



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2026 – 06:45 am BST

PDB ID : 2YFL / pdb_00002yfl
Title : Crystal Structure of Biphenyl dioxygenase variant RR41 with 2-chloro dibenzofuran
Authors : Kumar, P.; Bolin, J.T.
Deposited on : 2011-04-06
Resolution : 2.60 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

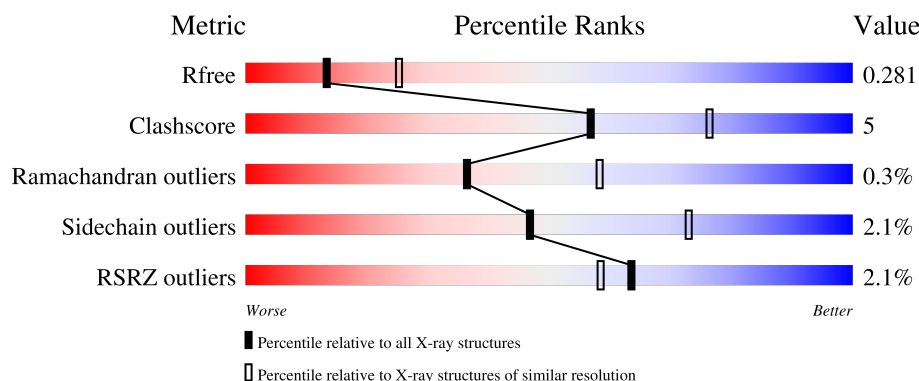
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	459	
1	C	459	
1	E	459	
1	G	459	
1	I	459	

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Mol	Chain	Length	Quality of chain
1	K	459	 4% 83% 10% • 6%
2	B	188	 % 82% 13% • •
2	D	188	 % 79% 16% • •
2	F	188	 81% 14% •
2	H	188	 82% 13% •
2	J	188	 86% 10% •
2	L	188	 86% 9% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FES	G	900	-	-	X	-
5	DC4	C	1460	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 29968 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	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			
1	C	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			
1	E	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			
1	G	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			
1	I	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			
1	K	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			

There are 30 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
A	338	GLN	ASN	engineered mutation	UNP P37333
A	341	VAL	ILE	engineered mutation	UNP P37333
A	409	PHE	LEU	engineered mutation	UNP P37333
C	335	ALA	THR	engineered mutation	UNP P37333
C	336	MET	PHE	engineered mutation	UNP P37333
C	338	GLN	ASN	engineered mutation	UNP P37333
C	341	VAL	ILE	engineered mutation	UNP P37333
C	409	PHE	LEU	engineered mutation	UNP P37333
E	335	ALA	THR	engineered mutation	UNP P37333
E	336	MET	PHE	engineered mutation	UNP P37333
E	338	GLN	ASN	engineered mutation	UNP P37333
E	341	VAL	ILE	engineered mutation	UNP P37333
E	409	PHE	LEU	engineered mutation	UNP P37333
G	335	ALA	THR	engineered mutation	UNP P37333
G	336	MET	PHE	engineered mutation	UNP P37333

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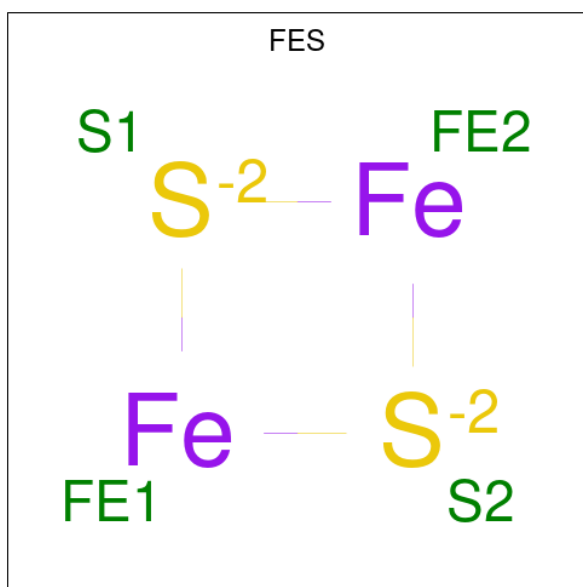
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Chain	Residue	Modelled	Actual	Comment	Reference
G	338	GLN	ASN	engineered mutation	UNP P37333
G	341	VAL	ILE	engineered mutation	UNP P37333
G	409	PHE	LEU	engineered mutation	UNP P37333
I	335	ALA	THR	engineered mutation	UNP P37333
I	336	MET	PHE	engineered mutation	UNP P37333
I	338	GLN	ASN	engineered mutation	UNP P37333
I	341	VAL	ILE	engineered mutation	UNP P37333
I	409	PHE	LEU	engineered mutation	UNP P37333
K	335	ALA	THR	engineered mutation	UNP P37333
K	336	MET	PHE	engineered mutation	UNP P37333
K	338	GLN	ASN	engineered mutation	UNP P37333
K	341	VAL	ILE	engineered mutation	UNP P37333
K	409	PHE	LEU	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 (CCD ID: FES) (formula: Fe₂S₂).

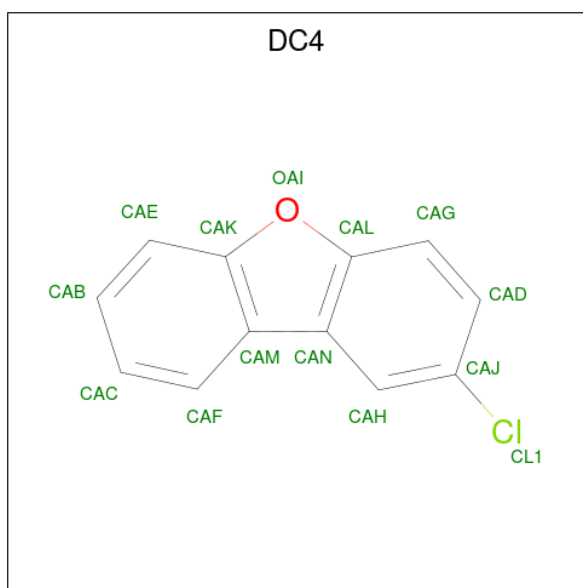


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	I	1	Total	Fe	S	0	0
			4	2	2		
3	K	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 5 is 2-CHLORODIBENZOFURAN (CCD ID: DC4) (formula: C₁₂H₇ClO).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	50	Total	O	0	0
			50	50		
6	B	26	Total	O	0	0
			26	26		
6	C	41	Total	O	0	0
			41	41		
6	D	24	Total	O	0	0
			24	24		
6	E	62	Total	O	0	0
			62	62		
6	F	21	Total	O	0	0
			21	21		
6	G	30	Total	O	0	0
			30	30		
6	H	19	Total	O	0	0
			19	19		
6	I	35	Total	O	0	0
			35	35		

