Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2023 – 01:55 PM EDT

PDB ID	:	4RM3
Title	:	Crystal structure of a benzoate coenzyme A ligase with 2-Furoic acid
Authors	:	Strom, S.; Nosrati, M.; Thornburg, C.; Walker, K.D.; Geiger, J.H.
Deposited on	:	2014-10-18
Resolution	:	1.76 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:

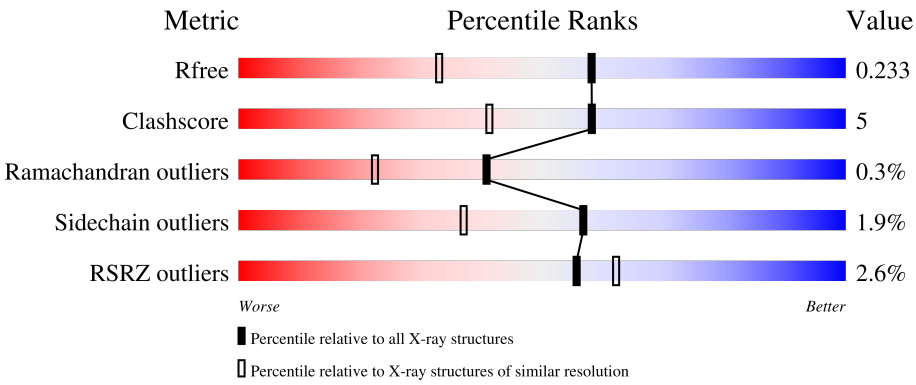
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

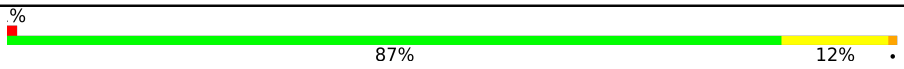
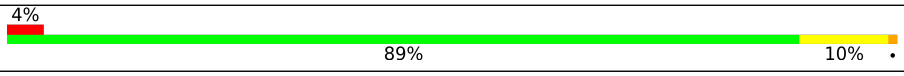
The reported resolution of this entry is 1.76 Å.

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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	520	
1	B	520	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8486 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.

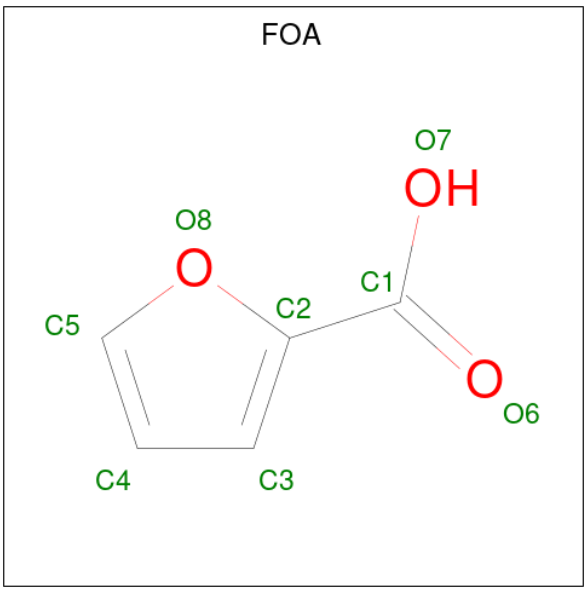
- Molecule 1 is a protein called Benzoate-coenzyme A ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	518	3940	2521	682	727	10	0	1	0
1	B	519	3898	2499	669	720	10	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ALA	THR	conflict	UNP Q93TK0
A	341	ASP	GLY	conflict	UNP Q93TK0
A	524	GLY	-	expression tag	UNP Q93TK0
B	83	ALA	THR	conflict	UNP Q93TK0
B	341	ASP	GLY	conflict	UNP Q93TK0
B	524	GLY	-	expression tag	UNP Q93TK0

- Molecule 2 is 2-FUROIC ACID (three-letter code: FOA) (formula: $C_5H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	8	5	3	0	0
			Total	C	O		
2	B	1	8	5	3	0	0

- Molecule 3 is water.

