Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2023 – 06:03 PM EDT

PDB ID	:	3GZY
Title	:	Crystal Structure of the Biphenyl Dioxygenase from Comamonas testosteroni Sp. Strain B-356
Authors	:	Kumar, P.; Colbert, C.L.; Bolin, J.T.
Deposited on	:	2009-04-08
Resolution	:	1.62 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:

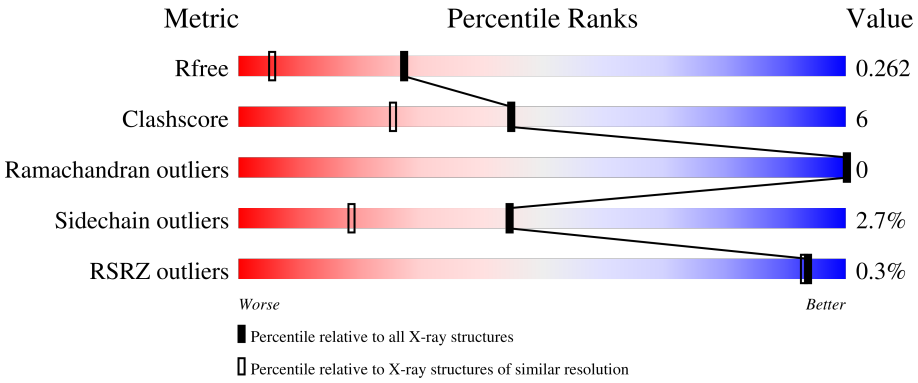
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.62 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	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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	457	79% 15%
2	B	186	83% 17%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5714 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 Biphenyl dioxygenase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	440	3577	2268	622	659	28	20	10	0

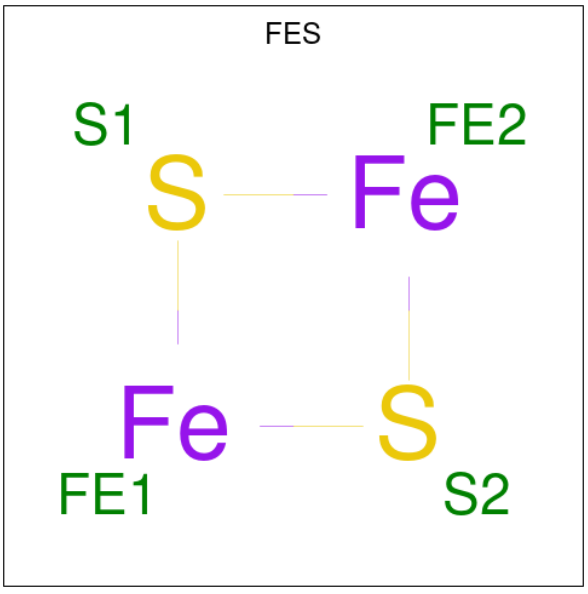
- Molecule 2 is a protein called Biphenyl dioxygenase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	186	1540	979	274	283	4	14	2	0

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

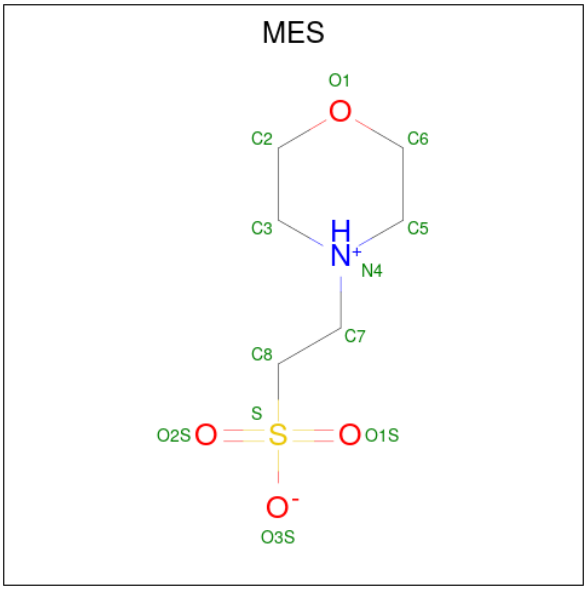
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
3	A	1	1	1	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 4 2 2	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 6 is water.

