



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:46 AM UTC

PDB ID : 3GZY / pdb_00003gzy
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	:	4-5-2 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

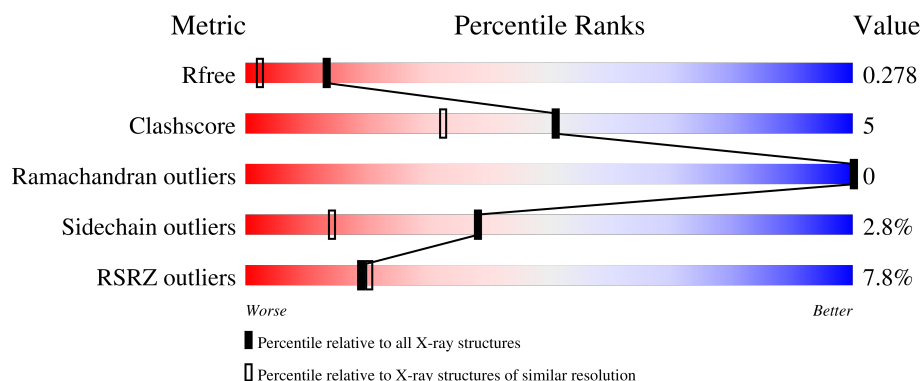
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (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 $\leq 5\%$. 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	457	
2	B	186	

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
1	A	440	Total	C	N	O	S	20	10	0
			3577	2268	622	659	28			

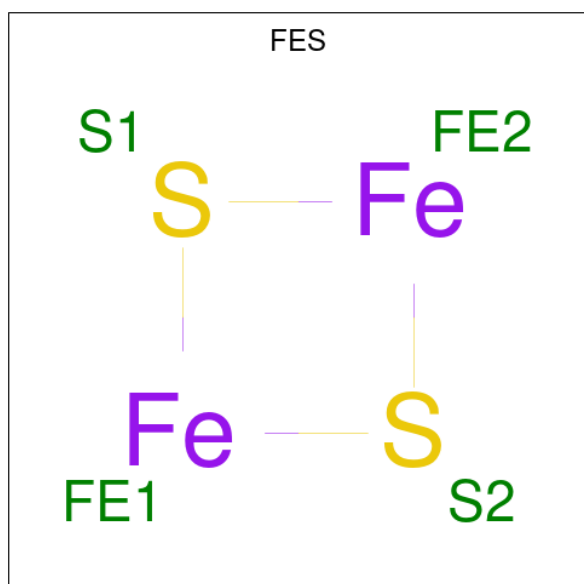
- Molecule 2 is a protein called Biphenyl dioxygenase subunit beta.

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

- Molecule 3 is FE (II) ION (CCD ID: FE2) (formula: Fe).

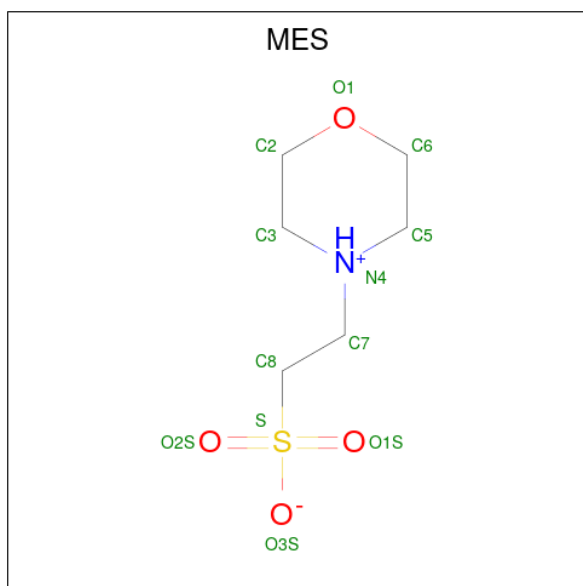
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