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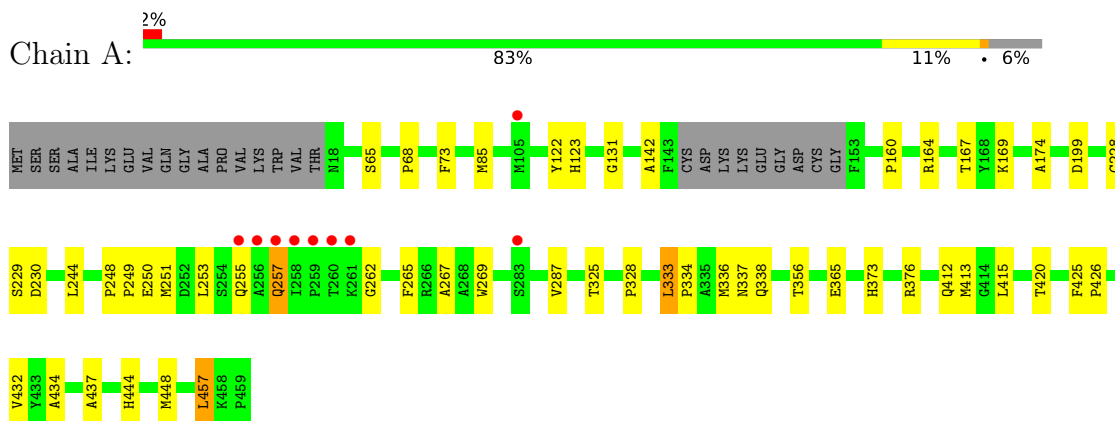
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	11	Total 11	O 11	0	0
6	K	20	Total 20	O 20	0	0
6	L	15	Total 15	O 15	0	0

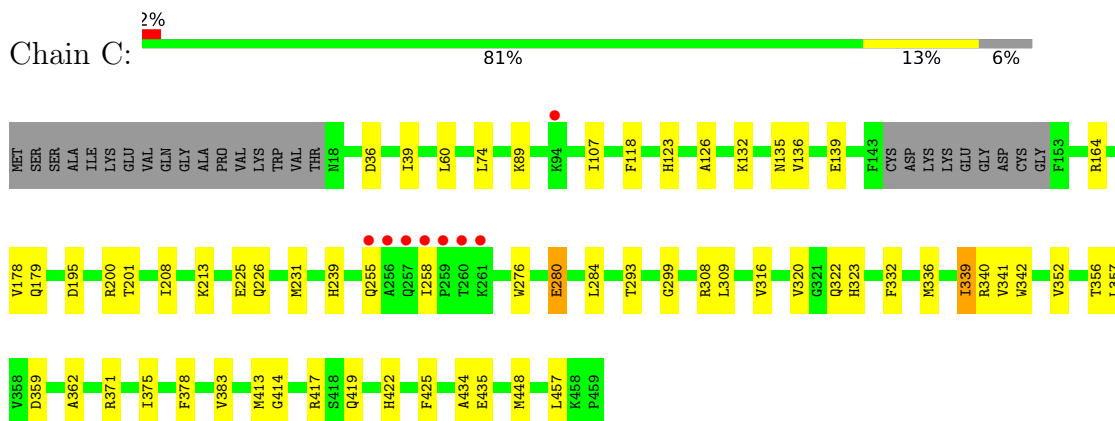
3 Residue-property plots

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.

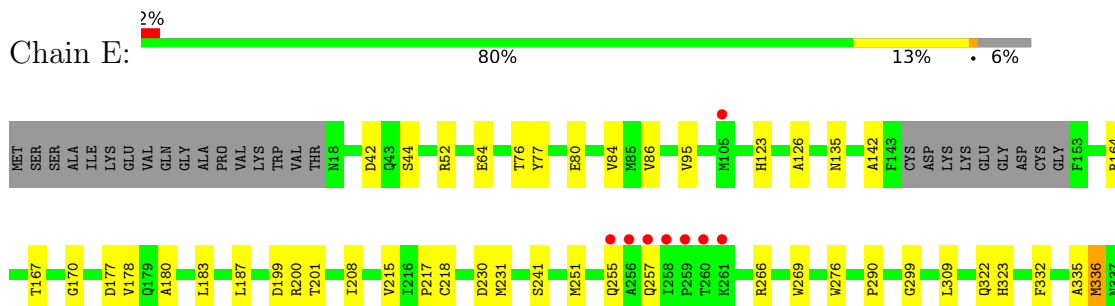
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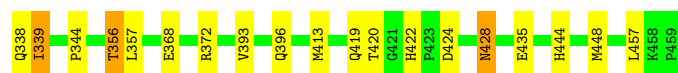


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

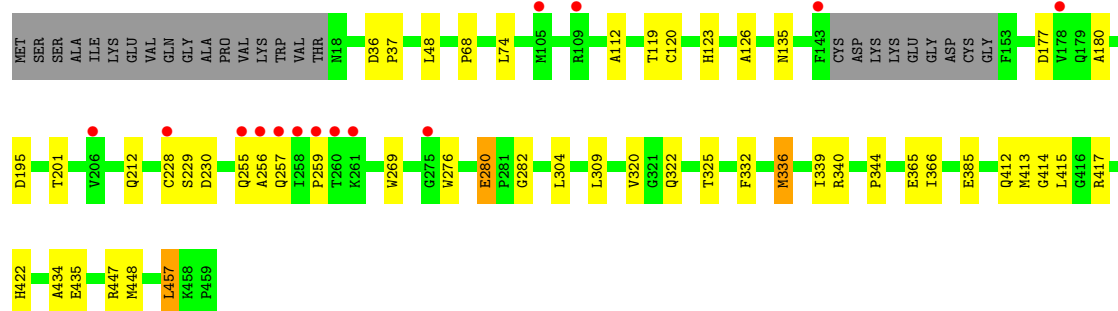
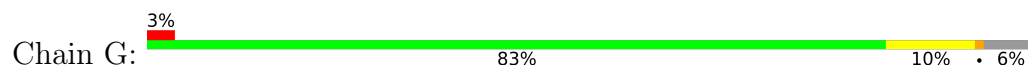


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

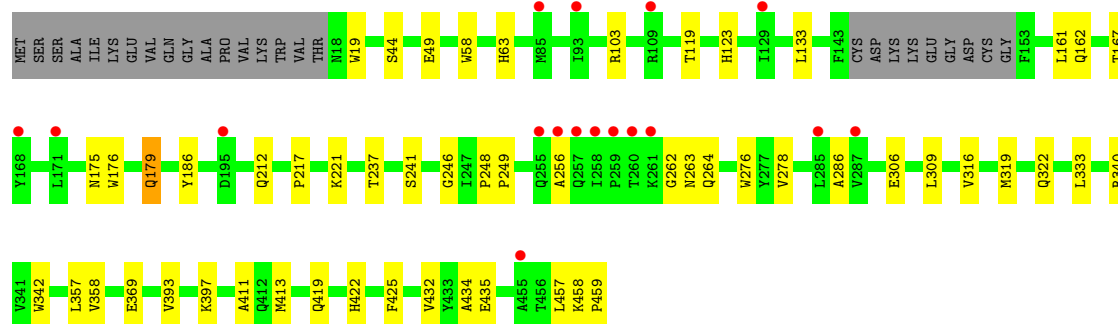
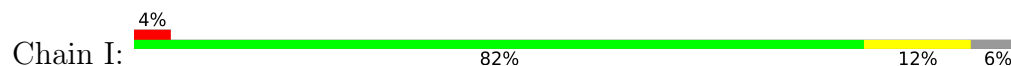




