



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:53 AM GMT

PDB ID : 2XSH
Title : CRYSTAL STRUCTURE OF P4 VARIANT OF BIPHENYL DIOXYGENASE FROM BURKHOLDERIA XENOVORANS LB400 IN COMPLEX WITH 2,6 DI CHLOROBIPHENYL
Authors : Kumar, P.; Bolin, J.T.
Deposited on : 2010-09-29
Resolution : 2.29 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

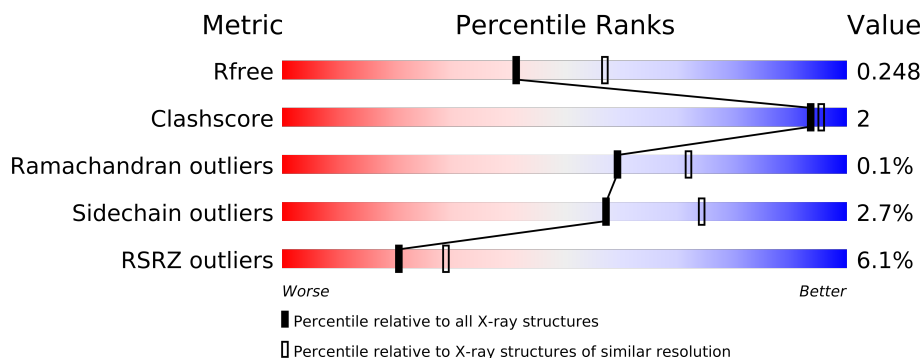
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.29 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	459	
1	C	459	
1	E	459	
1	G	459	
1	I	459	
1	K	459	
2	B	188	
2	D	188	
2	F	188	
2	H	188	
2	J	188	
2	L	188	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	FE2	A	901	-	X
5	DC5	A	902	-	X
5	DC5	C	902	-	X
5	DC5	E	900	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30603 atoms, of which 0 are hydrogen and 0 are deuterium.

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	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			
1	C	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			
1	E	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			
1	G	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			
1	I	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			
1	K	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			

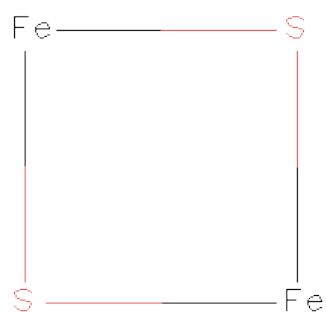
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	ALA	THR	ENGINEERED MUTATION	UNP P37333
A	336	MET	PHE	ENGINEERED MUTATION	UNP P37333
C	335	ALA	THR	ENGINEERED MUTATION	UNP P37333
C	336	MET	PHE	ENGINEERED MUTATION	UNP P37333
E	335	ALA	THR	ENGINEERED MUTATION	UNP P37333
E	336	MET	PHE	ENGINEERED MUTATION	UNP P37333
G	335	ALA	THR	ENGINEERED MUTATION	UNP P37333
G	336	MET	PHE	ENGINEERED MUTATION	UNP P37333
I	335	ALA	THR	ENGINEERED MUTATION	UNP P37333
I	336	MET	PHE	ENGINEERED MUTATION	UNP P37333
K	335	ALA	THR	ENGINEERED MUTATION	UNP P37333
K	336	MET	PHE	ENGINEERED MUTATION	UNP P37333

- Molecule 2 is a protein called BIPHENYL DIOXYGENASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			
2	D	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			
2	F	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			
2	H	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			
2	J	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			
2	L	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).

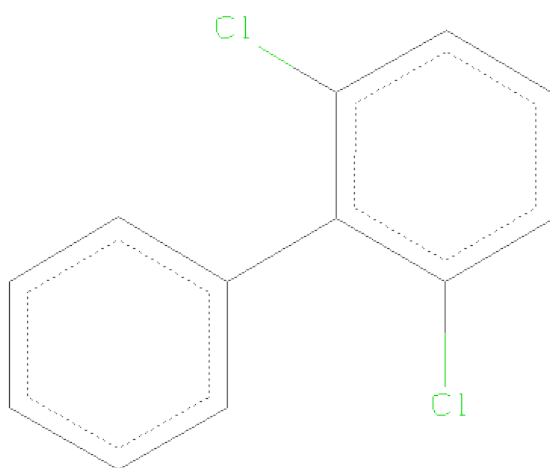


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	I	1	Total	Fe	S	0	0
			4	2	2		
3	K	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Fe 1	0	0
4	K	1	Total 1	Fe 1	0	0
4	E	1	Total 1	Fe 1	0	0
4	I	1	Total 1	Fe 1	0	0
4	C	1	Total 1	Fe 1	0	0
4	A	1	Total 1	Fe 1	0	0