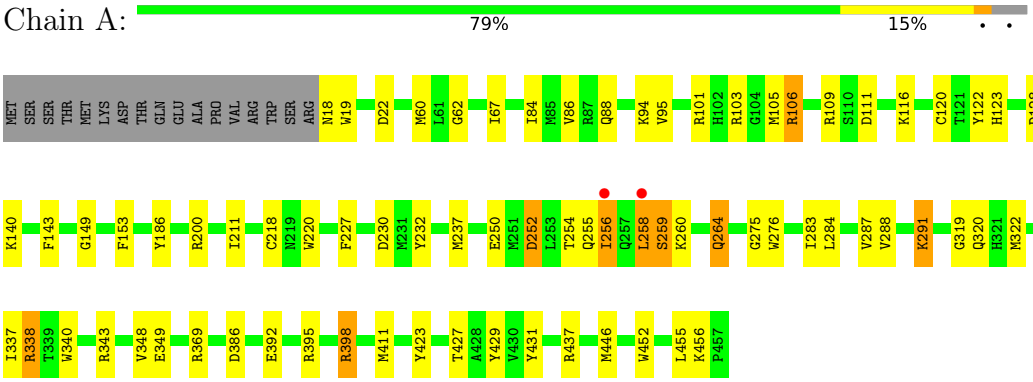
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	392	Total O 392 392	0	0
6	B	188	Total O 188 188	0	0

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.

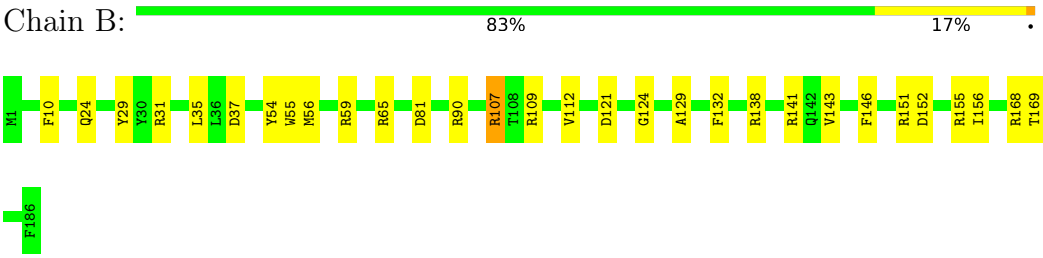
• Molecule 1: Biphenyl dioxygenase subunit alpha

Chain A:



• Molecule 2: Biphenyl dioxygenase subunit beta

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	136.23Å 136.23Å 106.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.33 – 1.62 39.33 – 1.63	Depositor EDS
% Data completeness (in resolution range)	93.5 (39.33-1.62) 98.6 (39.33-1.63)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	5.42 (at 1.63Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.118 , (Not available) 0.237 , 0.262	Depositor DCC
R_{free} test set	4713 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	12.0	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.366 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	5714	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, FES, FE2