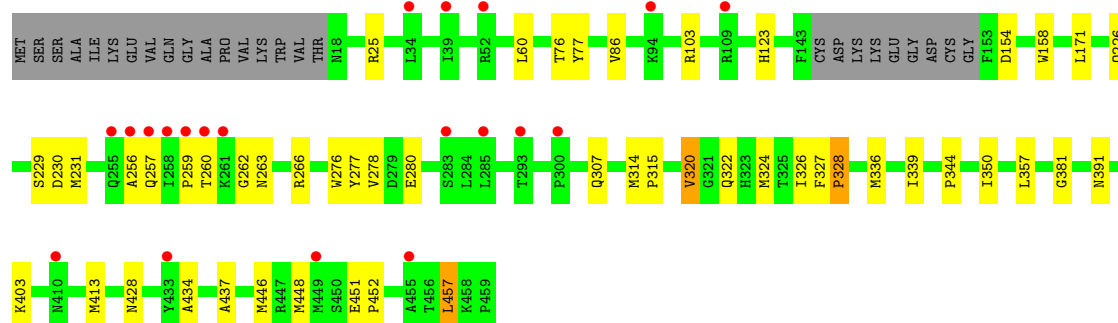
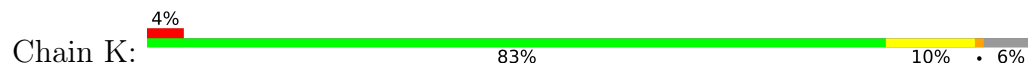
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



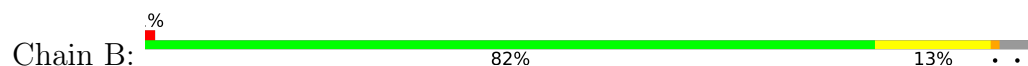
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



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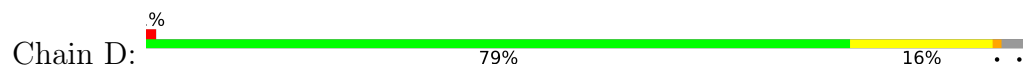


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

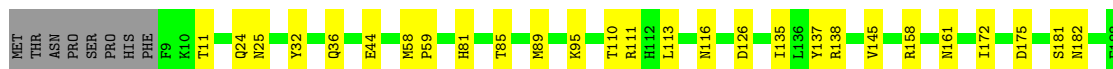
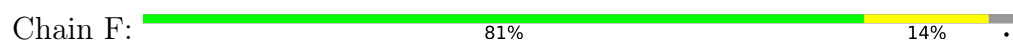




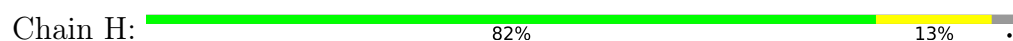
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



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• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.56Å 275.98Å 92.06Å 90.00° 117.46° 90.00°	Depositor
Resolution (Å)	137.36 – 2.60 137.36 – 2.60	Depositor EDS
% Data completeness (in resolution range)	77.7 (137.36-2.60) 81.8 (137.36-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.280 0.217 , 0.281	Depositor DCC
R_{free} test set	4927 reflections (4.21%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	29968	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: DC4, 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	0.44	0/3533	0.79	3/4796 (0.1%)
1	C	0.43	0/3533	0.79	2/4796 (0.0%)
1	E	0.46	0/3533	0.78	3/4796 (0.1%)
1	G	0.43	0/3533	0.79	0/4796
1	I	0.42	0/3533	0.80	3/4796 (0.1%)
1	K	0.42	0/3533	0.76	1/4796 (0.0%)
2	B	0.43	0/1530	0.71	0/2068
2	D	0.41	0/1530	0.72	0/2068
2	F	0.41	0/1530	0.71	0/2068
2	H	0.42	0/1530	0.73	0/2068
2	J	0.39	0/1530	0.70	0/2068
2	L	0.39	0/1530	0.69	0/2068
All	All	0.43	0/30378	0.76	12/41184 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	299	GLY	CA-C-N	7.16	126.69	119.24
1	E	299	GLY	C-N-CA	7.16	126.69	119.24
1	C	299	GLY	CA-C-N	5.66	124.86	118.97
1	C	299	GLY	C-N-CA	5.66	124.86	118.97
1	I	333	LEU	CA-C-N	5.52	126.74	119.84
1	I	333	LEU	C-N-CA	5.52	126.74	119.84
1	A	230	ASP	N-CA-C	5.48	116.27	108.54
1	K	231	MET	N-CA-C	-5.48	106.44	113.23
1	I	237	THR	N-CA-C	5.19	117.01	111.36
1	E	230	ASP	N-CA-C	5.09	116.34	109.11
1	A	333	LEU	CA-C-N	5.02	126.12	119.84
1	A	333	LEU	C-N-CA	5.02	126.12	119.84