- Molecule 5 is 2,6-DICHLOROBIPHENYL (three-letter code: DC5) (formula: C₁₂H₈Cl₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 14	C 12	Cl 2	0	0
5	C	1	Total 14	C 12	Cl 2	0	0
5	E	1	Total 14	C 12	Cl 2	0	0

- Molecule 6 is water.

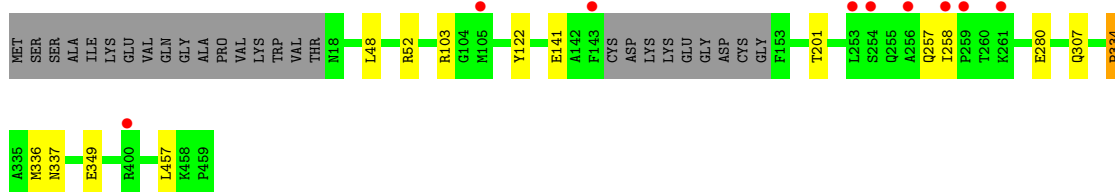
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	139	Total 139	O 139	0	0
6	B	82	Total 82	O 82	0	0
6	C	129	Total 129	O 129	0	0
6	D	81	Total 81	O 81	0	0
6	E	128	Total 128	O 128	0	0
6	F	79	Total 79	O 79	0	0
6	G	82	Total 82	O 82	0	0
6	H	51	Total 51	O 51	0	0
6	I	80	Total 80	O 80	0	0
6	J	32	Total 32	O 32	0	0
6	K	79	Total 79	O 79	0	0
6	L	31	Total 31	O 31	0	0

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.

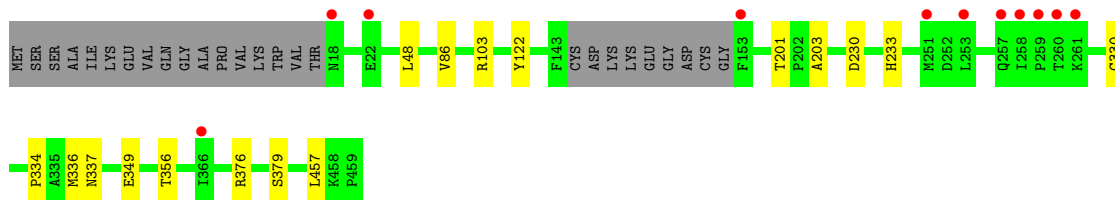
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain A: 



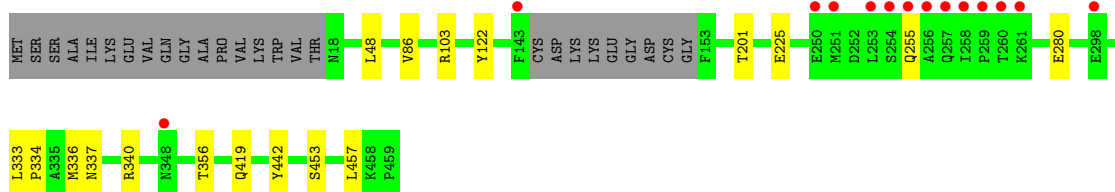
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain C: 



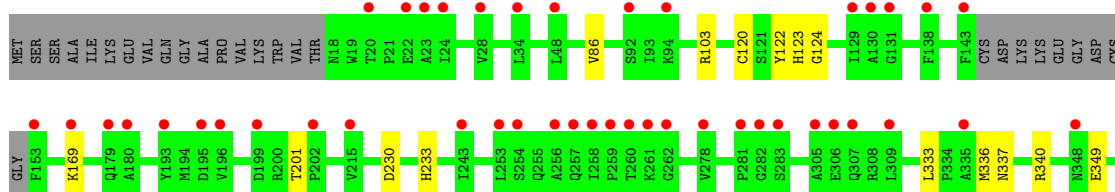
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain E: 



• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

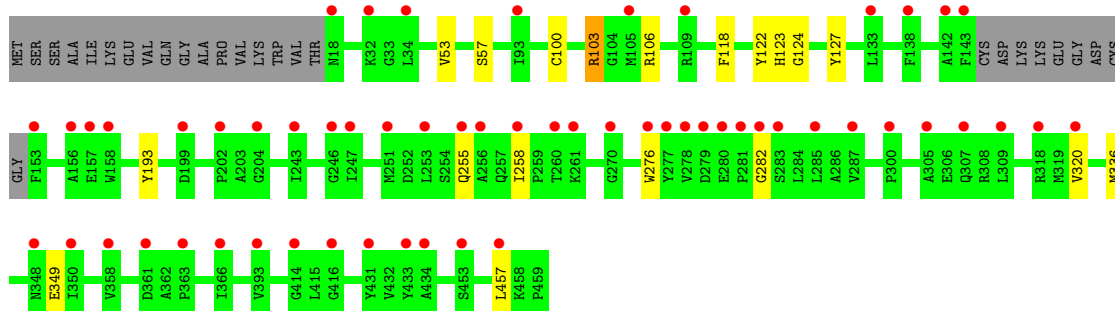
Chain G: 





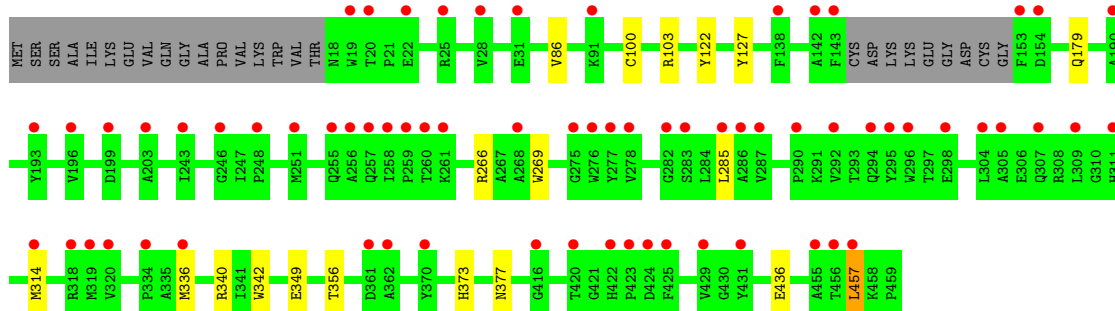
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain I:



• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain K:



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain B:



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain D:



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain F:



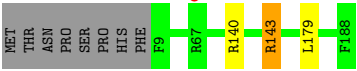
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain H: 



● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain J: 



● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.73Å 276.76Å 92.32Å 90.00° 117.37° 90.00°	Depositor
Resolution (Å)	138.68 – 2.29 46.47 – 2.29	Depositor EDS
% Data completeness (in resolution range)	87.7 (138.68-2.29) 87.7 (46.47-2.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.245 0.189 , 0.248	Depositor DCC
R_{free} test set	7632 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.6	EDS
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 152204 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	30603	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DC5, FE2, 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	0.50	0/3529	0.61	0/4791
1	C	0.50	0/3529	0.59	0/4791
1	E	0.48	0/3529	0.58	0/4791
1	G	0.39	0/3529	0.52	0/4791
1	I	0.38	0/3529	0.52	0/4791
1	K	0.37	0/3529	0.51	0/4791
2	B	0.51	0/1530	0.64	1/2068 (0.0%)
2	D	0.52	0/1530	0.61	0/2068
2	F	0.50	0/1530	0.62	1/2068 (0.0%)
2	H	0.46	0/1530	0.57	0/2068
2	J	0.43	0/1530	0.57	0/2068
2	L	0.44	0/1530	0.58	0/2068
All	All	0.45	0/30354	0.57	2/41154 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	143	ARG	NE-CZ-NH2	-6.43	117.09	120.30
2	F	143	ARG	NE-CZ-NH2	-5.22	117.69	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3427	0	0	3	0
1	C	3427	0	0	6	0
1	E	3427	0	0	3	0
1	G	3427	0	0	8	0
1	I	3427	0	0	9	0
1	K	3427	0	0	7	0
2	B	1496	0	0	2	0
2	D	1496	0	0	5	0
2	F	1496	0	0	8	0
2	H	1496	0	0	2	0
2	J	1496	0	0	1	0
2	L	1496	0	0	3	0
3	A	4	0	0	0	0
3	C	4	0	0	0	0
3	E	4	0	0	0	0
3	G	4	0	0	0	0
3	I	4	0	0	0	0
3	K	4	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
5	A	14	0	8	0	0
5	C	14	0	8	0	0
5	E	14	0	8	0	0
6	A	139	0	0	0	0
6	B	82	0	0	0	0
6	C	129	0	0	3	0
6	D	81	0	0	1	0
6	E	128	0	0	0	0
6	F	79	0	0	1	0
6	G	82	0	0	3	0
6	H	51	0	0	0	0
6	I	80	0	0	2	0
6	J	32	0	0	0	0
6	K	79	0	0	1	0
6	L	31	0	0	0	0
All	All	30603	0	24	48	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (48) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:334:PRO:O	1:A:337:ASN:OD1	2.10	0.68
2:D:58:MET:CE	2:D:81:HIS:CB	2.72	0.67
1:E:334:PRO:O	1:E:337:ASN:OD1	2.15	0.64
1:I:123:HIS:N	6:I:2025:HOH:O	2.31	0.63
1:G:124:GLY:N	6:G:2023:HOH:O	2.34	0.60
2:D:40:HIS:CE1	2:F:151:GLU:OE2	2.54	0.60
1:G:123:HIS:N	6:G:2023:HOH:O	2.35	0.60
2:B:143:ARG:NH2	1:C:349:GLU:OE2	2.34	0.60
1:G:120:CYS:SG	6:G:2023:HOH:O	2.58	0.56
2:H:55:HIS:NE2	2:H:83:ASP:OD2	2.39	0.55
1:C:376:ARG:NH1	6:C:2106:HOH:O	2.41	0.53
2:F:26:GLU:OE1	2:F:158:ARG:NH2	2.42	0.52
1:K:266:ARG:NH1	1:K:436:GLU:OE1	2.42	0.52
1:G:349:GLU:OE2	2:L:143:ARG:NH2	2.42	0.52
1:E:333:LEU:O	1:E:337:ASN:N	2.44	0.51
2:L:55:HIS:NE2	2:L:83:ASP:OD2	2.46	0.49
1:K:100:CYS:SG	1:K:127:TYR:OH	2.71	0.48
1:C:230:ASP:O	1:C:233:HIS:ND1	2.46	0.48
2:J:143:ARG:NH2	1:K:349:GLU:OE2	2.45	0.47
1:K:340:ARG:CD	1:K:342:TRP:CH2	2.99	0.45
1:I:193:TYR:CE2	1:I:276:TRP:CH2	3.05	0.44
1:E:225:GLU:OE2	1:E:442:TYR:OH	2.35	0.44
1:I:124:GLY:N	6:I:2025:HOH:O	2.49	0.44
2:F:41:ARG:NH1	6:F:2022:HOH:O	2.51	0.44
1:G:410:ASN:O	1:I:103:ARG:NH1	2.51	0.44
1:I:118:PHE:O	1:I:127:TYR:N	2.50	0.44
1:A:349:GLU:OE2	2:F:143:ARG:NH2	2.50	0.43
1:I:100:CYS:SG	1:I:127:TYR:OH	2.76	0.43
1:G:230:ASP:O	1:G:233:HIS:ND1	2.52	0.43
1:G:394:GLU:OE2	1:I:106:ARG:NE	2.52	0.43
1:A:141:GLU:OE1	1:A:141:GLU:N	2.52	0.43
1:C:201:THR:CB	6:C:2100:HOH:O	2.66	0.42
1:K:269:TRP:NE1	1:K:457:LEU:O	2.53	0.42
2:F:31:TYR:OH	2:F:154:ASP:OD1	2.38	0.42
1:K:373:HIS:O	1:K:377:ASN:ND2	2.52	0.42
2:F:55:HIS:NE2	2:F:83:ASP:OD2	2.53	0.42
1:K:314:MET:N	6:K:2058:HOH:O	2.52	0.42
2:D:41:ARG:CD	6:D:2019:HOH:O	2.67	0.42
1:G:333:LEU:O	1:G:337:ASN:N	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:58:MET:CE	2:F:81:HIS:CB	2.98	0.42
2:D:26:GLU:OE1	2:D:158:ARG:NH2	2.53	0.41
2:D:99:ASP:OD1	2:F:67:ARG:NE	2.52	0.41
1:C:203:ALA:N	6:C:2100:HOH:O	2.54	0.41
1:C:334:PRO:O	1:C:337:ASN:OD1	2.39	0.41
2:B:39:ASP:OD1	2:B:112:HIS:ND1	2.54	0.40
2:L:104:GLU:OE1	2:L:108:SER:N	2.54	0.40
2:H:143:ARG:NH2	1:I:349:GLU:OE2	2.54	0.40
1:I:53:VAL:O	1:I:57:SER:OG	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	429/459 (94%)	409 (95%)	20 (5%)	0	100	100
1	C	429/459 (94%)	411 (96%)	18 (4%)	0	100	100
1	E	429/459 (94%)	415 (97%)	14 (3%)	0	100	100
1	G	429/459 (94%)	405 (94%)	23 (5%)	1 (0%)	56	68
1	I	429/459 (94%)	403 (94%)	25 (6%)	1 (0%)	56	68
1	K	429/459 (94%)	401 (94%)	28 (6%)	0	100	100
2	B	178/188 (95%)	171 (96%)	7 (4%)	0	100	100
2	D	178/188 (95%)	172 (97%)	6 (3%)	0	100	100
2	F	178/188 (95%)	172 (97%)	6 (3%)	0	100	100
2	H	178/188 (95%)	174 (98%)	4 (2%)	0	100	100
2	J	178/188 (95%)	171 (96%)	7 (4%)	0	100	100
2	L	178/188 (95%)	173 (97%)	5 (3%)	0	100	100
All	All	3642/3882 (94%)	3477 (96%)	163 (4%)	2 (0%)	59	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	282	GLY
1	G	169	LYS