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



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

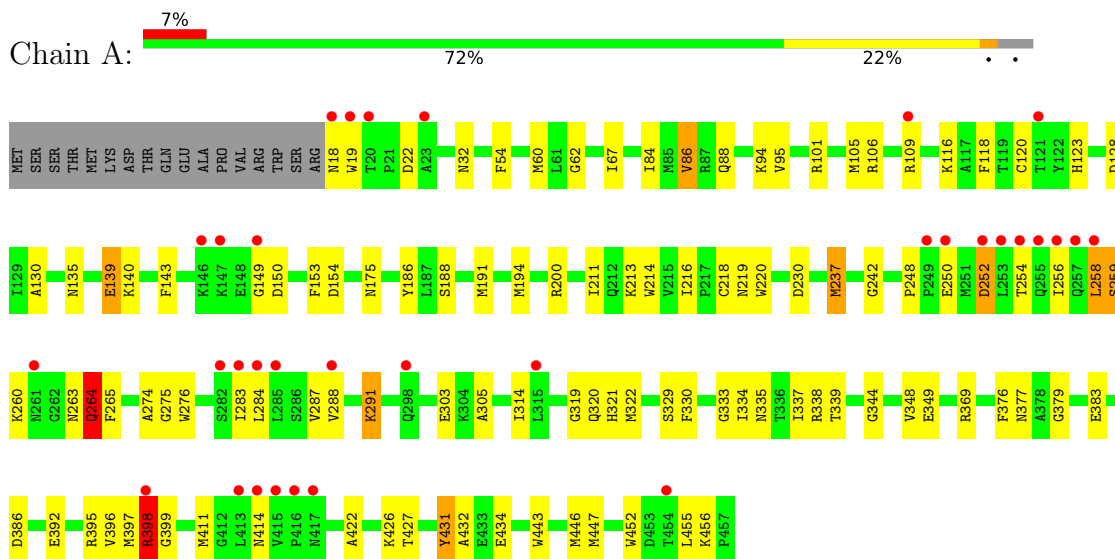
- Molecule 6 is water.

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

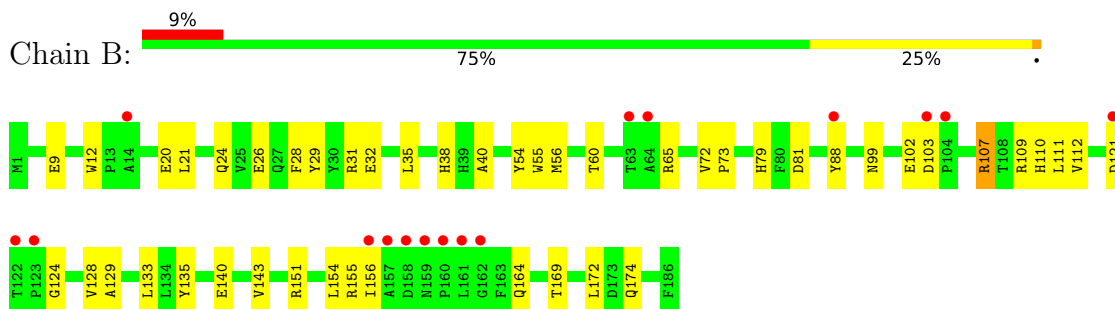
3 Residue-property plots [i](#)

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



- Molecule 2: Biphenyl dioxygenase subunit beta



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	5.42 (at 1.63Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.118 , (Not available) (Not available) , 0.278	Depositor DCC
R_{free} test set	4714 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)	0.36 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.366 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.88	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.*

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

5.1 Standard geometry

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

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	0.80	1/3681 (0.0%)	1.78	78/4991 (1.6%)
2	B	0.89	0/1579	1.93	58/2145 (2.7%)
All	All	0.83	1/5260 (0.0%)	1.83	136/7136 (1.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	GLU	CA-C	5.06	1.58	1.52