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	3430	0	3274	28	0
1	C	3430	0	3274	41	0
1	E	3430	0	3274	37	0
1	G	3430	0	3274	27	0
1	I	3430	0	3274	33	0
1	K	3430	0	3274	28	0
2	B	1496	0	1447	18	0
2	D	1496	0	1447	23	0
2	F	1496	0	1447	24	0
2	H	1496	0	1447	18	0
2	J	1496	0	1447	16	0
2	L	1496	0	1447	14	0
3	A	4	0	0	1	0
3	C	4	0	0	1	0
3	E	4	0	0	1	0
3	G	4	0	0	2	0
3	I	4	0	0	1	0
3	K	4	0	0	1	0
4	A	1	0	0	0	0
4	C	1	0	0	1	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	7	1	0
5	C	14	0	7	8	0
6	A	50	0	0	1	0
6	B	26	0	0	3	0
6	C	41	0	0	4	0
6	D	24	0	0	0	0
6	E	62	0	0	3	0
6	F	21	0	0	1	0
6	G	30	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	19	0	0	1	0
6	I	35	0	0	10	0
6	J	11	0	0	0	0
6	K	20	0	0	2	0
6	L	15	0	0	0	0
All	All	29968	0	28340	267	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 (267) 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:I:58:TRP:HA	6:I:2007:HOH:O	1.44	1.14
1:K:263:ASN:HA	6:K:2019:HOH:O	1.49	1.13
1:A:142:ALA:HB1	1:C:413:MET:HG3	1.53	0.90
1:C:378:PHE:HE1	5:C:1460:DC4:HAD	1.35	0.90
1:A:413:MET:HG3	1:E:142:ALA:HB1	1.57	0.85
1:G:259:PRO:HA	1:G:280:GLU:HG2	1.59	0.82
1:C:378:PHE:CE1	5:C:1460:DC4:HAD	2.15	0.80
1:I:264:GLN:HA	6:I:2021:HOH:O	1.85	0.77
2:J:180:LEU:HD11	2:L:145:VAL:HG21	1.67	0.76
1:G:126:ALA:HB3	1:G:135:ASN:HB3	1.69	0.74
1:C:226:GLN:O	5:C:1460:DC4:HAC	1.88	0.73
1:C:239:HIS:NE2	6:C:2027:HOH:O	2.22	0.72
3:G:900:FES:S2	6:G:2004:HOH:O	2.50	0.70
1:E:339:ILE:HD11	1:E:357:LEU:HG	1.76	0.68
1:I:123:HIS:HB2	3:I:900:FES:S2	2.35	0.67
1:G:414:GLY:HA2	1:G:417:ARG:HD2	1.76	0.66
1:A:413:MET:HG2	1:A:434:ALA:HA	1.77	0.66
1:G:413:MET:HG2	1:G:434:ALA:HA	1.79	0.65
1:G:123:HIS:HB2	3:G:900:FES:S2	2.35	0.65
1:C:339:ILE:HD11	1:C:357:LEU:HG	1.78	0.65
1:G:276:TRP:HB3	1:G:322:GLN:HG3	1.78	0.65
2:D:180:LEU:HD11	2:F:145:VAL:HG21	1.79	0.65
1:C:413:MET:HE2	1:C:435:GLU:HG3	1.77	0.64
4:C:901:FE2:FE	6:C:2027:HOH:O	1.49	0.64
2:B:175:ASP:OD2	2:D:111:ARG:HB2	1.97	0.64
1:E:251:MET:HG3	1:E:255:GLN:HB2	1.80	0.64
2:D:58:MET:HE2	2:D:81:HIS:HB2	1.80	0.63
2:J:49:LEU:HD21	2:J:163:LEU:HD13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:413:MET:HG2	1:I:434:ALA:HA	1.79	0.63
1:G:366:ILE:HB	6:G:2021:HOH:O	1.98	0.62
1:E:266:ARG:HB3	1:E:428:ASN:ND2	2.14	0.62
1:A:287:VAL:HG21	5:A:1460:DC4:HAD	1.82	0.62
2:J:60:LEU:HD23	2:J:81:HIS:CE1	2.37	0.59
1:E:199:ASP:HB3	1:E:309:LEU:HD21	1.85	0.59
1:I:133:LEU:HG	6:I:2014:HOH:O	2.02	0.59
1:A:265:PHE:CZ	1:A:267:ALA:HA	2.38	0.59
1:G:448:MET:HA	1:G:457:LEU:HD11	1.85	0.58
1:G:195:ASP:HB3	1:G:309:LEU:HD22	1.84	0.58
1:A:123:HIS:HB2	3:A:900:FES:S2	2.44	0.58
2:H:49:LEU:HD21	2:H:163:LEU:HD13	1.84	0.58
2:B:113:LEU:HD13	2:F:135:ILE:HG13	1.85	0.58
1:I:309:LEU:HD13	1:I:316:VAL:HG11	1.84	0.58
1:C:309:LEU:HD13	1:C:316:VAL:HG11	1.87	0.57
1:G:447:ARG:HH21	1:G:457:LEU:HA	1.69	0.57
1:I:319:MET:HG2	6:I:2022:HOH:O	2.05	0.57
1:C:123:HIS:HB2	3:C:900:FES:S2	2.45	0.57
1:C:339:ILE:CD1	1:C:357:LEU:HG	2.34	0.57
1:G:120:CYS:SG	6:G:2004:HOH:O	2.58	0.56
2:H:25:ASN:HD21	2:L:24:GLN:HG2	1.71	0.56
1:C:413:MET:HG2	1:C:434:ALA:HA	1.88	0.56
1:I:262:GLY:HA2	1:I:278:VAL:HG23	1.87	0.55
2:D:58:MET:HE2	2:D:81:HIS:CB	2.36	0.55
1:G:212:GLN:HG2	2:H:60:LEU:HD21	1.88	0.55
2:H:12:PHE:H	2:J:36:GLN:HE21	1.55	0.55
2:D:54:ILE:HA	2:D:168:ALA:O	2.05	0.55
1:A:373:HIS:HD2	1:A:376:ARG:HE	1.54	0.55
2:H:116:ASN:HA	2:J:32:TYR:CD1	2.42	0.55
1:E:332:PHE:HB3	1:E:339:ILE:HG23	1.89	0.55
2:H:135:ILE:HD12	2:J:113:LEU:HD22	1.89	0.54
1:C:378:PHE:HE1	5:C:1460:DC4:CAD	2.15	0.54
1:K:123:HIS:HB2	3:K:900:FES:S2	2.48	0.54
2:H:68:GLU:HB3	2:H:71:LEU:HD12	1.89	0.54
1:C:448:MET:HG2	1:C:457:LEU:HD21	1.89	0.54
1:E:266:ARG:HB3	1:E:428:ASN:HD22	1.73	0.54
1:I:422:HIS:HB2	6:I:2033:HOH:O	2.09	0.53
1:A:262:GLY:C	1:A:432:VAL:HB	2.33	0.53
1:C:414:GLY:HA2	1:C:417:ARG:HD2	1.90	0.53
1:C:231:MET:SD	5:C:1460:DC4:HAE	2.50	0.52
2:J:126:ASP:HB3	2:J:158:ARG:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:448:MET:HA	1:K:457:LEU:HD11	1.91	0.52
1:E:241:SER:HB2	2:F:95:LYS:HG3	1.92	0.52
2:D:24:GLN:HG2	2:F:25:ASN:HD21	1.75	0.52
1:I:241:SER:HB2	2:J:95:LYS:HG3	1.91	0.52
1:G:412:GLN:O	1:G:415:LEU:HB2	2.10	0.51
1:E:123:HIS:HB2	3:E:900:FES:S2	2.51	0.51
2:L:22:GLU:O	2:L:26:GLU:HG3	2.10	0.51
1:C:378:PHE:CE1	5:C:1460:DC4:CAD	2.90	0.51
2:D:12:PHE:H	2:F:36:GLN:NE2	2.08	0.51
2:H:126:ASP:O	2:H:157:ARG:HA	2.10	0.51
2:B:162:ASN:HB3	6:B:2020:HOH:O	2.10	0.51