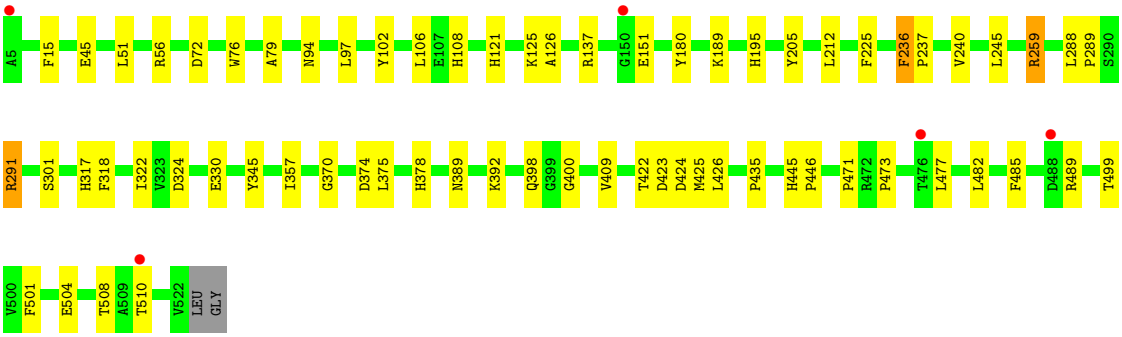
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	324	324	324	0	0
			Total	O		
3	B	308	308	308	0	0

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.

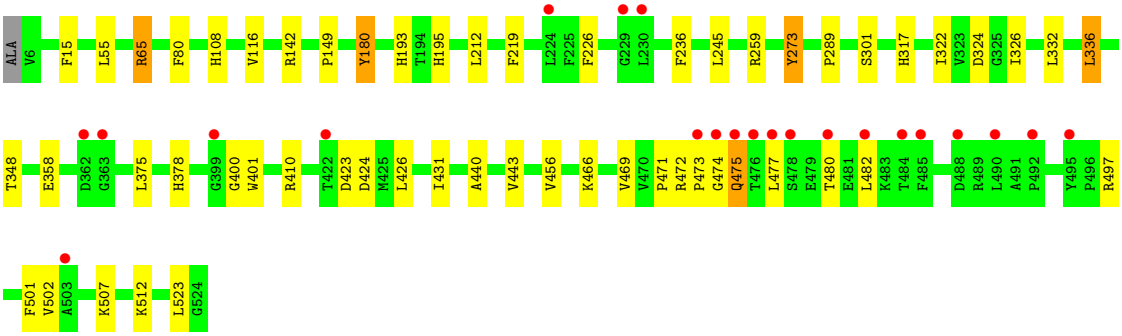
• Molecule 1: Benzoate-coenzyme A ligase

Chain A:



• Molecule 1: Benzoate-coenzyme A ligase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.64Å 95.11Å 95.33Å 90.00° 104.88° 90.00°	Depositor
Resolution (Å)	33.09 – 1.76 33.09 – 1.76	Depositor EDS
% Data completeness (in resolution range)	98.5 (33.09-1.76) 98.5 (33.09-1.76)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.184 , 0.229 0.186 , 0.233	Depositor DCC
R_{free} test set	4918 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8486	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: FOA

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	1.19	8/4048 (0.2%)	1.02	5/5520 (0.1%)
1	B	1.19	3/4009 (0.1%)	1.00	5/5476 (0.1%)
All	All	1.19	11/8057 (0.1%)	1.01	10/10996 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	330	GLU	CG-CD	5.82	1.60	1.51
1	B	116	VAL	CB-CG1	5.45	1.64	1.52
1	A	425	MET	CB-CG	5.33	1.68	1.51
1	A	345	TYR	CD2-CE2	5.33	1.47	1.39
1	A	504	GLU	CD-OE2	-5.32	1.19	1.25
1	B	80	PHE	CE1-CZ	5.32	1.47	1.37
1	A	205	TYR	CE1-CZ	5.29	1.45	1.38
1	B	180	TYR	CD1-CE1	5.11	1.47	1.39
1	A	45	GLU	CB-CG	5.08	1.61	1.52
1	A	240	VAL	CB-CG2	5.04	1.63	1.52
1	A	236	PHE	CD1-CE1	5.01	1.49	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	374	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	56	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	55	LEU	CB-CG-CD1	-5.35	101.91	111.00
1	B	375	LEU	CB-CG-CD1	-5.34	101.93	111.00
1	A	288	LEU	CB-CG-CD2	-5.29	102.00	111.00
1	A	106	LEU	CB-CG-CD1	-5.18	102.20	111.00
1	B	336	LEU	CB-CG-CD1	-5.08	102.36	111.00
1	A	72	ASP	CB-CG-OD2	-5.07	113.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	273	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	B	219	PHE	CB-CG-CD2	-5.03	117.28	120.80

