



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:52 AM GMT

PDB ID : 3CHT
Title : Crystal Structure of Di-iron AurF with partially bound Ligand
Authors : Zhang, H.; Brunzelle, J.S.; Nair, S.K.
Deposited on : 2008-03-10
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

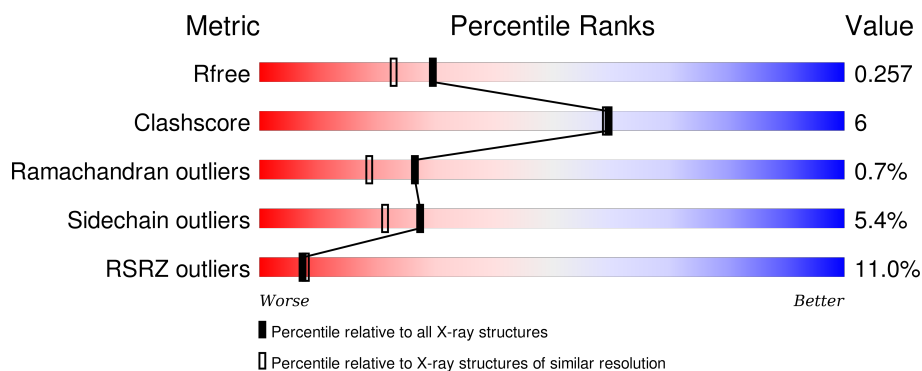
1 Overall quality at a glance

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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	

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	4NB	A	502	-	-	-	X

2 Entry composition [i](#)

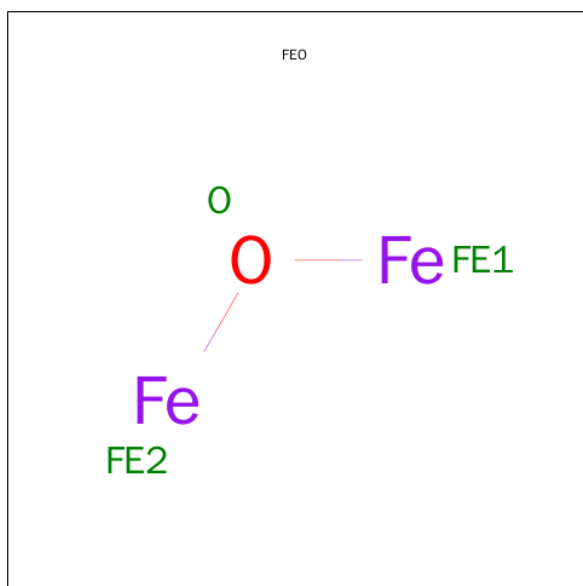
There are 4 unique types of molecules in this entry. The entry contains 5040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

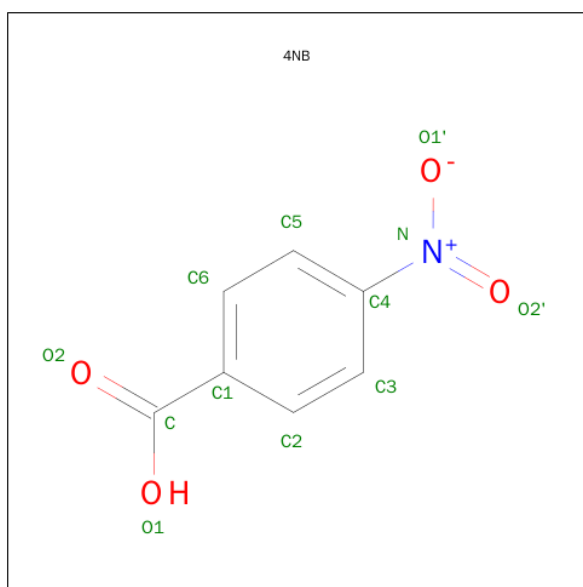
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2404	1525	431	438	10			
1	B	300	Total	C	N	O	S	0	0	0
			2388	1517	427	434	10			

- Molecule 2 is MU-OXO-DIIRON (three-letter code: FEO) (formula: Fe₂O).