1:G:201:THR:HG22	1:G:304:LEU:HD23	1.93	0.51
1:G:413:MET:HE2	1:G:435:GLU:HG3	1.92	0.51
1:C:60:LEU:HD23	1:C:341:VAL:HG22	1.92	0.50
2:F:126:ASP:HB3	2:F:158:ARG:HB2	1.92	0.50
2:D:110:THR:HG22	2:D:138:ARG:HG2	1.92	0.50
2:F:110:THR:HA	2:F:137:TYR:O	2.11	0.50
1:A:122:TYR:OH	1:C:226:GLN:NE2	2.44	0.50
1:K:60:LEU:HD11	1:K:171:LEU:HD22	1.94	0.50
2:B:116:ASN:HA	2:D:32:TYR:CD1	2.47	0.49
1:C:422:HIS:HD2	1:C:425:PHE:H	1.59	0.49
1:E:335:ALA:HB3	1:E:336:MET:HE3	1.94	0.49
1:C:340:ARG:HD2	1:C:342:TRP:CH2	2.48	0.49
2:J:180:LEU:HD11	2:L:145:VAL:CG2	2.42	0.49
1:C:276:TRP:HB3	1:C:322:GLN:HG3	1.94	0.49
1:E:126:ALA:HB3	1:E:135:ASN:HB3	1.94	0.49
1:A:169:LYS:HD3	1:A:199:ASP:HB2	1.95	0.48
2:H:150:GLY:HA2	2:H:175:ASP:OD2	2.13	0.48
1:G:228:CYS:HB2	1:G:325:THR:HB	1.95	0.48
1:E:52:ARG:HB3	1:E:448:MET:O	2.13	0.48
1:C:164:ARG:HD2	1:C:178:VAL:HA	1.94	0.48
1:K:344:PRO:HA	1:K:350:ILE:HG22	1.95	0.48
2:B:9:PHE:N	6:B:2001:HOH:O	2.45	0.48
1:E:200:ARG:HB2	6:E:2049:HOH:O	2.14	0.48
1:I:49:GLU:OE2	1:I:221:LYS:NZ	2.44	0.48
2:J:120:LYS:HB3	2:J:129:GLU:HB2	1.96	0.48
1:C:36:ASP:O	1:C:39:ILE:HG12	2.12	0.48
1:C:126:ALA:HB3	1:C:135:ASN:HB3	1.96	0.48
1:I:411:ALA:HA	1:I:435:GLU:OE1	2.14	0.48
2:J:81:HIS:CE1	2:J:179:LEU:HD11	2.49	0.48
1:G:344:PRO:HD3	6:G:2019:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:GLN:HE21	2:L:12:PHE:H	1.62	0.47
1:I:262:GLY:C	1:I:432:VAL:HB	2.39	0.47
1:G:435:GLU:OE2	1:K:103:ARG:NH2	2.44	0.47
1:I:276:TRP:HB3	1:I:322:GLN:HG3	1.97	0.47
1:C:419:GLN:HB2	6:C:2038:HOH:O	2.13	0.47
2:J:135:ILE:HD12	2:L:113:LEU:HD22	1.96	0.47
2:L:54:ILE:HA	2:L:168:ALA:O	2.15	0.47
1:C:359:ASP:HB2	1:C:362:ALA:HB2	1.95	0.47
2:J:118:ILE:HB	2:J:131:ASN:HB3	1.96	0.47
1:E:84:VAL:O	1:E:95:VAL:HA	2.15	0.47
1:G:177:ASP:HB3	1:G:180:ALA:HB2	1.96	0.47
1:E:164:ARG:HD2	1:E:178:VAL:HA	1.97	0.47
1:C:208:ILE:HD12	1:C:356:THR:OG1	2.15	0.47
1:I:58:TRP:HD1	1:I:186:TYR:CG	2.33	0.47
1:E:80:GLU:HG2	1:E:344:PRO:O	2.15	0.46
2:H:59:PRO:HD2	2:H:172:ILE:O	2.14	0.46
1:K:324:MET:HE2	1:K:326:ILE:HD11	1.96	0.46
1:E:183:LEU:O	1:E:187:LEU:HG	2.15	0.46
2:B:25:ASN:HD21	2:F:24:GLN:HG2	1.81	0.46
2:L:31:TYR:HE2	2:L:130:VAL:HG11	1.80	0.46
1:E:208:ILE:HD12	1:E:356:THR:OG1	2.16	0.46
1:E:231:MET:HE2	1:E:323:HIS:HD2	1.80	0.46
2:F:85:THR:O	2:F:89:MET:HG2	2.16	0.46
1:G:340:ARG:HH12	1:G:385:GLU:CD	2.23	0.46
2:D:175:ASP:OD2	2:F:111:ARG:HB2	2.16	0.46
1:I:263:ASN:HB2	1:I:276:TRP:NE1	2.31	0.46
1:I:306:GLU:C	6:I:2025:HOH:O	2.58	0.46
2:L:19:ALA:HB1	2:L:23:LEU:HD23	1.97	0.46
1:K:413:MET:HG2	1:K:434:ALA:HA	1.98	0.46
2:D:35:ALA:HB1	2:D:112:HIS:HB2	1.97	0.46
1:I:19:TRP:HE1	1:I:44:SER:HB2	1.81	0.46
1:I:176:TRP:HB3	1:K:403:LYS:HE3	1.97	0.46
2:L:179:LEU:HD21	2:L:184:LEU:HD11	1.98	0.46
2:B:35:ALA:HB1	2:B:112:HIS:HB2	1.97	0.46
1:C:371:ARG:HD2	2:D:78:ASP:O	2.15	0.46
1:I:217:PRO:HG2	1:I:393:VAL:HG22	1.98	0.45
1:K:229:SER:HB2	1:K:437:ALA:HB3	1.98	0.45
1:K:277:TYR:HB2	1:K:320:VAL:O	2.16	0.45
2:D:116:ASN:HA	2:F:32:TYR:CD1	2.52	0.45
1:A:131:GLY:O	1:A:160:PRO:HD2	2.16	0.45
1:C:332:PHE:HB3	1:C:339:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:ASN:HA	2:F:32:TYR:CG	2.51	0.45
1:E:231:MET:HE2	1:E:323:HIS:CD2	2.51	0.45
2:B:37:LEU:HD23	2:F:11:THR:HG21	1.99	0.45
1:C:195:ASP:HB3	1:C:309:LEU:HD21	1.99	0.45
1:E:215:VAL:O	2:F:182:ASN:HA	2.16	0.45
1:E:290:PRO:HD2	6:E:2052:HOH:O	2.16	0.45
1:E:76:THR:OG1	1:E:77:TYR:N	2.49	0.45
1:I:422:HIS:HD2	1:I:425:PHE:H	1.65	0.45
2:D:49:LEU:HD21	2:D:163:LEU:HD13	1.98	0.45
2:H:36:GLN:NE2	2:L:12:PHE:H	2.15	0.45
2:B:49:LEU:HD21	2:B:163:LEU:HD13	1.99	0.45
1:E:217:PRO:HG2	1:E:393:VAL:HG22	1.99	0.45
2:F:138:ARG:NH2	2:F:181:SER:OG	2.49	0.45
1:I:246:GLY:HA3	1:I:286:ALA:O	2.17	0.45
2:J:116:ASN:HA	2:L:32:TYR:CD1	2.52	0.45
1:A:229:SER:HB2	1:A:437:ALA:HB3	1.99	0.45
1:K:262:GLY:HA2	1:K:278:VAL:HG23	1.98	0.45
2:F:58:MET:HE2	2:F:81:HIS:CB	2.48	0.44
1:G:280:GLU:H	1:G:320:VAL:HG21	1.82	0.44
1:E:422:HIS:CD2	1:E:424:ASP:H	2.36	0.44
1:A:164:ARG:O	1:A:174:ALA:HA	2.18	0.44
1:I:162:GLN:HG2	6:I:2018:HOH:O	2.18	0.44
2:B:12:PHE:H	2:D:36:GLN:NE2	2.16	0.44
2:B:58:MET:HE2	2:B:81:HIS:HB2	2.00	0.44
2:D:19:ALA:HB1	2:D:23:LEU:HD23	1.99	0.44
2:D:135:ILE:HD12	2:F:113:LEU:HD22	2.00	0.44
2:B:126:ASP:HB3	2:B:158:ARG:HB2	1.99	0.43
1:E:339:ILE:CD1	1:E:357:LEU:HG	2.45	0.43
1:I:179:GLN:HE21	1:I:179:GLN:HA	1.82	0.43
1:I:397:LYS:NZ	6:I:2031:HOH:O	2.51	0.43