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	0.61	0/3681	1.47	36/4991 (0.7%)
2	B	0.63	0/1579	1.62	37/2145 (1.7%)
All	All	0.61	0/5260	1.52	73/7136 (1.0%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	200	ARG	NE-CZ-NH2	-11.45	114.58	120.30
1	A	338	ARG	NE-CZ-NH1	-11.05	114.77	120.30
1	A	200	ARG	NE-CZ-NH1	10.49	125.55	120.30
2	B	132	PHE	CB-CG-CD1	10.38	128.07	120.80
1	A	106[A]	ARG	NE-CZ-NH1	9.91	125.25	120.30
1	A	106[B]	ARG	NE-CZ-NH1	9.91	125.25	120.30
1	A	349	GLU	O-C-N	9.58	138.03	122.70
1	A	338	ARG	NE-CZ-NH2	9.01	124.81	120.30
2	B	152	ASP	CB-CG-OD2	8.92	126.33	118.30
1	A	369	ARG	NE-CZ-NH1	-8.65	115.97	120.30
2	B	31	ARG	NE-CZ-NH2	8.34	124.47	120.30
2	B	141	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	A	128	ASP	CB-CG-OD1	8.11	125.59	118.30
2	B	54	TYR	CB-CG-CD1	-8.10	116.14	121.00
2	B	109	ARG	NE-CZ-NH2	-8.01	116.30	120.30
2	B	132	PHE	CB-CG-CD2	-7.30	115.69	120.80
1	A	343	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	106[A]	ARG	CD-NE-CZ	7.16	133.63	123.60
1	A	106[B]	ARG	CD-NE-CZ	7.16	133.63	123.60
2	B	138	ARG	NE-CZ-NH1	7.13	123.87	120.30
2	B	168	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	A	386	ASP	CB-CG-OD1	7.05	124.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	330	PHE	CB-CG-CD2	7.02	125.71	120.80
1	A	111	ASP	CB-CG-OD1	-6.97	112.03	118.30
1	A	101	ARG	CG-CD-NE	6.95	126.40	111.80
1	A	429	TYR	CB-CG-CD1	6.87	125.12	121.00
1	A	276	TRP	CH2-CZ2-CE2	6.71	124.11	117.40
2	B	59	ARG	NE-CZ-NH1	-6.60	117.00	120.30
2	B	107	ARG	NE-CZ-NH2	6.50	123.55	120.30
2	B	59	ARG	NE-CZ-NH2	6.34	123.47	120.30
2	B	90	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	B	109	ARG	CD-NE-CZ	-6.32	114.75	123.60
1	A	340	TRP	CH2-CZ2-CE2	6.29	123.69	117.40
1	A	227	PHE	CG-CD2-CE2	6.27	127.70	120.80
2	B	155	ARG	NE-CZ-NH2	-6.23	117.19	120.30
2	B	169	THR	O-C-N	6.17	132.58	122.70
2	B	143	VAL	O-C-N	6.16	132.55	122.70
1	A	62	GLY	O-C-N	6.11	132.48	122.70
2	B	37	ASP	CB-CG-OD2	-6.11	112.80	118.30
2	B	10	PHE	CG-CD2-CE2	5.90	127.29	120.80
1	A	86	VAL	O-C-N	5.89	132.13	122.70
1	A	109	ARG	CD-NE-CZ	5.89	131.84	123.60
2	B	35	LEU	O-C-N	-5.85	113.33	122.70
2	B	81	ASP	O-C-N	5.80	131.98	122.70
2	B	10	PHE	CB-CG-CD1	5.80	124.86	120.80
2	B	151	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	A	232	TYR	CB-CG-CD1	-5.75	117.55	121.00
2	B	141	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	232	TYR	CB-CG-CD2	5.68	124.41	121.00
2	B	155	ARG	CD-NE-CZ	5.68	131.56	123.60
1	A	369	ARG	NE-CZ-NH2	5.66	123.13	120.30
2	B	138	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	423	TYR	CB-CG-CD1	5.65	124.39	121.00
1	A	319	GLY	O-C-N	-5.64	113.68	122.70
2	B	55	TRP	O-C-N	5.62	131.69	122.70
1	A	330	PHE	CG-CD2-CE2	5.57	126.93	120.80
2	B	129	ALA	O-C-N	5.57	131.61	122.70
2	B	146	PHE	CB-CG-CD1	-5.54	116.92	120.80
2	B	54	TYR	CG-CD1-CE1	-5.47	116.92	121.30
2	B	54	TYR	CA-CB-CG	5.45	123.76	113.40
1	A	186	TYR	CA-CB-CG	5.44	123.74	113.40
2	B	174	GLN	O-C-N	5.42	131.37	122.70
2	B	109	ARG	NE-CZ-NH1	5.41	123.00	120.30
2	B	24	GLN	O-C-N	-5.39	114.07	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	107	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	67	ILE	O-C-N	5.25	131.08	121.10
1	A	230	ASP	CA-C-O	5.21	131.03	120.10
1	A	437	ARG	CD-NE-CZ	5.16	130.83	123.60
1	A	103	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	101	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	A	322	MET	O-C-N	5.07	130.80	122.70
2	B	146	PHE	CZ-CE2-CD2	-5.02	114.07	120.10
2	B	31	ARG	CD-NE-CZ	5.01	130.61	123.60

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	3577	0	3434	58	0
2	B	1540	0	1501	7	0
3	A	1	0	0	0	0
4	A	4	0	0	1	0
5	B	12	0	13	1	0
6	A	392	0	0	3	0
6	B	188	0	0	3	0
All	All	5714	0	4948	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 6.