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	3940	0	3873	40	0
1	B	3898	0	3789	37	0
2	A	8	0	3	0	0
2	B	8	0	3	0	0
3	A	324	0	0	3	0
3	B	308	0	0	6	0
All	All	8486	0	7668	74	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 (74) 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:245:LEU:HD21	1:A:259:ARG:HG2	1.35	1.07
1:A:426:LEU:HD11	1:A:435:PRO:HG3	1.38	1.05
1:A:489:ARG:HD3	3:A:1331:HOH:O	1.58	1.02
1:A:510:THR:HG21	3:A:1387:HOH:O	1.70	0.92
1:A:15:PHE:H	1:A:195:HIS:HD2	1.19	0.89
1:B:15:PHE:H	1:B:195:HIS:HD2	1.22	0.86
1:A:426:LEU:N	1:A:426:LEU:HD12	1.94	0.82
1:A:245:LEU:HD21	1:A:259:ARG:CG	2.12	0.79
1:A:245:LEU:CD2	1:A:259:ARG:HG2	2.19	0.70
1:B:456:VAL:HG21	1:B:466:LYS:HD3	1.74	0.69
1:B:348[B]:THR:HG23	3:B:1200:HOH:O	1.94	0.67
1:B:108:HIS:HD2	1:B:180:TYR:OH	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PHE:H	1:A:195:HIS:CD2	2.10	0.64
1:B:497:ARG:HB3	3:B:1166:HOH:O	1.98	0.62
1:B:326:ILE:HG22	1:B:348[A]:THR:HG21	1.82	0.61
1:B:289:PRO:O	1:B:317:HIS:HE1	1.83	0.61
1:A:426:LEU:CD1	1:A:435:PRO:HG3	2.23	0.61
1:A:510:THR:HG23	1:B:149:PRO:HG3	1.84	0.60
1:A:195:HIS:HE1	3:A:1246:HOH:O	1.85	0.60
1:B:15:PHE:H	1:B:195:HIS:CD2	2.10	0.60
1:A:108:HIS:HD2	1:A:180:TYR:OH	1.87	0.57
1:B:65:ARG:N	1:B:65:ARG:HD3	2.20	0.57
1:B:423:ASP:O	1:B:424:ASP:CB	2.53	0.56
1:B:456:VAL:HG21	1:B:466:LYS:CD	2.36	0.56
1:B:472:ARG:C	1:B:474:GLY:H	2.09	0.56
1:A:389:ASN:ND2	1:A:392:LYS:HD2	2.23	0.54
1:A:426:LEU:HD11	1:A:435:PRO:CG	2.27	0.54
1:B:348[B]:THR:HG22	3:B:1360:HOH:O	2.08	0.53
1:A:189:LYS:HD3	1:A:392:LYS:HD3	1.90	0.53
1:B:226:PHE:CE1	1:B:431:ILE:HG12	2.43	0.53
1:B:477:LEU:HD11	1:B:482:LEU:HD13	1.90	0.52
1:A:357:ILE:HG23	1:A:375:LEU:CD1	2.40	0.52
1:B:226:PHE:HE1	1:B:431:ILE:HG12	1.74	0.52
1:A:301:SER:HB2	1:A:322:ILE:CG2	2.40	0.51
1:B:245:LEU:HD21	1:B:259:ARG:HG2	1.92	0.51
1:A:97:LEU:HB2	1:A:102:TYR:CZ	2.45	0.51
1:B:482:LEU:CA	3:B:1397:HOH:O	2.59	0.51
1:B:480:THR:C	1:B:482:LEU:H	2.14	0.51
1:A:485:PHE:O	1:A:489:ARG:HG2	2.11	0.51
1:A:121:HIS:NE2	1:A:151:GLU:OE2	2.34	0.50
1:A:426:LEU:N	1:A:426:LEU:CD1	2.70	0.50
1:A:126:ALA:HA	1:B:440:ALA:HB1	1.94	0.49
1:B:469:VAL:O	1:B:471:PRO:HD3	2.13	0.48
1:B:301:SER:HB2	1:B:322:ILE:CG2	2.43	0.48
1:B:477:LEU:HD23	1:B:501:PHE:CE1	2.48	0.48
1:A:94:ASN:HA	1:A:225:PHE:CD1	2.49	0.48
1:A:289:PRO:O	1:A:317:HIS:HE1	1.97	0.48
1:B:502:VAL:HG11	1:B:523:LEU:HD13	1.96	0.47
1:A:508:THR:OG1	1:A:510:THR:HG22	2.14	0.47
1:A:482:LEU:HD23	1:A:499:THR:HG21	1.96	0.47
1:A:236:PHE:HB2	1:A:237:PRO:HD3	1.97	0.46
1:B:477:LEU:CD2	1:B:501:PHE:CE1	2.99	0.45
1:A:212:LEU:HD12	1:A:236:PHE:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:PRO:HG3	1:A:501:PHE:HD1	1.82	0.45
1:A:51:LEU:CD2	1:A:79:ALA:HA	2.46	0.45
1:B:193:HIS:CE1	1:B:332:LEU:HB2	2.51	0.45
1:B:378:HIS:HD2	1:B:400:GLY:O	2.00	0.45
1:A:357:ILE:HG23	1:A:375:LEU:HD11	1.98	0.45
1:A:125:LYS:HD3	1:B:443:VAL:HG21	1.98	0.44
1:B:195:HIS:HE1	3:B:1196:HOH:O	2.00	0.44
1:B:358:GLU:HG3	1:B:401:TRP:CH2	2.52	0.44
1:B:474:GLY:O	1:B:475:GLN:CB	2.65	0.44
1:B:507:LYS:HA	1:B:512:LYS:O	2.18	0.44
1:A:212:LEU:CD1	1:A:236:PHE:HB3	2.48	0.44
1:B:212:LEU:CD1	1:B:236:PHE:HB3	2.49	0.43
1:A:378:HIS:HD2	1:A:400:GLY:O	2.01	0.43
1:A:445:HIS:CE1	1:A:477:LEU:HD13	2.55	0.42
1:A:291:ARG:HD2	1:A:318:PHE:O	2.20	0.41
1:B:472:ARG:O	1:B:474:GLY:N	2.50	0.41
1:A:370:GLY:HA2	1:A:409:VAL:HG13	2.01	0.41
1:B:142:ARG:HH11	1:B:142:ARG:HD3	1.69	0.41
1:A:423:ASP:C	1:A:423:ASP:OD1	2.58	0.41
1:A:291:ARG:HD2	1:A:318:PHE:C	2.41	0.41
1:B:348[B]:THR:HG21	3:B:1263:HOH:O	2.21	0.40