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

- Molecule 3 is 4-NITROBENZOIC ACID (three-letter code: 4NB) (formula: C₇H₅NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	7	1	4		

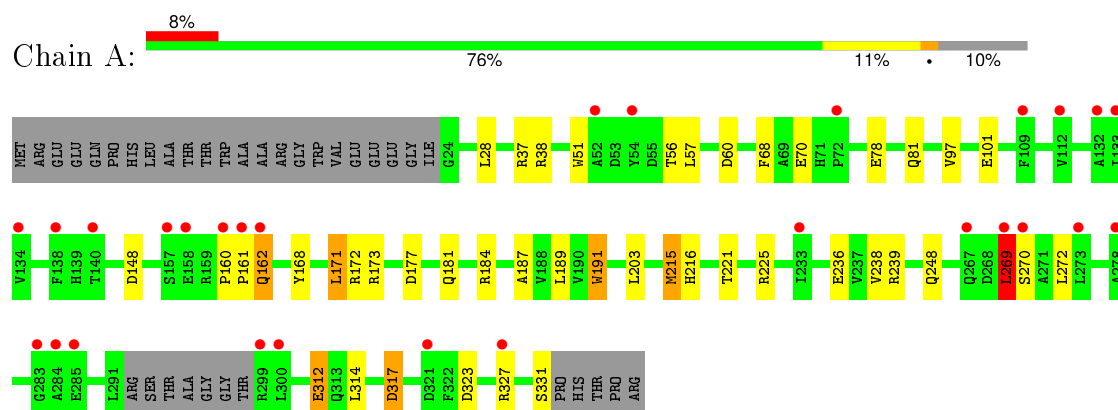
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total	O	0	0
			139	139		
4	B	91	Total	O	0	0
			91	91		

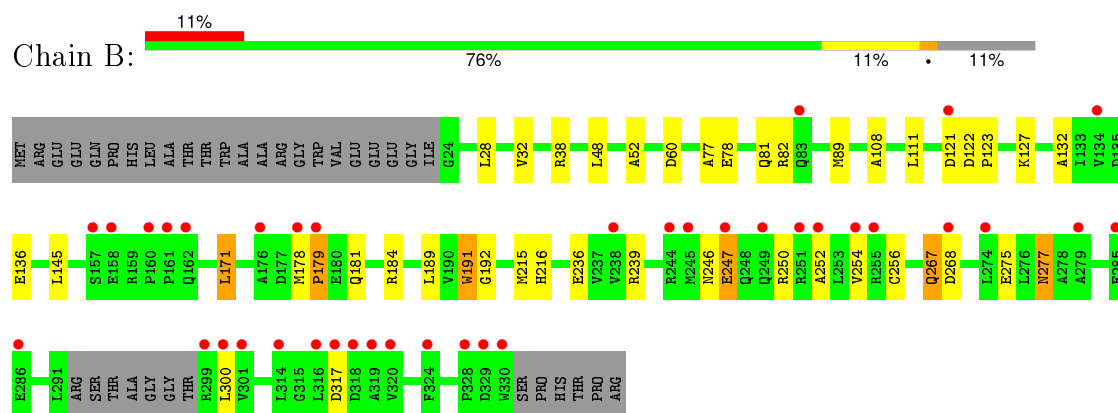
3 Residue-property plots

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.

- Molecule 1: p-Aminobenzoate N-Oxygenase



- Molecule 1: p-Aminobenzoate N-Oxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.14Å 77.19Å 140.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 44.09 – 1.99	Depositor EDS
% Data completeness (in resolution range)	96.6 (25.00-2.00) 95.9 (44.09-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.203 , 0.256 0.204 , 0.257	Depositor DCC
R_{free} test set	2129 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 42121 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5040	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: FEO, 4NB

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	0.54	0/2454	0.63	2/3338 (0.1%)
1	B	0.58	4/2438 (0.2%)	0.61	1/3318 (0.0%)
All	All	0.56	4/4892 (0.1%)	0.62	3/6656 (0.0%)

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	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	247	GLU	C-N	8.02	1.52	1.34
1	B	246	ASN	CG-OD1	7.79	1.41	1.24
1	B	247	GLU	C-O	6.64	1.35	1.23
1	B	246	ASN	CG-ND2	6.53	1.49	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	269	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	38	ARG	NE-CZ-NH1	-5.22	117.69	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	GLN	Peptide
1	B	178	MET	Peptide

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	2404	0	2403	30	0
1	B	2388	0	2383	24	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	12	0	4	3	0
4	A	139	0	0	8	0
4	B	91	0	0	2	0
All	All	5040	0	4790	55	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 6.

