Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 03:27 PM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

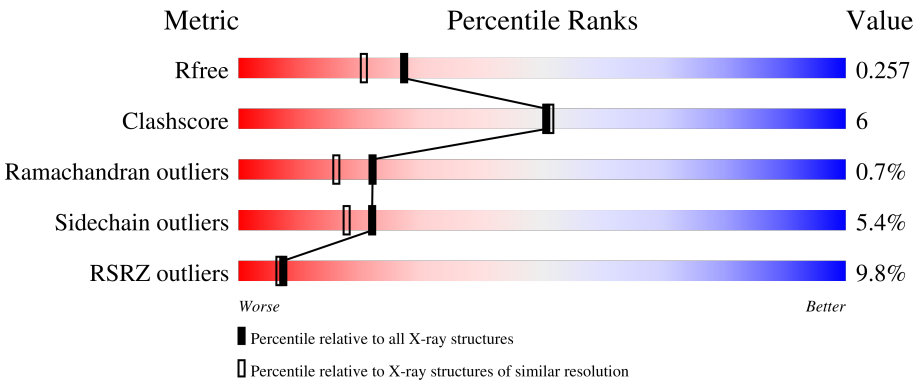
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	7%, 76%, 11%, •, 10%
1	B	336	10%, 76%, 11%, •, 11%

2 Entry composition (i)

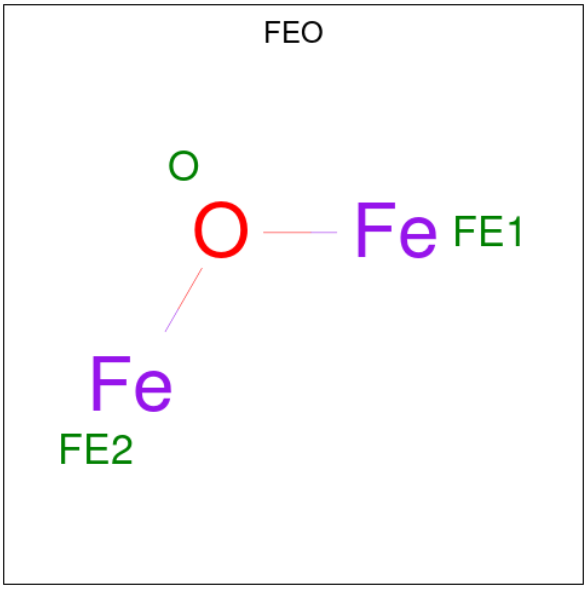
There are 4 unique types of molecules in this entry. The entry contains 5040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

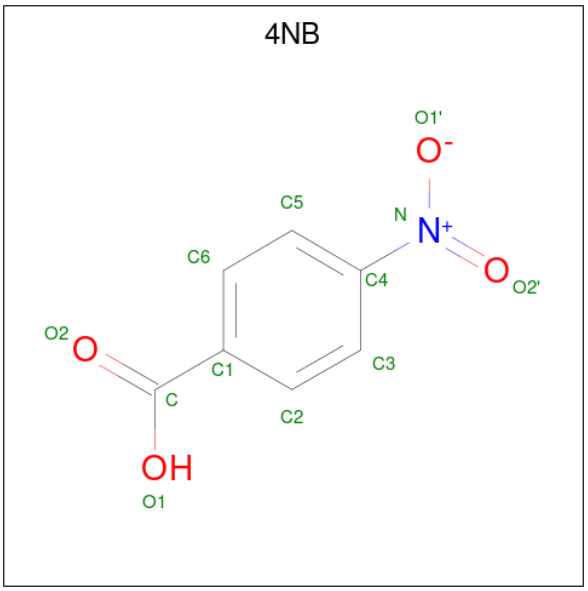
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	301	2404	1525	431	438	10	0	0	0
1	B	300	2388	1517	427	434	10	0	0	0

- Molecule 2 is MU-OXO-DIIRON (three-letter code: FEO) (formula: Fe_2O).



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 4-NITROBENZOIC ACID (three-letter code: 4NB) (formula: $C_7H_5NO_4$).



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

- Molecule 4 is water.

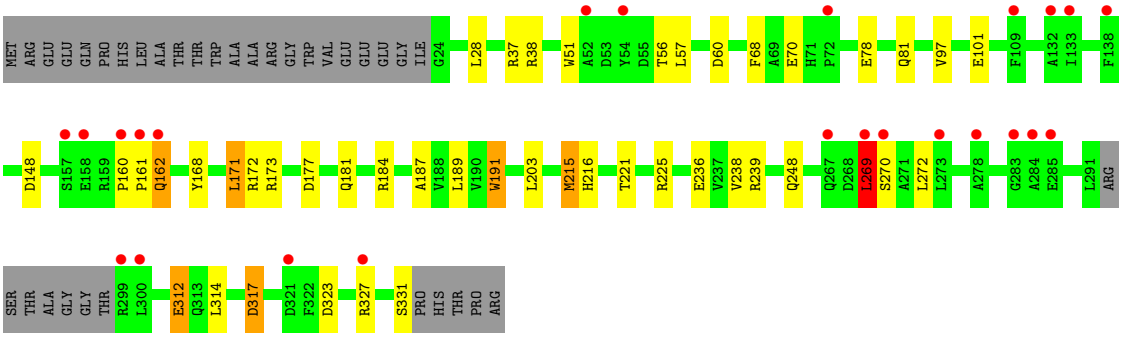
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	139	139	139	0	0
			Total	O		
4	B	91	91	91	0	0

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.

