



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:30 PM UTC

PDB ID : 2XSH / pdb_00002xsh
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 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

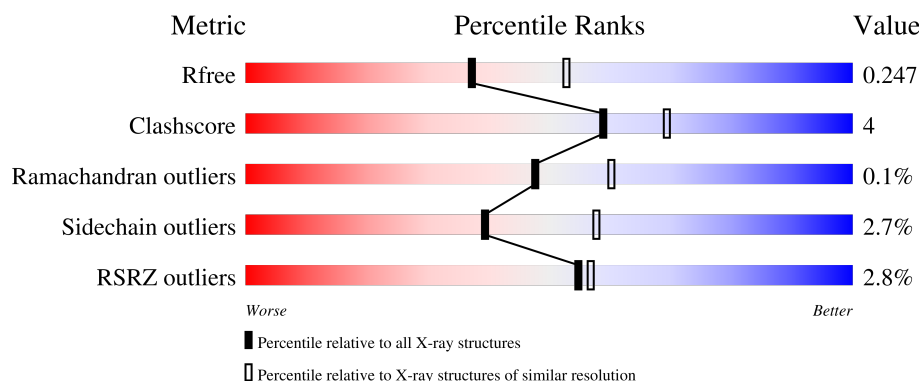
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	2% 85% 8% 6%
1	C	459	2% 83% 12% 6%
1	E	459	2% 81% 12% 6%
1	G	459	5% 83% 11% 6%
1	I	459	5% 82% 12% 6%

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Mol	Chain	Length	Quality of chain
1	K	459	7% 81% 14% 6%
2	B	188	84% 11% 5%
2	D	188	% 82% 13% 3%
2	F	188	% 81% 14% 3%
2	H	188	86% 10% 4%
2	J	188	89% 6% 5%
2	L	188	87% 8% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30603 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
			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			

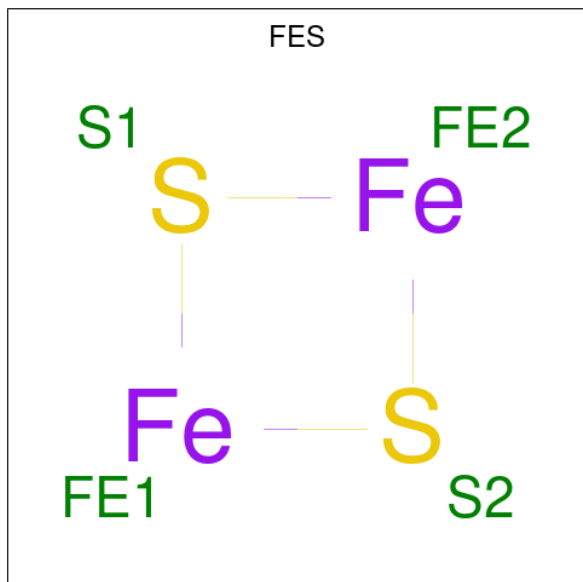
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	ALA	THR	engineered mutation	UNP P37333
C	335	ALA	THR	engineered mutation	UNP P37333
E	335	ALA	THR	engineered mutation	UNP P37333
G	335	ALA	THR	engineered mutation	UNP P37333
I	335	ALA	THR	engineered mutation	UNP P37333
K	335	ALA	THR	engineered mutation	UNP P37333
A	336	MET	PHE	engineered mutation	UNP P37333
C	336	MET	PHE	engineered mutation	UNP P37333
E	336	MET	PHE	engineered mutation	UNP P37333
G	336	MET	PHE	engineered mutation	UNP P37333
I	336	MET	PHE	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 (CCD ID: FES) (formula: Fe_2S_2).

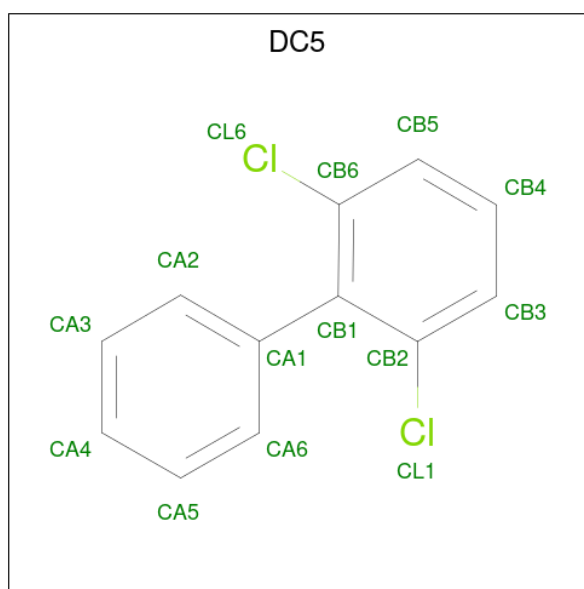


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	I	1	Total	Fe	S	0	0
			4	2	2		
3	K	1	Total	Fe	S	0	0
			4	2	2		

- 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 2,6-DICHLOROBIPHENYL (CCD ID: DC5) (formula: C₁₂H₈Cl₂).