All (55) 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:187:ALA:HB1	4:A:637:HOH:O	1.16	1.25
3:A:502:4NB:H2	4:A:599:HOH:O	1.84	0.77
1:A:323:ASP:HB2	4:A:630:HOH:O	1.84	0.76
1:A:78:GLU:H	1:A:81:GLN:HE21	1.33	0.74
1:B:78:GLU:H	1:B:81:GLN:HE21	1.35	0.74
1:A:168:TYR:CE1	1:A:172:ARG:HD2	2.27	0.69
1:B:267:GLN:HA	1:B:267:GLN:HE21	1.57	0.68
1:A:168:TYR:CE1	1:A:172:ARG:CD	2.78	0.65
1:A:225:ARG:HD2	4:A:567:HOH:O	1.95	0.65
1:A:225:ARG:NH2	4:A:639:HOH:O	2.00	0.63
1:A:68:PHE:HE2	1:A:272:LEU:HD12	1.65	0.60
1:B:48:LEU:HD13	1:B:145:LEU:HD22	1.84	0.59
1:B:78:GLU:H	1:B:81:GLN:NE2	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HD22	3:A:502:4NB:H6	1.89	0.55
1:A:68:PHE:CE2	1:A:272:LEU:HD12	2.41	0.54
1:A:148:ASP:OD2	4:A:636:HOH:O	2.18	0.53
1:A:221:THR:O	1:A:225:ARG:HG3	2.09	0.53
1:A:168:TYR:CE1	1:A:172:ARG:HD3	2.44	0.52
1:B:32:VAL:HG11	1:B:127:LYS:HE2	1.92	0.52
1:A:168:TYR:CZ	1:A:172:ARG:HD2	2.45	0.51
1:A:37:ARG:NH1	4:A:561:HOH:O	2.43	0.51
1:B:181:GLN:NE2	1:B:184:ARG:HH11	2.09	0.51
1:A:78:GLU:H	1:A:81:GLN:NE2	2.06	0.50
1:A:51:TRP:CE2	1:A:215:MET:HG3	2.46	0.50
1:B:267:GLN:NE2	1:B:268:ASP:H	2.10	0.49
1:B:77:ALA:O	1:B:82:ARG:NH2	2.46	0.48
1:A:312:GLU:HG3	1:A:317:ASP:OD1	2.13	0.48
1:B:267:GLN:HE21	1:B:268:ASP:H	1.61	0.48
1:B:267:GLN:CA	1:B:267:GLN:HE21	2.25	0.48
1:B:171:LEU:HG	1:B:191:TRP:CG	2.49	0.48
1:B:179:PRO:HA	4:B:553:HOH:O	2.14	0.47
1:A:216:HIS:HE1	4:A:521:HOH:O	1.97	0.47
1:A:269:LEU:CD2	1:A:269:LEU:H	2.28	0.47
1:A:51:TRP:CD1	1:A:215:MET:HE3	2.50	0.47
1:A:238:VAL:HG12	1:A:314:LEU:HD21	1.97	0.47
1:B:60:ASP:O	1:B:216:HIS:HD2	1.98	0.46
1:B:179:PRO:HD3	4:B:541:HOH:O	2.16	0.45
1:B:252:ALA:O	1:B:256:CYS:HB2	2.16	0.45
1:A:181:GLN:NE2	1:A:184:ARG:HH11	2.15	0.45
1:B:89:MET:HG3	1:B:275:GLU:HG3	1.98	0.44
1:A:171:LEU:HG	1:A:191:TRP:CG	2.52	0.44
1:A:272:LEU:HD13	1:A:272:LEU:HA	1.93	0.43
1:B:171:LEU:HG	1:B:191:TRP:CD1	2.54	0.43
1:B:132:ALA:O	1:B:136:GLU:HG2	2.19	0.43
1:A:97:VAL:O	1:A:101:GLU:HG2	2.20	0.42
1:A:203:LEU:HB2	3:A:502:4NB:O1	2.20	0.42
1:B:122:ASP:HA	1:B:123:PRO:HD3	1.94	0.42
1:A:236:GLU:CD	1:A:239:ARG:HH12	2.23	0.41
1:A:160:PRO:HA	1:A:161:PRO:HD3	1.86	0.41
1:B:111:LEU:HA	1:B:111:LEU:HD23	1.91	0.41
1:B:108:ALA:HB2	1:B:192:GLY:HA3	2.02	0.41
1:B:277:ASN:HD22	1:B:277:ASN:HA	1.62	0.41
1:B:236:GLU:CD	1:B:239:ARG:HH12	2.23	0.41
1:A:60:ASP:O	1:A:216:HIS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ARG:O	1:B:254:VAL:HG23	2.21	0.41

There are no symmetry-related clashes.