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	350/372 (94%)	338 (97%)	12 (3%)	49	64
1	C	350/372 (94%)	341 (97%)	9 (3%)	59	76
1	E	350/372 (94%)	337 (96%)	13 (4%)	45	60
1	G	350/372 (94%)	342 (98%)	8 (2%)	63	80
1	I	350/372 (94%)	343 (98%)	7 (2%)	68	84
1	K	350/372 (94%)	342 (98%)	8 (2%)	63	80
2	B	159/167 (95%)	154 (97%)	5 (3%)	52	68
2	D	159/167 (95%)	153 (96%)	6 (4%)	44	59
2	F	159/167 (95%)	155 (98%)	4 (2%)	60	77
2	H	159/167 (95%)	156 (98%)	3 (2%)	69	85
2	J	159/167 (95%)	156 (98%)	3 (2%)	69	85
2	L	159/167 (95%)	154 (97%)	5 (3%)	52	68
All	All	3054/3234 (94%)	2971 (97%)	83 (3%)	57	74

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	52	ARG
1	A	103	ARG
1	A	122	TYR
1	A	201	THR
1	A	257	GLN
1	A	258	ILE
1	A	280	GLU
1	A	307	GLN
1	A	334	PRO

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Mol	Chain	Res	Type
1	A	336	MET
1	A	457	LEU
2	B	44	GLU
2	B	76	ASP
2	B	140	ARG
2	B	143	ARG
2	B	179	LEU
1	C	48	LEU
1	C	86	VAL
1	C	103	ARG
1	C	122	TYR
1	C	330	CYS
1	C	336	MET
1	C	356	THR
1	C	379	SER
1	C	457	LEU
2	D	44	GLU
2	D	76	ASP
2	D	94	ARG
2	D	113	LEU
2	D	121	GLU
2	D	179	LEU
1	E	48	LEU
1	E	86	VAL
1	E	103	ARG
1	E	122	TYR
1	E	201	THR
1	E	255	GLN
1	E	280	GLU
1	E	336	MET
1	E	340	ARG
1	E	356	THR
1	E	419	GLN
1	E	453	SER
1	E	457	LEU
2	F	44	GLU
2	F	94	ARG
2	F	140	ARG
2	F	179	LEU
1	G	86	VAL
1	G	103	ARG
1	G	122	TYR