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	GLU	O-C-N	12.49	138.03	123.29
1	A	248	PRO	O-C-N	11.52	126.56	121.15
2	B	99	ASN	CA-CB-CG	9.85	122.45	112.60
1	A	319	GLY	O-C-N	-9.77	113.68	122.57
2	B	81	ASP	O-C-N	9.22	131.98	123.50
1	A	349	GLU	CA-C-O	-8.87	110.72	120.38
1	A	274	ALA	CA-C-O	-8.81	111.45	121.40
2	B	143	VAL	O-C-N	8.78	132.55	123.07
1	A	67	ILE	O-C-N	8.75	131.08	121.10
2	B	35	LEU	CA-C-O	8.65	129.90	120.82
2	B	35	LEU	O-C-N	-8.48	113.33	122.07
1	A	86	VAL	O-C-N	7.91	132.13	123.03
2	B	169	THR	O-C-N	7.80	132.58	123.30
2	B	24	GLN	O-C-N	-7.71	114.07	122.09
1	A	319	GLY	CA-C-O	7.66	129.22	120.03
2	B	107	ARG	CA-C-O	-7.66	112.39	120.58
1	A	230	ASP	CA-C-O	7.62	131.03	121.58
1	A	175	ASN	OD1-CG-ND2	-7.53	115.07	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	135	TYR	CA-C-O	-7.47	112.28	120.43
1	A	62	GLY	O-C-N	7.43	132.48	124.15
1	A	305	ALA	CA-C-O	7.39	128.39	120.55
1	A	396	VAL	O-C-N	-7.37	114.72	121.87
2	B	174	GLN	O-C-N	7.12	131.37	123.33
1	A	139	GLU	O-C-N	7.09	129.63	122.12
1	A	62	GLY	CA-C-O	-7.05	114.70	121.05
1	A	349	GLU	CA-C-N	-6.97	113.37	122.37
1	A	349	GLU	C-N-CA	-6.97	113.37	122.37
2	B	151	ARG	CA-C-O	-6.92	113.13	120.40
1	A	194	MET	CA-C-O	6.91	127.75	120.42
2	B	55	TRP	O-C-N	6.91	131.69	123.33
2	B	109	ARG	CD-NE-CZ	-6.89	114.75	124.40
2	B	72	VAL	O-C-N	-6.86	113.52	121.07
1	A	219	ASN	OD1-CG-ND2	-6.86	115.74	122.60
1	A	230	ASP	O-C-N	-6.77	115.46	122.64
2	B	20	GLU	CA-C-O	6.75	127.65	120.70
2	B	174	GLN	CA-C-O	-6.74	113.44	120.99
1	A	338	ARG	NE-CZ-NH1	-6.73	114.77	121.50
2	B	129	ALA	O-C-N	6.71	131.61	123.16
2	B	169	THR	CA-C-O	-6.68	113.14	120.36
2	B	99	ASN	CA-C-O	-6.55	114.00	121.66
1	A	101	ARG	CG-CD-NE	6.54	126.40	112.00
1	A	322	MET	O-C-N	6.54	130.80	123.48
1	A	333	GLY	CA-C-O	6.52	126.59	119.55
1	A	434	GLU	O-C-N	6.48	129.09	122.09
2	B	40	ALA	CA-C-O	-6.46	113.79	122.44
2	B	55	TRP	CA-C-O	-6.39	112.93	120.60
1	A	303	GLU	CA-C-O	6.34	127.27	120.55
2	B	133	LEU	CA-C-O	-6.34	113.48	120.33
1	A	338	ARG	NE-CZ-NH2	6.23	124.81	119.20
2	B	32	GLU	CA-C-O	6.22	127.56	120.90
2	B	140	GLU	O-C-N	6.21	129.69	122.17
1	A	263	ASN	O-C-N	6.18	130.21	123.10
1	A	216	ILE	CA-C-O	6.14	125.26	119.98
1	A	379	GLY	O-C-N	6.08	129.95	122.29
2	B	32	GLU	O-C-N	-6.08	115.77	122.09
2	B	129	ALA	CA-C-O	-6.08	114.29	121.16
2	B	81	ASP	CA-C-O	-6.05	114.28	120.63
1	A	329	SER	O-C-N	-6.05	115.80	123.24
2	B	164	GLN	CA-C-O	-5.95	114.39	121.11
1	A	376	PHE	CA-CB-CG	-5.93	107.87	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	72	VAL	CA-C-O	5.91	125.21	119.71
1	A	274	ALA	O-C-N	5.86	130.26	123.17
1	A	258	LEU	CA-C-N	-5.85	114.74	122.99
1	A	258	LEU	C-N-CA	-5.85	114.74	122.99
2	B	31	ARG	NE-CZ-NH2	5.85	124.47	119.20
2	B	88	TYR	O-C-N	-5.79	116.11	122.07
1	A	242	GLY	O-C-N	-5.70	116.71	122.18