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:A:258:LEU:CD1	1:A:259:SER:N	1.68	1.52
1:A:258:LEU:HD13	1:A:259:SER:N	1.30	1.25
1:A:258:LEU:HD12	1:A:259:SER:N	1.44	1.08
1:A:258:LEU:HD12	1:A:258:LEU:C	1.76	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:HD12	1:A:259:SER:CA	1.99	0.92
1:A:258:LEU:CD1	1:A:258:LEU:C	2.24	0.92
1:A:258:LEU:HD11	1:A:259:SER:O	1.70	0.91
1:A:258:LEU:CD1	1:A:259:SER:CA	2.53	0.85
1:A:258:LEU:CD1	1:A:259:SER:C	2.45	0.84
1:A:446[B]:MET:SD	1:A:455:LEU:HD21	2.25	0.76
1:A:255:GLN:C	1:A:256:ILE:HD13	2.08	0.73
1:A:258:LEU:HD12	1:A:259:SER:C	2.10	0.71
1:A:258:LEU:CD1	1:A:259:SER:O	2.38	0.70
1:A:258:LEU:HD11	1:A:259:SER:C	2.13	0.66
1:A:256:ILE:HD13	1:A:256:ILE:N	2.11	0.65
1:A:395:ARG:HD2	6:B:507:HOH:O	1.97	0.64
1:A:398:ARG:HH11	1:A:398:ARG:HB3	1.63	0.62
1:A:105[B]:MET:HG3	1:A:106[B]:ARG:N	2.16	0.60
1:A:411:MET:HE1	1:A:431:TYR:HB3	1.85	0.58
1:A:452:TRP:O	1:A:456:LYS:HG2	2.03	0.58
1:A:60[B]:MET:HE2	1:A:337:ILE:HD11	1.87	0.56
1:A:446[B]:MET:CE	1:A:455:LEU:HD21	2.36	0.56
1:A:220:TRP:HA	1:A:348:VAL:HG11	1.88	0.55
1:A:398:ARG:HH11	1:A:398:ARG:CB	2.19	0.54
1:A:105[B]:MET:HG3	1:A:106[B]:ARG:O	2.09	0.53
1:A:256:ILE:N	1:A:256:ILE:CD1	2.73	0.52
1:A:252:ASP:OD2	1:A:254:THR:HG23	2.10	0.51
1:A:22:ASP:HB2	6:A:556:HOH:O	2.11	0.51
2:B:121:ASP:OD1	5:B:702:MES:O3S	2.30	0.50
1:A:334[B]:ILE:HG12	6:A:516:HOH:O	2.12	0.49
2:B:56:MET:HE1	2:B:172:LEU:HD22	1.94	0.48
1:A:283:ILE:HG13	1:A:284:LEU:N	2.28	0.48
1:A:255:GLN:C	1:A:256:ILE:CD1	2.81	0.48
1:A:252:ASP:OD2	1:A:254:THR:OG1	2.32	0.48
1:A:275:GLY:O	1:A:320:GLN:HA	2.13	0.47
1:A:411:MET:CE	1:A:431:TYR:HB3	2.44	0.47
2:B:56:MET:CE	2:B:172:LEU:HD22	2.45	0.47
1:A:18:ASN:ND2	1:A:19:TRP:HD1	2.12	0.47
1:A:60[B]:MET:HE1	1:A:337:ILE:HG12	1.96	0.46
1:A:149:GLY:HA2	1:A:153:PHE:O	2.16	0.46
1:A:392:GLU:CD	1:A:395:ARG:HH21	2.19	0.46
1:A:105[B]:MET:HB3	1:A:120:CYS:SG	2.56	0.46
1:A:105[A]:MET:HB3	1:A:120:CYS:SG	2.56	0.45
1:A:287:VAL:HG11	1:A:334[A]:ILE:CD1	2.46	0.45
1:A:250:GLU:N	1:A:250:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106[B]:ARG:NH1	6:A:642:HOH:O	2.50	0.45
1:A:123:HIS:HB2	4:A:700:FES:S1	2.57	0.45
1:A:18:ASN:ND2	1:A:19:TRP:CD1	2.85	0.44
1:A:105[B]:MET:HE3	1:A:105[B]:MET:HB2	1.63	0.44
1:A:283:ILE:HG13	1:A:284:LEU:H	1.82	0.44
1:A:291:LYS:HB2	1:A:291:LYS:HE2	1.60	0.44
2:B:29:TYR:HB3	2:B:112:VAL:HG11	2.00	0.43
1:A:218:CYS:O	1:A:348:VAL:HG13	2.19	0.43
1:A:88:GLN:CG	1:A:94[B]:LYS:HG3	2.49	0.42
1:A:284:LEU:O	1:A:288:VAL:HG22	2.19	0.42
1:A:446[B]:MET:SD	1:A:455:LEU:HD11	2.60	0.42
2:B:107:ARG:NH2	6:B:527:HOH:O	2.53	0.41
1:A:105[B]:MET:HG2	1:A:120:CYS:SG	2.60	0.41
1:A:211:ILE:HD13	1:A:211:ILE:HG21	1.87	0.41
2:B:124:GLY:HA3	2:B:156:ILE:HG12	2.03	0.41
1:A:264:GLN:O	1:A:427:THR:HA	2.21	0.41
1:A:287:VAL:CG1	1:A:334[A]:ILE:HG12	2.51	0.41
1:A:84:ILE:O	1:A:95:VAL:HA	2.20	0.41
2:B:65:ARG:HG2	6:B:332:HOH:O	2.22	0.40
1:A:139:GLU:HA	1:A:143:PHE:CD1	2.57	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	448/457 (98%)	433 (97%)	15 (3%)	0	100	100
2	B	186/186 (100%)	179 (96%)	7 (4%)	0	100	100
All	All	634/643 (99%)	612 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	376/382 (98%)	362 (96%)	14 (4%)	34 10
2	B	164/162 (101%)	164 (100%)	0	100 100
All	All	540/544 (99%)	526 (97%)	14 (3%)	44 19