1:K:154:ASP:O	1:K:158:TRP:HD1	2.01	0.43
2:B:32:TYR:CD1	2:F:116:ASN:HA	2.54	0.43
1:C:213:LYS:HA	1:C:352:VAL:O	2.18	0.43
1:G:336:MET:H	1:G:336:MET:HG2	1.56	0.43
2:H:12:PHE:H	2:J:36:GLN:NE2	2.16	0.43
1:K:381:GLY:HA3	2:L:184:LEU:HB2	2.00	0.43
1:K:259:PRO:HA	1:K:280:GLU:HG2	2.01	0.43
1:K:76:THR:OG1	1:K:77:TYR:N	2.51	0.43
1:A:425:PHE:HA	1:A:426:PRO:HD3	1.86	0.43
1:C:280:GLU:H	1:C:320:VAL:HG21	1.84	0.43
2:D:47:PHE:HB2	2:D:93:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:58:MET:HE2	2:F:81:HIS:HB2	2.00	0.43
1:G:269:TRP:HZ2	1:G:457:LEU:HD22	1.84	0.43
1:E:368:GLU:HG3	1:E:372:ARG:HE	1.84	0.43
2:H:116:ASN:HA	2:J:32:TYR:CG	2.54	0.42
1:I:319:MET:HE3	6:I:2022:HOH:O	2.19	0.42
1:K:266:ARG:HB3	1:K:428:ASN:HB3	2.00	0.42
1:K:339:ILE:HD13	1:K:357:LEU:HG	2.01	0.42
1:A:73:PHE:HA	1:A:85:MET:O	2.19	0.42
1:A:228:CYS:HB2	1:A:325:THR:HB	2.00	0.42
1:A:373:HIS:CD2	1:A:376:ARG:HE	2.37	0.42
2:B:16:SER:HA	6:B:2003:HOH:O	2.19	0.42
2:D:113:LEU:HD23	2:F:113:LEU:CD2	2.49	0.42
1:I:248:PRO:HA	1:I:249:PRO:HD3	1.85	0.42
1:C:383:VAL:HB	2:D:95:LYS:HD3	2.01	0.42
1:G:332:PHE:HB3	1:G:339:ILE:HG23	2.01	0.42
1:I:161:LEU:HD21	1:K:403:LYS:HD2	2.01	0.42
1:A:251:MET:HG3	1:A:255:GLN:HB2	2.01	0.42
1:A:412:GLN:O	1:A:415:LEU:HB2	2.18	0.42
1:K:451:GLU:HA	1:K:452:PRO:HD3	1.88	0.42
2:L:58:MET:HE2	2:L:81:HIS:CB	2.50	0.42
2:H:60:LEU:HG	2:H:80:ALA:HA	2.02	0.42
1:E:413:MET:HE2	1:E:435:GLU:HG3	2.02	0.42
2:H:104:GLU:HG2	2:H:185:SER:HB2	2.01	0.42
1:A:269:TRP:CZ2	1:A:444:HIS:HE1	2.37	0.42
1:A:333:LEU:HD12	1:A:338:GLN:HB3	2.02	0.42
1:E:276:TRP:HB3	1:E:322:GLN:HG3	2.01	0.42
2:F:58:MET:HG3	2:F:172:ILE:HB	2.01	0.42
1:I:340:ARG:HD3	1:I:342:TRP:CH2	2.55	0.42
1:A:334:PRO:O	1:A:337:ASN:OD1	2.37	0.41
1:K:391:ASN:HD22	1:K:391:ASN:HA	1.64	0.41
1:A:365:GLU:H	1:A:365:GLU:CD	2.28	0.41
1:C:323:HIS:CD2	5:C:1460:DC4:HAB	2.55	0.41
2:F:161:ASN:HB2	6:F:2018:HOH:O	2.19	0.41
2:B:58:MET:HE1	2:B:184:LEU:HD13	2.01	0.41
2:B:168:ALA:O	2:B:169:LYS:HG2	2.21	0.41
1:E:336:MET:H	1:E:336:MET:HG2	1.60	0.41
1:G:36:ASP:HA	1:G:37:PRO:HD3	1.89	0.41
1:E:177:ASP:HB3	1:E:180:ALA:HB2	2.02	0.41
2:B:51:ASP:OD2	2:B:157:ARG:NH1	2.53	0.41
2:B:111:ARG:HB2	2:F:175:ASP:OD2	2.21	0.41
2:H:54:ILE:HA	2:H:168:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:212:GLN:HE21	1:I:212:GLN:HB2	1.62	0.41
1:I:458:LYS:HA	1:I:459:PRO:HD3	1.92	0.41
1:C:284:LEU:HD23	1:C:293:THR:HG23	2.02	0.41
1:E:257:GLN:HG2	6:E:2040:HOH:O	2.20	0.41
1:G:230:ASP:OD2	1:K:123:HIS:NE2	2.45	0.41
1:K:314:MET:HA	1:K:315:PRO:HD3	1.92	0.41
1:A:244:LEU:HD13	1:A:253:LEU:HG	2.03	0.41
1:I:175:ASN:HB2	6:I:2007:HOH:O	2.21	0.41
1:K:307:GLN:HB3	6:K:2014:HOH:O	2.20	0.41
1:A:248:PRO:HA	1:A:249:PRO:HD2	1.86	0.41
1:C:231:MET:HE2	1:C:323:HIS:HD2	1.86	0.41
1:C:375:ILE:HD11	2:D:79:LEU:HA	2.02	0.41
5:C:1460:DC4:CAH	6:C:2027:HOH:O	2.69	0.41
2:D:125:PRO:O	2:D:126:ASP:HB2	2.20	0.41
1:E:218:CYS:HA	1:E:396:GLN:HG2	2.03	0.41
1:C:136:VAL:O	1:C:139:GLU:HB2	2.21	0.41
1:C:336:MET:H	1:C:336:MET:HG2	1.56	0.41
1:E:42:ASP:OD2	1:E:44:SER:HB2	2.21	0.41
1:E:413:MET:HB2	1:E:435:GLU:OE1	2.21	0.41
1:I:63:HIS:CD2	1:I:357:LEU:HD21	2.56	0.41
1:E:269:TRP:CZ2	1:E:444:HIS:HE1	2.40	0.40
1:K:276:TRP:HB3	1:K:322:GLN:HG3	2.02	0.40
1:C:107:ILE:HG22	1:C:118:PHE:HB3	2.03	0.40
2:F:58:MET:HA	2:F:59:PRO:HD2	1.98	0.40
1:A:65:SER:O	1:A:68:PRO:HG3	2.22	0.40
1:A:257:GLN:HG2	6:A:2034:HOH:O	2.21	0.40
2:H:161:ASN:HB3	6:H:2018:HOH:O	2.21	0.40
1:K:25:ARG:HG2	1:K:446:MET:SD	2.61	0.40
1:K:226:GLN:HA	1:K:230:ASP:CB	2.52	0.40
1:A:448:MET:HA	1:A:457:LEU:HD11	2.04	0.40
1:K:327:PHE:HA	1:K:328:PRO:HA	1.92	0.40
1:C:200:ARG:O	1:C:308:ARG:HD3	2.21	0.40
1:E:64:GLU:HG3	1:E:170:GLY:O	2.21	0.40
1:G:74:LEU:HD12	1:G:112:ALA:HB2	2.03	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%)	405 (94%)	23 (5%)	1 (0%)	43	66
1	C	429/459 (94%)	404 (94%)	25 (6%)	0	100	100
1	E	429/459 (94%)	409 (95%)	20 (5%)	0	100	100
1	G	429/459 (94%)	399 (93%)	25 (6%)	5 (1%)	10	23
1	I	429/459 (94%)	400 (93%)	28 (6%)	1 (0%)	43	66
1	K	429/459 (94%)	394 (92%)	32 (8%)	3 (1%)	18	38
2	B	178/188 (95%)	171 (96%)	7 (4%)	0	100	100
2	D	178/188 (95%)	171 (96%)	7 (4%)	0	100	100
2	F	178/188 (95%)	168 (94%)	10 (6%)	0	100	100
2	H	178/188 (95%)	168 (94%)	10 (6%)	0	100	100
2	J	178/188 (95%)	169 (95%)	9 (5%)	0	100	100
2	L	178/188 (95%)	167 (94%)	11 (6%)	0	100	100
All	All	3642/3882 (94%)	3425 (94%)	207 (6%)	10 (0%)	36	58