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

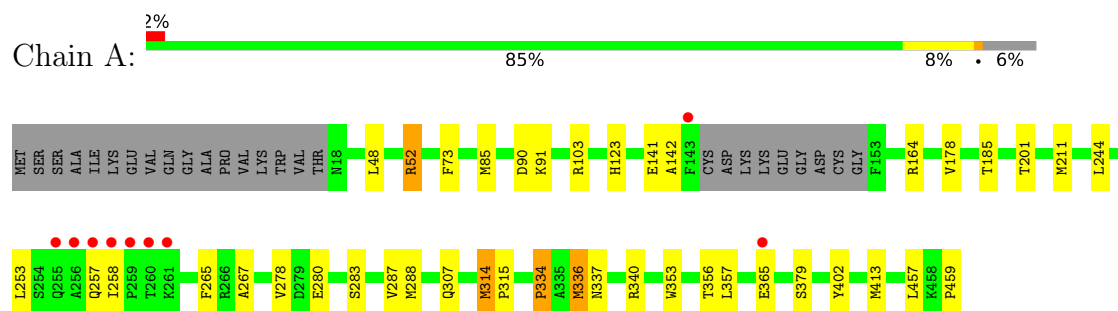
- Molecule 6 is water.

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

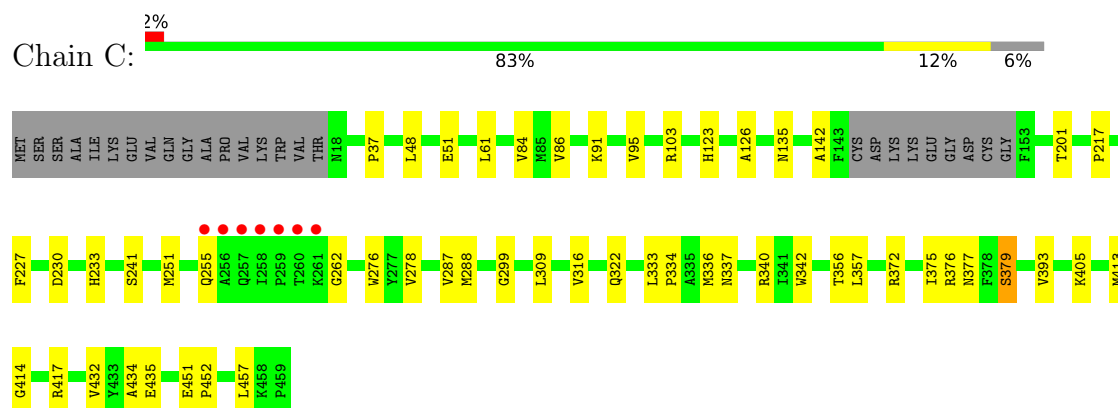
3 Residue-property plots [i](#)

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.

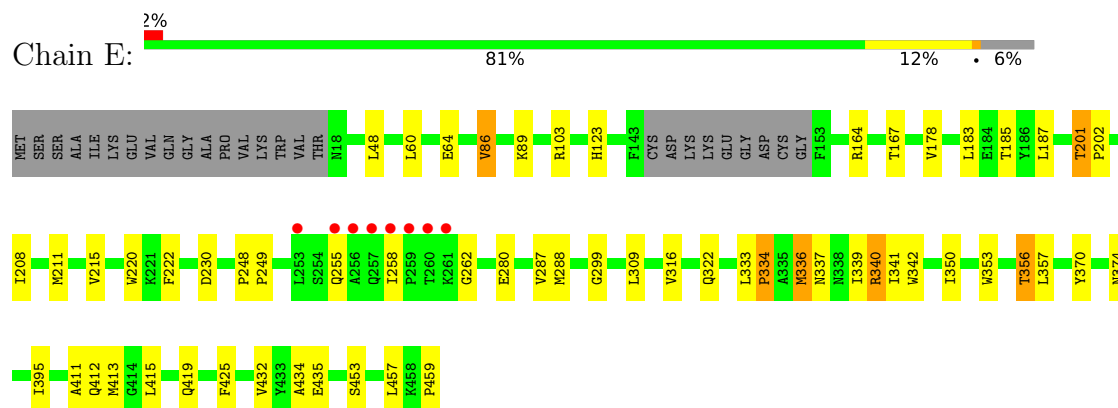
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