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LYS
1	A	122	TYR
1	A	135	ASN
1	A	140	LYS
1	A	237	MET
1	A	252	ASP
1	A	256	ILE
1	A	258	LEU
1	A	259	SER
1	A	260	LYS
1	A	264	GLN
1	A	291	LYS
1	A	338	ARG
1	A	398	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	135	ASN
2	B	38	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)

Of 3 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
5	MES	B	702	-	12,12,12	1.19	1 (8%)	14,16,16	1.64	2 (14%)
4	FES	A	700	1	0,4,4	-	-	-		

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
5	MES	B	702	-	-	0/6/14/14	0/1/1/1
4	FES	A	700	1	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	702	MES	C8-S	3.68	1.82	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	702	MES	O2S-S-C8	-4.03	102.06	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	702	MES	C6-C5-N4	2.02	113.17	110.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	702	MES	1	0
4	A	700	FES	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, 95^{th} 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	440/457 (96%)	-0.96	2 (0%) 91 90	7, 13, 26, 55	27 (6%)
2	B	186/186 (100%)	-1.00	0 100 100	6, 12, 26, 46	12 (6%)
All	All	626/643 (97%)	-0.97	2 (0%) 94 93	6, 13, 26, 55	39 (6%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	LEU	3.0
1	A	256	ILE	2.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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
5	MES	B	702	12/12	0.98	0.07	16,24,31,42	0
3	FE2	A	701	1/1	0.99	0.05	17,17,17,17	0
4	FES	A	700	4/4	1.00	0.05	9,10,10,11	0

6.5 Other polymers (i)

There are no such residues in this entry.