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%)	289 (97%)	7 (2%)	1 (0%)	46	41
1	B	296/336 (88%)	286 (97%)	7 (2%)	3 (1%)	19	11
All	All	593/672 (88%)	575 (97%)	14 (2%)	4 (1%)	26	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	52	ALA
1	B	179	PRO
1	A	162	GLN
1	B	300	LEU

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%)	236 (93%)	17 (7%)	20	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	250/281 (89%)	240 (96%)	10 (4%)	38	33
All	All	503/562 (90%)	476 (95%)	27 (5%)	27	21

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	56	THR
1	A	57	LEU
1	A	70	GLU
1	A	171	LEU
1	A	173	ARG
1	A	177	ASP
1	A	189	LEU
1	A	191	TRP
1	A	215	MET
1	A	248	GLN
1	A	269	LEU
1	A	270	SER
1	A	312	GLU
1	A	317	ASP
1	A	327	ARG
1	A	331	SER
1	B	28	LEU
1	B	121	ASP
1	B	171	LEU
1	B	189	LEU
1	B	191	TRP
1	B	215	MET
1	B	247	GLU
1	B	267	GLN
1	B	277	ASN
1	B	317	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	181	GLN
1	A	213	GLN
1	A	216	HIS

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Mol	Chain	Res	Type
1	A	248	GLN
1	A	277	ASN
1	B	81	GLN
1	B	181	GLN
1	B	213	GLN
1	B	216	HIS
1	B	267	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 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	0,2,2	0.00	-	0,1,1	0.00	-
3	4NB	A	502	-	7,12,12	0.36	0	11,16,16	1.19	1 (9%)
2	FEO	B	501	1	0,2,2	0.00	-	0,1,1	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	FEO	A	501	1	-	0/0/0/0	0/0/0/0
3	4NB	A	502	-	-	0/4/8/8	0/1/1/1
2	FEO	B	501	1	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	4NB	C5-C4-N	2.04	121.13	119.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	4NB	3	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%)	0.90	28 (9%) 11 11	27, 40, 56, 65	0
1	B	300/336 (89%)	0.92	38 (12%) 5 5	29, 39, 55, 64	0
All	All	601/672 (89%)	0.91	66 (10%) 7 8	27, 40, 55, 65	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	GLN	7.4
1	A	299	ARG	6.6
1	B	320	VAL	6.0
1	B	299	ARG	5.0
1	B	301	VAL	4.7
1	A	161	PRO	4.6
1	B	328	PRO	4.5
1	A	52	ALA	4.5
1	A	72	PRO	4.5
1	B	329	ASP	4.4
1	B	319	ALA	4.1
1	B	245	MET	4.1
1	B	157	SER	4.1
1	B	121	ASP	4.0
1	A	157	SER	3.9
1	B	247	GLU	3.9
1	B	161	PRO	3.8
1	B	318	ASP	3.8
1	B	314	LEU	3.6
1	A	327	ARG	3.5
1	B	158	GLU	3.4
1	B	179	PRO	3.4
1	B	274	LEU	3.4
1	B	255	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	252	ALA	3.3
1	B	251	ARG	3.2
1	A	54	TYR	3.2
1	B	249	GLN	3.2
1	B	316	LEU	3.2
1	A	283	GLY	3.1
1	A	278	ALA	3.0
1	B	300	LEU	3.0
1	B	268	ASP	2.9
1	A	273	LEU	2.9
1	A	284	ALA	2.8
1	B	162	GLN	2.8
1	A	269	LEU	2.8
1	A	160	PRO	2.6
1	A	133	ILE	2.5
1	B	134	VAL	2.5
1	A	132	ALA	2.5
1	B	285	GLU	2.5
1	A	300	LEU	2.5
1	A	270	SER	2.4
1	A	285	GLU	2.4
1	A	158	GLU	2.4
1	B	279	ALA	2.3
1	B	238	VAL	2.3
1	B	160	PRO	2.3
1	B	83	GLN	2.3
1	B	330	TRP	2.3
1	B	176	ALA	2.2
1	B	324	PHE	2.2
1	B	244	ARG	2.2
1	A	109	PHE	2.2
1	A	138	PHE	2.2
1	B	317	ASP	2.2
1	A	267	GLN	2.1
1	A	321	ASP	2.1
1	A	134	VAL	2.1
1	A	140	THR	2.1
1	B	254	VAL	2.1
1	A	233	ILE	2.1
1	B	178	MET	2.1
1	A	112	VAL	2.1
1	B	286	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	4NB	A	502	12/12	0.73	0.28	6.21	62,64,65,65	0
2	FEO	A	501	3/3	1.00	0.04	-6.55	25,25,25,26	0
2	FEO	B	501	3/3	0.99	0.03	-6.58	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.