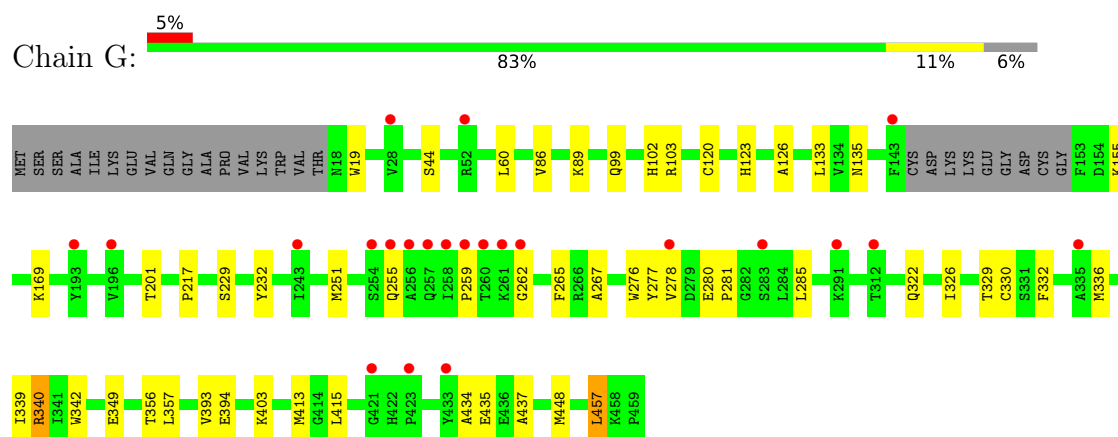
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



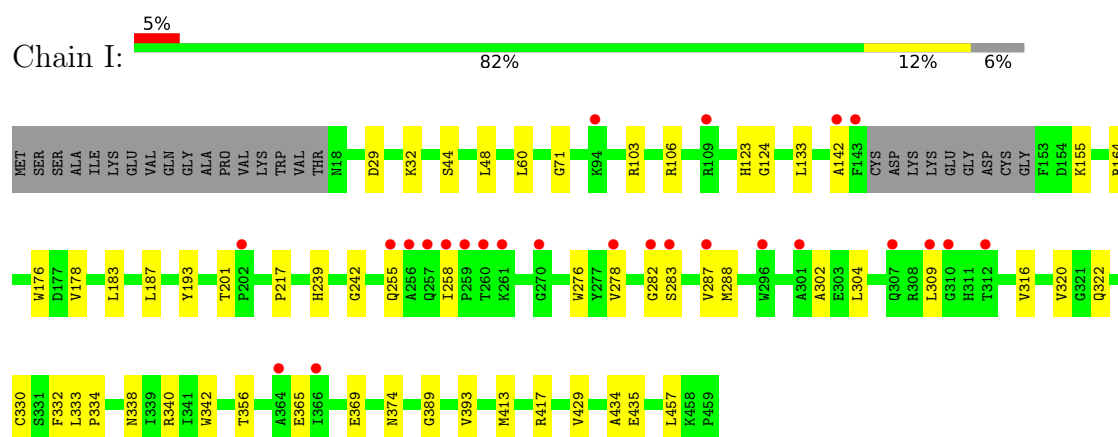
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



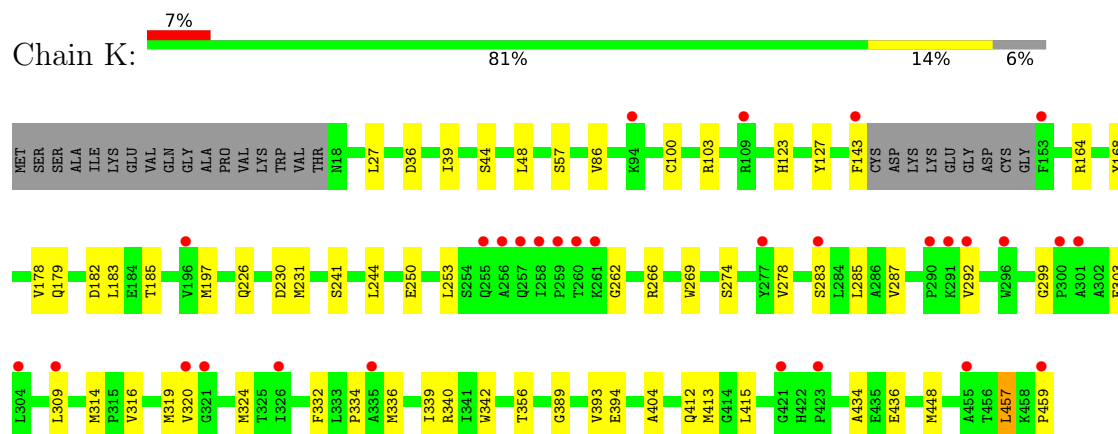
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



