAL	2.7
1	B	117	PHE	2.6
1	A	214	PRO	2.6
1	A	156	ILE	2.6
1	B	250	ARG	2.6
1	B	123	PRO	2.6
1	B	189	LEU	2.6
1	B	112	VAL	2.6
1	B	231	GLY	2.6
1	A	67	PRO	2.6
1	B	177	ASP	2.6
1	A	316	LEU	2.6
1	B	109	PHE	2.5
1	B	164	GLU	2.5
1	B	266	GLU	2.5
1	B	259	ILE	2.5
1	B	35	TRP	2.5
1	B	42	VAL	2.5
1	B	280	GLY	2.5
1	B	284	ALA	2.5
1	B	241	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	192	GLY	2.5
1	A	254	VAL	2.4
1	B	321	ASP	2.4
1	B	323	ASP	2.4
1	B	214	PRO	2.4
1	B	30	ARG	2.4
1	B	38	ARG	2.4
1	B	131	GLN	2.4
1	B	66	VAL	2.4
1	B	157	SER	2.4
1	B	64	GLU	2.4
1	B	182	TRP	2.4
1	B	82	ARG	2.4
1	B	308	ARG	2.4
1	A	54	TYR	2.4
1	B	200	ASN	2.4
1	B	212	ILE	2.4
1	A	114	HIS	2.4
1	B	75	LEU	2.3
1	B	316	LEU	2.3
1	A	299	ARG	2.3
1	A	322	PHE	2.3
1	B	72	PRO	2.3
1	B	40	ALA	2.3
1	B	168	TYR	2.3
1	B	225	ARG	2.3
1	B	186	ILE	2.3
1	A	57	LEU	2.3
1	A	43	ASN	2.3
1	A	84	ARG	2.3
1	B	187	ALA	2.3
1	B	303	ASP	2.3
1	A	218	LEU	2.3
1	B	286	GLU	2.2
1	B	125	ILE	2.2
1	A	277	ASN	2.2
1	B	173	ARG	2.2
1	B	111	LEU	2.2
1	B	261	LEU	2.2
1	B	312	GLU	2.2
1	A	320	VAL	2.2
1	B	315	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	40	ALA	2.2
1	A	262	GLU	2.2
1	B	108	ALA	2.2
1	A	269	LEU	2.2
1	B	113	MET	2.2
1	B	121	ASP	2.2
1	B	105	ALA	2.2
1	A	36	PRO	2.1
1	A	163	PRO	2.1
1	B	52	ALA	2.1
1	B	326	GLU	2.1
1	B	140	THR	2.1
1	A	324	PHE	2.1
1	A	157	SER	2.1
1	A	331	SER	2.1
1	B	273	LEU	2.1
1	A	198	CYS	2.1
1	B	110	ASP	2.1
1	A	207	ALA	2.1
1	B	175	LEU	2.0
1	A	268	ASP	2.0
1	B	221	THR	2.0
1	B	183	GLU	2.0
1	A	278	ALA	2.0
1	B	229	ALA	2.0
1	A	267	GLN	2.0
1	B	46	ASP	2.0
1	A	59	PRO	2.0
1	A	258	PRO	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(Å ²)	Q<0.9
2	FEO	A	501	3/3	0.99	0.12	19,19,20,22	0
2	FEO	B	501	3/3	0.99	0.10	26,26,29,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.