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Mol	Chain	Res	Type
1	G	201	THR
1	G	336	MET
1	G	340	ARG
1	G	415	LEU
1	G	457	LEU
2	H	10	LYS
2	H	140	ARG
2	H	179	LEU
1	I	103	ARG
1	I	122	TYR
1	I	255	GLN
1	I	258	ILE
1	I	320	VAL
1	I	336	MET
1	I	457	LEU
2	J	140	ARG
2	J	143	ARG
2	J	179	LEU
1	K	86	VAL
1	K	103	ARG
1	K	122	TYR
1	K	179	GLN
1	K	285	LEU
1	K	336	MET
1	K	356	THR
1	K	457	LEU
2	L	10	LYS
2	L	44	GLU
2	L	94	ARG
2	L	140	ARG
2	L	179	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	$\# Z > 2$
3	FES	A	900	1	0,4,4	0.00	-	0,4,4	0.00	-
5	DC5	A	902	-	15,15,15	1.24	1 (6%)	20,20,20	0.59	0
3	FES	C	900	1	0,4,4	0.00	-	0,4,4	0.00	-
5	DC5	C	902	-	15,15,15	1.20	1 (6%)	20,20,20	0.81	0
5	DC5	E	900	-	15,15,15	1.30	1 (6%)	20,20,20	0.89	1 (5%)
3	FES	E	901	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	G	900	1,6	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	I	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	K	900	1	0,4,4	0.00	-	0,4,4	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
3	FES	A	900	1	-	0/0/4/4	0/0/1/1
5	DC5	A	902	-	-	0/4/4/4	0/2/2/2
3	FES	C	900	1	-	0/0/4/4	0/0/1/1
5	DC5	C	902	-	-	0/4/4/4	0/2/2/2
5	DC5	E	900	-	-	0/4/4/4	0/2/2/2
3	FES	E	901	1	-	0/0/4/4	0/0/1/1
3	FES	G	900	1,6	-	0/0/4/4	0/0/1/1
3	FES	I	900	1	-	0/0/4/4	0/0/1/1
3	FES	K	900	1	-	0/0/4/4	0/0/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	900	DC5	CB1-CA1	-4.82	1.40	1.50
5	A	902	DC5	CB1-CA1	-4.31	1.41	1.50
5	C	902	DC5	CB1-CA1	-4.19	1.41	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	900	DC5	CB6-CB1-CB2	2.21	118.22	115.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	433/459 (94%)	-0.30	9 (2%) 60 70	24, 38, 56, 70	18 (4%)
1	C	433/459 (94%)	-0.18	11 (2%) 54 65	27, 41, 61, 76	18 (4%)
1	E	433/459 (94%)	-0.10	14 (3%) 45 55	24, 43, 68, 78	18 (4%)
1	G	433/459 (94%)	0.67	53 (12%) 5 8	43, 82, 116, 130	18 (4%)
1	I	433/459 (94%)	0.74	58 (13%) 4 6	39, 84, 136, 163	18 (4%)
1	K	433/459 (94%)	0.89	69 (15%) 3 4	42, 87, 151, 175	18 (4%)
2	B	180/188 (95%)	-0.22	1 (0%) 86 92	26, 36, 57, 65	4 (2%)
2	D	180/188 (95%)	-0.19	3 (1%) 67 76	28, 40, 58, 62	4 (2%)
2	F	180/188 (95%)	-0.28	2 (1%) 77 85	26, 38, 56, 62	4 (2%)
2	H	180/188 (95%)	-0.15	2 (1%) 77 85	34, 49, 67, 79	4 (2%)
2	J	180/188 (95%)	-0.04	1 (0%) 86 92	35, 56, 76, 83	4 (2%)
2	L	180/188 (95%)	-0.05	1 (0%) 86 92	34, 53, 76, 87	4 (2%)
All	All	3678/3882 (94%)	0.16	224 (6%) 21 29	24, 51, 113, 175	132 (3%)

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	258	ILE	17.4
1	G	258	ILE	9.3
1	I	282	GLY	8.7
1	K	282	GLY	8.5
1	G	257	GLN	8.1
1	C	258	ILE	7.3
1	K	257	GLN	7.0
1	G	260	THR	6.7
1	K	320	VAL	6.5
1	I	258	ILE	6.3
1	I	143	PHE	6.3