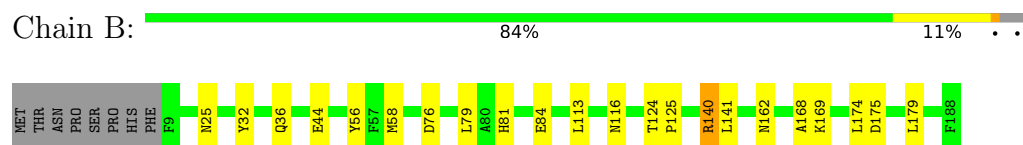
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



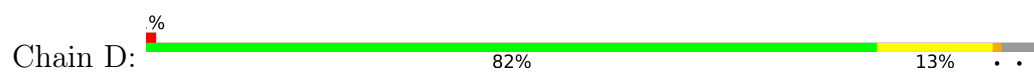
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



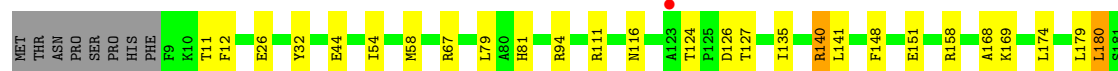
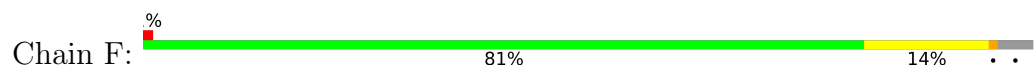
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



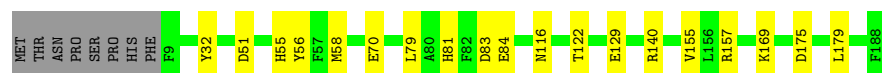
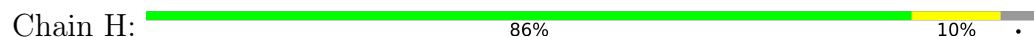
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



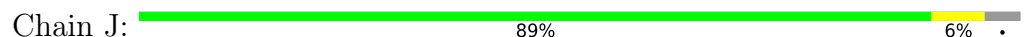
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



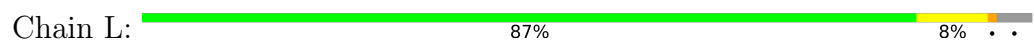
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



• 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	86.73Å 276.76Å 92.32Å 90.00° 117.37° 90.00°	Depositor
Resolution (Å)	138.68 – 2.29 138.38 – 2.29	Depositor EDS
% Data completeness (in resolution range)	87.7 (138.68-2.29) 88.1 (138.38-2.29)	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 0.188 , 0.247	Depositor DCC
R_{free} test set	7632 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	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.