2	B	73	PRO	O-C-N	5.70	130.09	123.14
1	A	344	GLY	O-C-N	5.69	127.46	121.77
1	A	154	ASP	CA-C-O	-5.67	114.22	120.24
1	A	265	PHE	O-C-N	5.67	130.60	123.23
2	B	9	GLU	CA-C-O	5.67	127.56	121.55
1	A	383	GLU	CA-C-O	-5.66	114.52	120.63
1	A	339	THR	CA-C-O	-5.65	114.72	120.71
1	A	213	LYS	CA-C-O	-5.62	114.29	120.36
2	B	128	VAL	O-C-N	-5.61	117.14	123.20
2	B	133	LEU	O-C-N	5.54	130.43	123.12
1	A	369	ARG	NE-CZ-NH1	-5.53	115.97	121.50
2	B	107	ARG	O-C-N	5.53	129.56	122.93
1	A	264	GLN	CA-C-O	5.51	127.63	121.40
1	A	330	PHE	O-C-N	5.51	129.05	123.26
1	A	377	ASN	OD1-CG-ND2	5.51	128.11	122.60
1	A	322	MET	CA-C-O	-5.48	114.86	120.89
2	B	54	TYR	CA-CB-CG	5.48	123.76	113.90
2	B	111	LEU	CA-C-O	-5.47	114.45	120.69
1	A	186	TYR	CA-CB-CG	5.46	123.74	113.90
2	B	135	TYR	O-C-N	5.46	129.44	123.27
1	A	265	PHE	CA-C-O	-5.45	114.81	120.70
1	A	338	ARG	O-C-N	-5.45	117.59	123.42
2	B	110	HIS	CA-C-N	-5.44	113.72	121.50
2	B	110	HIS	C-N-CA	-5.44	113.72	121.50
1	A	339	THR	O-C-N	5.42	130.09	123.21
1	A	32	ASN	CA-CB-CG	-5.41	107.19	112.60
1	A	431	TYR	CA-C-O	5.39	127.43	121.39
2	B	60	THR	CA-C-O	-5.36	115.35	121.68
1	A	188	SER	CB-CA-C	-5.36	110.42	116.63
1	A	321	HIS	O-C-N	-5.35	115.94	123.11
1	A	128	ASP	O-C-N	5.33	129.32	122.23
1	A	335	ASN	CA-CB-CG	-5.33	107.27	112.60
1	A	109	ARG	CD-NE-CZ	5.32	131.84	124.40
2	B	140	GLU	CA-C-O	-5.32	114.86	120.55
1	A	150	ASP	CA-CB-CG	5.31	117.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	102	GLU	CA-C-N	-5.31	116.36	122.52
2	B	102	GLU	C-N-CA	-5.31	116.36	122.52
1	A	191	MET	O-C-N	-5.29	115.74	120.71
2	B	28	PHE	O-C-N	-5.28	116.63	122.07
1	A	118	PHE	O-C-N	5.28	129.78	123.13
2	B	103	ASP	CA-CB-CG	-5.24	107.36	112.60
1	A	54	PHE	CA-CB-CG	-5.24	108.56	113.80
1	A	414	ASN	CA-C-N	5.23	126.16	122.60
1	A	414	ASN	C-N-CA	5.23	126.16	122.60
2	B	38	HIS	CA-CB-CG	-5.23	108.57	113.80
2	B	12	TRP	CA-C-N	5.18	125.08	119.85
2	B	12	TRP	C-N-CA	5.18	125.08	119.85
2	B	154	LEU	CA-C-O	5.17	126.19	120.71
2	B	21	LEU	O-C-N	-5.17	116.26	122.15
1	A	259	SER	O-C-N	5.17	129.45	123.30
1	A	329	SER	CA-C-O	5.16	127.15	121.11
1	A	399	GLY	O-C-N	-5.15	116.58	122.91
1	A	200	ARG	NE-CZ-NH2	-5.14	114.58	119.20
2	B	88	TYR	CA-C-O	5.13	126.20	120.82
2	B	26	GLU	O-C-N	5.12	127.42	122.09
1	A	154	ASP	O-C-N	5.12	129.26	123.27
1	A	432	ALA	O-C-N	5.12	128.90	123.42
2	B	28	PHE	CA-CB-CG	-5.12	108.69	113.80
2	B	155	ARG	CD-NE-CZ	5.11	131.56	124.40
2	B	54	TYR	CA-C-O	5.09	125.74	120.40
2	B	151	ARG	O-C-N	5.09	129.83	123.12
1	A	276	TRP	CH2-CZ2-CE2	5.08	124.11	117.50
1	A	398	ARG	CA-C-O	5.05	125.78	119.97
1	A	426	LYS	O-C-N	-5.05	116.81	123.02
1	A	386	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	214	TRP	CA-CB-CG	5.04	123.17	113.60
1	A	118	PHE	CA-C-O	-5.03	115.08	120.46
1	A	422	ALA	CA-C-O	5.03	125.54	119.31
1	A	62	GLY	N-CA-C	-5.00	103.95	110.45