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Mol	Chain	Res	Type	RSRZ
1	K	248	PRO	6.1
1	K	292	VAL	6.1
1	I	142	ALA	6.0
1	K	290	PRO	5.9
1	K	22	GLU	5.9
1	A	258	ILE	5.7
1	K	277	TYR	5.7
1	I	278	VAL	5.5
1	K	260	THR	5.4
1	K	294	GLN	5.4
1	K	361	ASP	5.4
1	K	278	VAL	5.3
1	G	254	SER	5.3
1	I	281	PRO	5.2
1	I	366	ILE	5.2
1	K	455	ALA	4.9
1	G	253	LEU	4.8
1	K	256	ALA	4.8
1	K	420	THR	4.7
1	C	257	GLN	4.6
1	E	260	THR	4.5
1	G	282	GLY	4.4
1	K	153	PHE	4.4
1	K	276	TRP	4.4
1	K	305	ALA	4.3
1	G	261	LYS	4.2
1	G	202	PRO	4.1
1	K	295	TYR	4.1
1	G	259	PRO	4.0
1	G	256	ALA	4.0
1	I	246	GLY	3.9
1	I	305	ALA	3.9
1	I	204	GLY	3.8
1	G	196	VAL	3.8
1	I	277	TYR	3.8
1	K	143	PHE	3.8
1	K	370	TYR	3.8
1	E	256	ALA	3.7
1	K	138	PHE	3.7
1	G	243	ILE	3.7
1	K	422	HIS	3.6
1	A	254	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	I	280	GLU	3.6
1	G	433	TYR	3.5
1	K	259	PRO	3.5
1	K	314	MET	3.5
1	E	253	LEU	3.4
1	E	258	ILE	3.4
1	I	361	ASP	3.4
1	A	143	PHE	3.4
1	I	199	ASP	3.4
1	I	156	ALA	3.4
1	K	261	LYS	3.3
1	K	319	MET	3.3
1	E	261	LYS	3.3
1	G	92	SER	3.3
1	I	153	PHE	3.3
1	G	283	SER	3.2
1	G	199	ASP	3.2
1	K	268	ALA	3.2
1	G	34	LEU	3.2
1	I	279	ASP	3.2
1	K	424	ASP	3.2
1	G	262	GLY	3.2
1	G	129	ILE	3.2
1	E	250	GLU	3.2
1	E	254	SER	3.2
1	G	94	LYS	3.2
1	G	335	ALA	3.1
1	G	305	ALA	3.1
1	I	300	PRO	3.1
1	K	20	THR	3.1
1	C	259	PRO	3.1
1	G	169	LYS	3.1
1	G	307	GLN	3.0
1	K	196	VAL	3.0
1	C	260	THR	3.0
1	G	348	ASN	3.0
1	K	307	GLN	3.0
1	K	283	SER	3.0
2	J	67	ARG	3.0
1	K	199	ASP	3.0
1	K	318	ARG	3.0
1	I	253	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	270	GLY	2.9
1	C	153	PHE	2.9
1	K	457	LEU	2.9
1	I	285	LEU	2.9
1	G	400	ARG	2.9
1	E	257	GLN	2.9
1	I	158	TRP	2.9
1	I	307	GLN	2.9
1	G	457	LEU	2.8
1	I	243	ILE	2.8
1	K	19	TRP	2.8
1	K	362	ALA	2.8
1	K	311	HIS	2.8
1	I	256	ALA	2.8
1	E	255	GLN	2.8
1	E	259	PRO	2.8
1	I	431	TYR	2.8
1	K	203	ALA	2.7
1	K	336	MET	2.7
2	B	123	ALA	2.7
1	K	423	PRO	2.7
1	K	285	LEU	2.7
1	C	22	GLU	2.7
1	C	261	LYS	2.7
1	I	138	PHE	2.7
1	K	309	LEU	2.7
1	A	256	ALA	2.7
1	E	251	MET	2.7
1	I	287	VAL	2.6
2	H	52	LYS	2.6
1	K	246	GLY	2.6
1	A	261	LYS	2.6
1	G	138	PHE	2.6
1	G	130	ALA	2.6
1	G	143	PHE	2.6
1	G	193	TYR	2.6
1	I	18	ASN	2.6
1	I	414	GLY	2.6
2	D	16	SER	2.6
1	K	429	VAL	2.6
1	I	433	TYR	2.5
1	I	260	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	143	PHE	2.5
1	I	416	GLY	2.5