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	256	ALA
1	G	257	GLN
1	I	256	ALA
1	K	256	ALA
1	K	257	GLN
1	G	255	GLN
1	G	68	PRO
1	G	282	GLY
1	A	328	PRO
1	K	328	PRO

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%)	343 (98%)	7 (2%)	48	74
1	C	350/372 (94%)	340 (97%)	10 (3%)	37	65
1	E	350/372 (94%)	339 (97%)	11 (3%)	35	63
1	G	350/372 (94%)	342 (98%)	8 (2%)	44	71
1	I	350/372 (94%)	342 (98%)	8 (2%)	44	71
1	K	350/372 (94%)	345 (99%)	5 (1%)	59	81
2	B	159/167 (95%)	156 (98%)	3 (2%)	50	75
2	D	159/167 (95%)	155 (98%)	4 (2%)	42	69
2	F	159/167 (95%)	158 (99%)	1 (1%)	78	91
2	H	159/167 (95%)	156 (98%)	3 (2%)	50	75
2	J	159/167 (95%)	158 (99%)	1 (1%)	78	91
2	L	159/167 (95%)	157 (99%)	2 (1%)	61	82
All	All	3054/3234 (94%)	2991 (98%)	63 (2%)	47	73

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	THR
1	A	250	GLU
1	A	257	GLN
1	A	336	MET
1	A	356	THR
1	A	420	THR
1	A	457	LEU
2	B	10	LYS
2	B	87	GLU
2	B	113	LEU
1	C	74	LEU
1	C	89	LYS
1	C	132	LYS
1	C	179	GLN

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Mol	Chain	Res	Type
1	C	201	THR
1	C	225	GLU
1	C	255	GLN
1	C	258	ILE
1	C	280	GLU
1	C	339	ILE
2	D	94	ARG
2	D	124	THR
2	D	140	ARG
2	D	180	LEU
1	E	86	VAL
1	E	167	THR
1	E	201	THR
1	E	336	MET
1	E	338	GLN
1	E	339	ILE
1	E	356	THR
1	E	419	GLN
1	E	420	THR
1	E	428	ASN
1	E	457	LEU
2	F	44	GLU
1	G	48	LEU
1	G	119	THR
1	G	229	SER
1	G	280	GLU
1	G	336	MET
1	G	365	GLU
1	G	422	HIS
1	G	457	LEU
2	H	70	GLU
2	H	99	ASP
2	H	179	LEU
1	I	103	ARG
1	I	119	THR
1	I	167	THR
1	I	179	GLN
1	I	358	VAL
1	I	369	GLU
1	I	419	GLN
1	I	457	LEU
2	J	10	LYS

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Mol	Chain	Res	Type
1	K	86	VAL
1	K	260	THR
1	K	320	VAL
1	K	336	MET
1	K	457	LEU
2	L	113	LEU
2	L	143	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	43	GLN
1	A	226	GLN
1	A	264	GLN
1	A	373	HIS
1	A	377	ASN
1	A	391	ASN
1	A	407	GLN
1	A	410	ASN
1	A	444	HIS
2	B	25	ASN
1	C	88	GLN
1	C	212	GLN
1	C	226	GLN
1	C	257	GLN
1	C	263	ASN
1	C	322	GLN
1	C	348	ASN
1	C	373	HIS
1	C	377	ASN
1	C	386	GLN
1	C	391	ASN
1	C	407	GLN
1	C	410	ASN
1	C	422	HIS
1	C	443	HIS
2	D	25	ASN
2	D	36	GLN
2	D	131	ASN
1	E	43	GLN
1	E	179	GLN

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Mol	Chain	Res	Type
1	E	212	GLN
1	E	226	GLN
1	E	338	GLN
1	E	343	HIS
1	E	373	HIS
1	E	374	ASN
1	E	386	GLN
1	E	391	ASN
1	E	410	ASN
1	E	422	HIS
1	E	428	ASN
1	E	443	HIS
1	E	444	HIS
2	F	25	ASN
2	F	36	GLN
2	F	77	GLN
1	G	43	GLN
1	G	88	GLN
1	G	212	GLN
1	G	226	GLN
1	G	337	ASN
1	G	407	GLN
1	G	419	GLN
1	G	444	HIS
2	H	25	ASN
2	H	36	GLN
2	H	77	GLN
2	H	131	ASN
1	I	99	GLN
1	I	179	GLN
1	I	212	GLN
1	I	419	GLN
1	I	422	HIS
1	I	443	HIS
1	I	444	HIS
2	J	25	ASN
2	J	36	GLN
2	J	131	ASN
1	K	88	GLN
1	K	99	GLN
1	K	226	GLN
1	K	263	ASN