There are no chirality outliers.

There are no planarity outliers.

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	3577	0	3434	44	0
2	B	1540	0	1501	8	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	52	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 (52) 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:446[B]:MET:SD	1:A:455:LEU:HD21	2.25	0.76
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: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
2:B:56:MET:HE3	2:B:172:LEU:HD22	1.86	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: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
1:A:392:GLU:CD	1:A:395:ARG:HH21	2.19	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
1:A:237:MET:HB3	1:A:237:MET:HE2	1.63	0.48
1:A:283:ILE:HG13	1:A:284:LEU:N	2.28	0.48
1:A:252:ASP:OD2	1:A:254:THR:OG1	2.32	0.48
1:A:411:MET:CE	1:A:431:TYR:HB3	2.44	0.48
1:A:275:GLY:O	1:A:320:GLN:HA	2.13	0.47
1:A:252:ASP:CG	1:A:254:THR:HG1	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:443:TRP:CZ2	1:A:447:MET:HE2	2.53	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
1:A:94[B]:LYS:NZ	1:A:130:ALA:O	2.49	0.40
2:B:65:ARG:HG2	6:B:332:HOH:O	2.22	0.40
2:B:56:MET:HE2	2:B:79:HIS:CD2	2.56	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 ⓘ

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%)	361 (96%)	15 (4%)	28	7
2	B	164/162 (101%)	164 (100%)	0	100	100
All	All	540/544 (99%)	525 (97%)	15 (3%)	38	14

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

Mol	Chain	Res	Type
1	A	86	VAL
1	A	116	LYS
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	314	ILE
1	A	397	MET
1	A	398	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	99	GLN
1	A	135	ASN
1	A	226	GLN
1	A	389	ASN
2	B	93	GLN

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](#)

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%)	15,16,16	1.39	2 (13%)
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	3.67	1.82	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	702	MES	O2S-S-C8	-3.09	102.06	106.73
5	B	702	MES	C6-C5-N4	2.01	113.17	110.12

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, 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	440/457 (96%)	0.67	33 (7%)	20 21	6, 13, 25, 55	36 (8%)
2	B	186/186 (100%)	0.55	16 (8%)	16 17	6, 12, 26, 43	14 (7%)
All	All	626/643 (97%)	0.64	49 (7%)	19 20	6, 13, 25, 55	50 (7%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	LEU	9.9
1	A	256	ILE	8.2
1	A	255	GLN	6.7
1	A	257	GLN	5.9
1	A	18	ASN	5.6
1	A	254	THR	5.5
2	B	158	ASP	5.1
2	B	121	ASP	4.7
1	A	19	TRP	4.1
2	B	159	ASN	4.1
2	B	14	ALA	4.0
2	B	156	ILE	3.9
1	A	250	GLU	3.9
2	B	160	PRO	3.6
2	B	122	THR	3.5
1	A	253	LEU	3.5
1	A	285	LEU	3.4
1	A	454	THR	3.2
1	A	398	ARG	3.0
2	B	63	THR	2.9
1	A	416	PRO	2.9
2	B	157	ALA	2.9
1	A	147	LYS	2.9
1	A	417	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	23	ALA	2.8
1	A	283	ILE	2.8
1	A	249	PRO	2.8
1	A	121	THR	2.8
1	A	415	VAL	2.7
2	B	88	TYR	2.7
1	A	414	ASN	2.7
1	A	20	THR	2.7
1	A	149	GLY	2.6
1	A	288	VAL	2.6
2	B	123	PRO	2.5
1	A	282	SER	2.5
1	A	261[A]	ASN	2.5
1	A	413	LEU	2.5
1	A	109	ARG	2.4
2	B	64	ALA	2.3
1	A	284	LEU	2.3
2	B	103	ASP	2.3
1	A	298	GLN	2.3
1	A	252	ASP	2.2
1	A	146	LYS	2.2
1	A	315	LEU	2.1
2	B	161	LEU	2.1
2	B	104	PRO	2.1
2	B	162	GLY	2.0

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 oligosaccharides 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, 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($\text{\AA}^2$)	Q<0.9
5	MES	B	702	12/12	0.94	0.11	16,24,31,42	0
4	FES	A	700	4/4	0.99	0.03	9,10,10,11	0
3	FE2	A	701	1/1	0.99	0.03	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.