1	K	286	ALA	2.5
1	I	276	TRP	2.5
1	I	318	ARG	2.5
1	G	446	MET	2.5
1	I	348	ASN	2.5
1	G	306	GLU	2.5
1	I	309	LEU	2.5
1	C	18	ASN	2.5
1	C	253	LEU	2.4
1	G	215	VAL	2.4
1	I	34	LEU	2.4
1	K	28	VAL	2.4
1	C	366	ILE	2.4
1	K	416	GLY	2.4
1	I	247	ILE	2.4
1	K	25	ARG	2.4
1	K	334	PRO	2.4
1	K	91	LYS	2.4
1	G	48	LEU	2.4
2	L	123	ALA	2.4
1	K	31	GLU	2.4
1	I	363	PRO	2.4
1	K	193	TYR	2.4
1	I	457	LEU	2.4
1	I	32	LYS	2.4
1	I	105	MET	2.4
1	E	348	ASN	2.3
1	G	131	GLY	2.3
1	A	105	MET	2.3
1	I	283	SER	2.3
1	I	93	ILE	2.3
1	K	190	ALA	2.3
1	K	456	THR	2.3
1	G	309	LEU	2.3
1	G	365	GLU	2.3
1	I	434	ALA	2.3
1	K	142	ALA	2.3
1	G	278	VAL	2.3
1	K	251	MET	2.3
1	K	298	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	154	ASP	2.2
1	K	304	LEU	2.2
1	G	28	VAL	2.2
1	K	287	VAL	2.2
1	K	255	GLN	2.2
2	D	13	GLU	2.2
1	G	24	ILE	2.2
1	I	202	PRO	2.2
1	G	455	ALA	2.2
1	I	358	VAL	2.2
2	F	145	VAL	2.2
1	G	180	ALA	2.2
2	D	145	VAL	2.2
1	K	431	TYR	2.2
1	I	393	VAL	2.2
1	I	109	ARG	2.1
1	A	259	PRO	2.1
1	I	453	SER	2.1
1	G	281	PRO	2.1
1	I	350	ILE	2.1
1	K	243	ILE	2.1
1	G	23	ALA	2.1
1	E	298	GLU	2.1
2	F	67	ARG	2.1
1	I	251	MET	2.1
1	G	179	GLN	2.1
1	I	255	GLN	2.1
1	K	296	TRP	2.1
1	G	22	GLU	2.1
1	I	157	GLU	2.1
1	G	361	ASP	2.1
1	C	251	MET	2.0
2	H	58	MET	2.0
1	A	253	LEU	2.0
1	I	261	LYS	2.0
1	G	20	THR	2.0
1	K	425	PHE	2.0
1	G	195	ASP	2.0
1	I	320	VAL	2.0
1	A	400	ARG	2.0
1	G	407	GLN	2.0
1	G	456	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	275	GLY	2.0
1	G	153	PHE	2.0
1	I	133	LEU	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 carbohydrates 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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	DC5	C	902	14/14	0.23	5.62	71,73,74,74	0
4	FE2	A	901	1/1	0.14	2.64	34,34,34,34	0
5	DC5	E	900	14/14	0.16	2.41	72,74,76,76	0
5	DC5	A	902	14/14	0.16	2.15	54,58,61,61	0
4	FE2	E	902	1/1	0.12	1.52	40,40,40,40	0
4	FE2	C	901	1/1	0.12	0.61	37,37,37,37	0
3	FES	E	901	4/4	0.12	0.24	36,38,38,40	0
3	FES	C	900	4/4	0.11	0.06	27,31,32,33	0
3	FES	G	900	4/4	0.12	-0.05	72,73,73,74	0
3	FES	A	900	4/4	0.11	-0.08	38,39,39,40	0
4	FE2	G	901	1/1	0.12	-0.31	58,58,58,58	0
3	FES	K	900	4/4	0.12	-0.47	56,57,57,59	0
3	FES	I	900	4/4	0.11	-0.47	62,62,64,66	0
4	FE2	K	901	1/1	0.10	-1.49	74,74,74,74	0
4	FE2	I	901	1/1	0.09	-2.15	58,58,58,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.