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Mol	Chain	Res	Type
1	K	307	GLN
1	K	348	ASN
1	K	391	ASN
1	K	396	GLN
1	K	407	GLN
1	K	410	ASN
1	K	443	HIS
2	L	25	ASN
2	L	36	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 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	C	900	1	0,4,4	-	-	-		
5	DC4	C	1460	-	16,16,16	0.99	1 (6%)	23,23,23	2.60	8 (34%)
5	DC4	A	1460	-	16,16,16	0.94	1 (6%)	23,23,23	2.39	7 (30%)
3	FES	A	900	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FES	I	900	1	0,4,4	-	-	-		
3	FES	E	900	1	0,4,4	-	-	-		
3	FES	K	900	1	0,4,4	-	-	-		
3	FES	G	900	1,6	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
3	FES	C	900	1	-	-	0/1/1/1
5	DC4	C	1460	-	-	-	0/3/3/3
5	DC4	A	1460	-	-	-	0/3/3/3
3	FES	A	900	1	-	-	0/1/1/1
3	FES	I	900	1	-	-	0/1/1/1
3	FES	E	900	1	-	-	0/1/1/1
3	FES	K	900	1	-	-	0/1/1/1
3	FES	G	900	1,6	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1460	DC4	CAM-CAN	-3.21	1.38	1.46
5	A	1460	DC4	CAM-CAN	-2.78	1.39	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1460	DC4	OAI-CAL-CAG	5.94	132.18	124.14
5	C	1460	DC4	OAI-CAK-CAE	5.88	132.11	124.14
5	A	1460	DC4	OAI-CAL-CAG	5.57	131.68	124.14
5	A	1460	DC4	OAI-CAK-CAE	5.56	131.68	124.14
5	C	1460	DC4	CAE-CAK-CAM	-4.41	119.36	123.64
5	C	1460	DC4	CAG-CAL-CAN	-4.15	119.60	123.64
5	A	1460	DC4	CAL-OAI-CAK	4.02	109.16	105.41
5	A	1460	DC4	CAG-CAL-CAN	-3.54	120.20	123.64
5	A	1460	DC4	OAI-CAK-CAM	-3.34	107.84	111.68
5	A	1460	DC4	CAE-CAK-CAM	-3.25	120.49	123.64
5	C	1460	DC4	CAL-OAI-CAK	3.15	108.35	105.41
5	A	1460	DC4	OAI-CAL-CAN	-3.10	108.12	111.68
5	C	1460	DC4	OAI-CAL-CAN	-3.02	108.21	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1460	DC4	OAI-CAK-CAM	-2.74	108.53	111.68
5	C	1460	DC4	CAF-CAM-CAK	2.46	121.21	118.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	900	FES	1	0
5	C	1460	DC4	8	0
5	A	1460	DC4	1	0
3	A	900	FES	1	0
3	I	900	FES	1	0
3	E	900	FES	1	0
3	K	900	FES	1	0
3	G	900	FES	2	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	433/459 (94%)	0.03	9 (2%) 63 58	30, 49, 66, 74	18 (4%)
1	C	433/459 (94%)	0.16	8 (1%) 67 63	31, 54, 79, 88	18 (4%)
1	E	433/459 (94%)	0.04	8 (1%) 67 63	29, 51, 72, 81	18 (4%)
1	G	433/459 (94%)	0.52	14 (3%) 50 44	46, 93, 141, 162	18 (4%)
1	I	433/459 (94%)	0.57	17 (3%) 43 38	46, 93, 140, 162	18 (4%)
1	K	433/459 (94%)	0.61	20 (4%) 37 32	46, 94, 137, 156	18 (4%)
2	B	180/188 (95%)	-0.07	1 (0%) 85 83	30, 46, 61, 68	4 (2%)
2	D	180/188 (95%)	-0.05	1 (0%) 85 83	33, 48, 62, 70	4 (2%)
2	F	180/188 (95%)	-0.06	0 100 100	31, 48, 67, 74	4 (2%)
2	H	180/188 (95%)	0.09	0 100 100	37, 61, 84, 95	4 (2%)
2	J	180/188 (95%)	0.09	0 100 100	39, 64, 84, 94	4 (2%)
2	L	180/188 (95%)	0.06	0 100 100	38, 61, 80, 91	4 (2%)
All	All	3678/3882 (94%)	0.23	78 (2%) 63 58	29, 61, 120, 162	132 (3%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	256	ALA	6.4
1	I	257	GLN	6.0
1	C	256	ALA	6.0
1	E	256	ALA	6.0
1	C	257	GLN	5.9
1	I	258	ILE	5.6
1	E	259	PRO	5.6
1	I	259	PRO	5.4
1	K	260	THR	5.3
1	G	256	ALA	5.3
1	G	259	PRO	5.2

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Mol	Chain	Res	Type	RSRZ
1	K	257	GLN	5.2
1	A	259	PRO	5.2
1	I	256	ALA	5.1
1	E	257	GLN	5.1
1	C	259	PRO	5.1
1	E	258	ILE	5.0
1	A	256	ALA	5.0
1	A	260	THR	4.7
1	G	258	ILE	4.5
1	A	258	ILE	4.4
1	K	259	PRO	4.2
1	A	257	GLN	4.2
1	G	257	GLN	4.2
1	E	255	GLN	3.9
1	K	34	LEU	3.9
1	K	255	GLN	3.9
1	K	258	ILE	3.9
1	E	260	THR	3.8
1	G	260	THR	3.6
1	G	109	ARG	3.6
1	A	283	SER	3.6
2	D	188	PHE	3.5
1	A	261	LYS	3.3
1	I	260	THR	3.2
1	G	261	LYS	3.2
1	C	258	ILE	3.2
1	A	255	GLN	3.1
1	E	261	LYS	3.1
1	A	105	MET	3.1
1	I	285	LEU	3.1
1	G	143	PHE	3.1
1	I	255	GLN	3.0
1	I	261	LYS	3.0
1	I	109	ARG	2.9
1	G	255	GLN	2.8
1	C	261	LYS	2.7
1	C	260	THR	2.7
1	K	52	ARG	2.6
1	K	283	SER	2.5
1	I	195	ASP	2.5
1	I	93	ILE	2.4
1	G	178	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	293	THR	2.3
1	G	275	GLY	2.3
1	K	455	ALA	2.3
2	B	163	LEU	2.3
1	K	109	ARG	2.3
1	E	105	MET	2.2
1	I	168	TYR	2.2
1	K	410	ASN	2.2
1	C	94	LYS	2.2
1	K	94	LYS	2.2
1	G	228	CYS	2.1
1	K	433	TYR	2.1
1	C	255	GLN	2.1
1	K	285	LEU	2.1
1	I	129	ILE	2.1
1	I	287	VAL	2.1
1	G	105	MET	2.1
1	K	39	ILE	2.1
1	K	300	PRO	2.1
1	I	85	MET	2.1
1	I	171	LEU	2.1
1	G	206	VAL	2.1
1	I	455	ALA	2.0
1	K	261	LYS	2.0
1	K	449	MET	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	DC4	C	1460	14/14	0.80	0.30	53,53,53,53	14
5	DC4	A	1460	14/14	0.91	0.23	49,49,49,49	14
3	FES	K	900	4/4	0.97	0.05	71,72,72,72	0
3	FES	C	900	4/4	0.97	0.05	46,49,49,50	0
3	FES	I	900	4/4	0.97	0.05	76,76,76,77	0
4	FE2	K	901	1/1	0.98	0.03	76,76,76,76	0
3	FES	E	900	4/4	0.98	0.05	40,40,41,41	0
3	FES	G	900	4/4	0.98	0.04	65,67,68,68	0
4	FE2	G	901	1/1	0.99	0.04	89,89,89,89	0
4	FE2	I	901	1/1	0.99	0.03	67,67,67,67	0
3	FES	A	900	4/4	0.99	0.04	46,46,46,48	0
4	FE2	C	901	1/1	0.99	0.04	57,57,57,57	0
4	FE2	E	901	1/1	0.99	0.03	41,41,41,41	0
4	FE2	A	901	1/1	1.00	0.02	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.