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	517/520 (99%)	506 (98%)	10 (2%)	1 (0%)	47	29
1	B	519/520 (100%)	503 (97%)	14 (3%)	2 (0%)	34	17
All	All	1036/1040 (100%)	1009 (97%)	24 (2%)	3 (0%)	41	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	ASP
1	B	475	GLN
1	B	473	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	402/412 (98%)	393 (98%)	9 (2%)	52	29
1	B	391/412 (95%)	385 (98%)	6 (2%)	65	49
All	All	793/824 (96%)	778 (98%)	15 (2%)	57	37

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	TRP
1	A	137	ARG
1	A	259	ARG
1	A	291	ARG
1	A	324	ASP
1	A	398	GLN
1	A	422	THR
1	A	446	PRO
1	A	473	PRO
1	B	65	ARG
1	B	273	TYR
1	B	324	ASP
1	B	336	LEU
1	B	410	ARG
1	B	426	LEU

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	50	GLN
1	A	108	HIS
1	A	171	GLN
1	A	195	HIS
1	A	317	HIS
1	A	378	HIS
1	B	108	HIS
1	B	112	GLN
1	B	195	HIS
1	B	317	HIS
1	B	378	HIS
1	B	460	HIS

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)

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	FOA	A	1000	-	3,8,8	1.41	0	4,10,10	1.60	0
2	FOA	B	1000	-	3,8,8	0.73	0	4,10,10	1.83	2 (50%)

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	FOA	A	1000	-	-	0/0/4/4	0/1/1/1
2	FOA	B	1000	-	-	0/0/4/4	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1000	FOA	O7-C1-C2	2.65	120.72	114.69
2	B	1000	FOA	O7-C1-O6	-2.49	117.82	123.35

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 (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	518/520 (99%)	-0.13	5 (0%)	82	87	11, 19, 34, 47	0
1	B	519/520 (99%)	0.08	22 (4%)	36	42	12, 20, 37, 61	0
All	All	1037/1040 (99%)	-0.03	27 (2%)	56	62	11, 20, 35, 61	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	474	GLY	12.2
1	B	475	GLN	8.0
1	B	484	THR	6.1
1	B	477	LEU	6.0
1	B	473	PRO	5.7
1	B	480	THR	5.4
1	B	476	THR	5.1
1	B	490	LEU	4.5
1	B	399	GLY	4.4
1	B	422	THR	4.2
1	A	150	GLY	3.8
1	B	492	PRO	3.6
1	B	362	ASP	3.3
1	B	485	PHE	3.3
1	A	5	ALA	3.0
1	B	503	ALA	2.9
1	A	476	THR	2.9
1	B	488	ASP	2.5
1	B	363	GLY	2.5
1	B	224	LEU	2.4
1	B	230	LEU	2.3
1	B	495	TYR	2.3
1	A	488	ASP	2.2
1	B	478	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	510	THR	2.0
1	B	229	GLY	2.0
1	B	482	LEU	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
2	FOA	A	1000	8/8	0.97	0.09	11,17,19,20	0
2	FOA	B	1000	8/8	0.97	0.11	8,16,17,18	0

6.5 Other polymers (i)

There are no such residues in this entry.