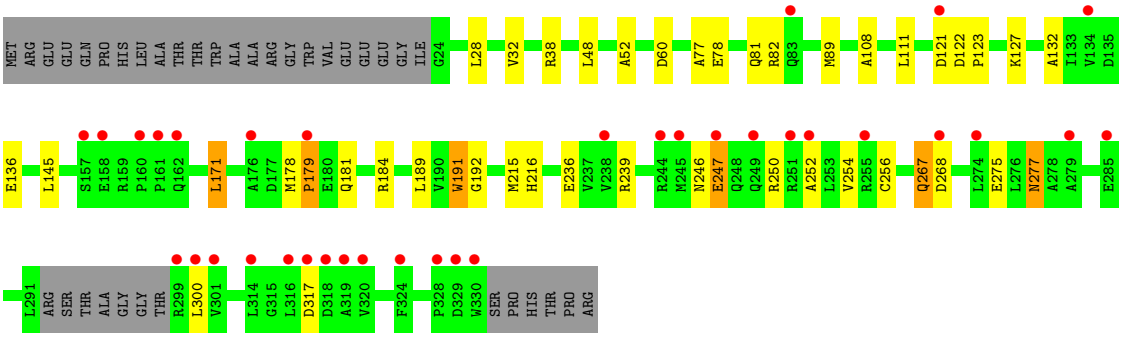
- Molecule 1: p-Aminobenzoate N-Oxygenase

Chain A:



- Molecule 1: p-Aminobenzoate N-Oxygenase

Chain B:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	2135 reflections (5.07%)	wwPDB-VP
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
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 4NB, 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	0.54	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(^{o})	Ideal(^{o})
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 (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	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:HE21	1:B:267:GLN:HA	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

Continued on next page...

Continued from previous page...

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:HE21	1:B:267:GLN:CA	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:H	1:A:269:LEU:CD2	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:160:PRO:HA	1:A:161:PRO:HD3	1.86	0.41
1:A:236:GLU:CD	1:A:239:ARG:HH12	2.23	0.41
1:B:111:LEU:HD23	1:B:111:LEU:HA	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

Continued on next page...

Continued from previous page...

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%)	41 37
1	B	296/336 (88%)	286 (97%)	7 (2%)	3 (1%)	15 9
All	All	593/672 (88%)	575 (97%)	14 (2%)	4 (1%)	22 16

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%)	16 11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	250/281 (89%)	240 (96%)	10 (4%)	31	29
All	All	503/562 (90%)	476 (95%)	27 (5%)	22	18

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

Sometimes 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

Continued on next page...

Continued from previous page...

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 monosaccharides 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	$\#\|Z\| > 2$
3	4NB	A	502	-	12,12,12	1.13	2 (16%)	14,16,16	1.07	1 (7%)
2	FEO	A	501	1	0,2,2	-	-	-		
2	FEO	B	501	1	0,2,2	-	-	-		

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
3	4NB	A	502	-	-	3/6/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	4NB	C4-N	-2.29	1.39	1.45
3	A	502	4NB	O1-C	-2.10	1.24	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	4NB	C5-C4-N	2.06	121.13	119.34

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	4NB	C3-C4-N-O2'
3	A	502	4NB	C5-C4-N-O2'
3	A	502	4NB	O1-C-C1-C2

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.81	24 (7%) 12 11	27, 40, 56, 65	0
1	B	300/336 (89%)	0.84	35 (11%) 4 4	29, 39, 55, 64	0
All	All	601/672 (89%)	0.83	59 (9%) 7 7	27, 40, 55, 65	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	GLN	7.2
1	A	299	ARG	6.5
1	B	320	VAL	5.6
1	B	299	ARG	4.8
1	A	161	PRO	4.4
1	B	301	VAL	4.4
1	B	328	PRO	4.4
1	A	72	PRO	4.3
1	A	52	ALA	4.3
1	B	329	ASP	4.2
1	B	245	MET	4.0
1	B	319	ALA	3.9
1	B	157	SER	3.9
1	B	121	ASP	3.8
1	B	247	GLU	3.7
1	A	157	SER	3.7
1	B	161	PRO	3.7
1	B	318	ASP	3.6
1	B	314	LEU	3.4
1	A	327	ARG	3.4
1	B	158	GLU	3.3
1	B	255	ARG	3.3
1	B	179	PRO	3.3
1	B	274	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	252	ALA	3.1
1	B	249	GLN	3.1
1	B	251	ARG	3.1
1	A	54	TYR	3.0
1	A	283	GLY	3.0
1	B	316	LEU	3.0
1	B	300	LEU	2.8
1	A	278	ALA	2.8
1	B	268	ASP	2.8
1	A	273	LEU	2.7
1	B	162	GLN	2.7
1	A	284	ALA	2.7
1	A	269	LEU	2.6
1	A	160	PRO	2.5
1	B	285	GLU	2.4
1	A	300	LEU	2.3
1	A	285	GLU	2.3
1	A	133	ILE	2.3
1	A	132	ALA	2.3
1	A	158	GLU	2.3
1	A	270	SER	2.3
1	B	134	VAL	2.3
1	B	83	GLN	2.2
1	B	160	PRO	2.2
1	B	279	ALA	2.2
1	B	238	VAL	2.2
1	B	330	TRP	2.1
1	B	244	ARG	2.1
1	A	267	GLN	2.1
1	B	176	ALA	2.1
1	B	324	PHE	2.1
1	B	317	ASP	2.0
1	A	321	ASP	2.0
1	A	109	PHE	2.0
1	A	138	PHE	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 monosaccharides 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
3	4NB	A	502	12/12	0.73	0.28	62,64,65,65	0
2	FEO	B	501	3/3	0.99	0.03	30,30,30,30	0
2	FEO	A	501	3/3	1.00	0.04	25,25,25,26	0

6.5 Other polymers (i)

There are no such residues in this entry.