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, FES, DC5

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	0.62	0/3529	0.87	2/4791 (0.0%)
1	C	0.62	0/3529	0.87	4/4791 (0.1%)
1	E	0.59	0/3529	0.87	6/4791 (0.1%)
1	G	0.49	0/3529	0.82	1/4791 (0.0%)
1	I	0.49	0/3529	0.82	0/4791
1	K	0.48	0/3529	0.81	4/4791 (0.1%)
2	B	0.62	0/1530	0.80	0/2068
2	D	0.60	0/1530	0.79	0/2068
2	F	0.59	0/1530	0.80	0/2068
2	H	0.53	0/1530	0.76	0/2068
2	J	0.51	0/1530	0.76	0/2068
2	L	0.51	0/1530	0.73	0/2068
All	All	0.56	0/30354	0.82	17/41154 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	299	GLY	CA-C-N	7.42	126.96	119.24
1	E	299	GLY	C-N-CA	7.42	126.96	119.24
1	C	299	GLY	CA-C-N	6.78	126.02	118.97
1	C	299	GLY	C-N-CA	6.78	126.02	118.97
1	E	230	ASP	N-CA-C	5.95	117.56	109.11
1	C	333	LEU	CA-C-N	5.77	125.89	119.32
1	C	333	LEU	C-N-CA	5.77	125.89	119.32
1	G	329	THR	N-CA-C	5.58	117.58	110.61
1	A	340	ARG	N-CA-C	5.37	117.56	109.23
1	K	231	MET	N-CA-C	-5.36	106.58	113.23
1	A	314	MET	N-CA-C	5.26	117.84	109.64
1	K	320	VAL	N-CA-C	5.18	114.24	106.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	86	VAL	N-CA-C	5.17	115.72	108.17
1	E	425	PHE	CA-C-N	5.07	124.97	119.85
1	E	425	PHE	C-N-CA	5.07	124.97	119.85
1	K	299	GLY	CA-C-N	5.07	124.68	119.05
1	K	299	GLY	C-N-CA	5.07	124.68	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3427	0	3276	25	0
1	C	3427	0	3276	30	0
1	E	3427	0	3276	36	0
1	G	3427	0	3276	29	0
1	I	3427	0	3276	36	0
1	K	3427	0	3276	36	0
2	B	1496	0	1447	18	0
2	D	1496	0	1447	27	0
2	F	1496	0	1447	24	0
2	H	1496	0	1447	13	0
2	J	1496	0	1447	6	0
2	L	1496	0	1447	12	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	1	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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
6	B	82	0	0	2	0
6	C	129	0	0	2	0
6	D	81	0	0	2	0
6	E	128	0	0	0	0
6	F	79	0	0	0	0
6	G	82	0	0	3	0
6	H	51	0	0	0	0
6	I	80	0	0	10	0
6	J	32	0	0	1	0
6	K	79	0	0	5	0
6	L	31	0	0	1	0
All	All	30603	0	28362	254	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 4.

All (254) 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)
2:D:58:MET:HE2	2:D:81:HIS:HB2	1.54	0.87
2:F:58:MET:HE2	2:F:81:HIS:CB	2.05	0.87
1:I:155:LYS:HD2	6:I:2029:HOH:O	1.81	0.81
1:C:287:VAL:HG12	1:C:288:MET:HE3	1.64	0.79
2:D:58:MET:HE1	2:D:184:LEU:HD13	1.65	0.79
1:I:133:LEU:HG	6:I:2029:HOH:O	1.83	0.78
1:E:413:MET:HE2	1:E:435:GLU:HG3	1.65	0.77
1:I:302:ALA:HB3	6:I:2055:HOH:O	1.84	0.77
1:A:287:VAL:HG12	1:A:288:MET:HE2	1.67	0.76
2:F:58:MET:HE2	2:F:81:HIS:HB2	1.69	0.75
1:C:201:THR:HB	6:C:2100:HOH:O	1.86	0.75
2:D:58:MET:CE	2:D:81:HIS:HB2	2.17	0.74
2:D:58:MET:HE2	2:D:81:HIS:CB	2.17	0.74
2:D:40:HIS:HE1	2:F:151:GLU:OE2	1.71	0.73
1:G:232:TYR:HB2	6:G:2049:HOH:O	1.89	0.73
2:D:58:MET:HE1	2:D:184:LEU:CD1	2.20	0.72
1:E:123:HIS:HB2	3:E:901:FES:S2	2.29	0.72
2:D:36:GLN:HE21	2:F:12:PHE:H	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:HIS:HB2	3:G:900:FES:S2	2.30	0.70
2:B:162:ASN:HB3	6:B:2075:HOH:O	1.90	0.70
1:K:389:GLY:O	1:K:393:VAL:HG23	1.92	0.69
1:I:309:LEU:HD13	1:I:316:VAL:HG11	1.74	0.69
1:A:287:VAL:HG12	1:A:288:MET:CE	2.22	0.69
1:A:334:PRO:O	1:A:337:ASN:OD1	2.10	0.68
1:G:339:ILE:HD13	1:G:357:LEU:HG	1.75	0.67
2:D:58:MET:CE	2:D:81:HIS:CB	2.72	0.67
1:K:292:VAL:HA	6:K:2053:HOH:O	1.94	0.66
2:B:58:MET:HE3	2:B:174:LEU:HD22	1.78	0.66
2:D:41:ARG:HD3	6:D:2019:HOH:O	1.96	0.66
1:K:314:MET:HA	6:K:2073:HOH:O	1.96	0.65
1:E:334:PRO:O	1:E:337:ASN:OD1	2.15	0.64
1:K:413:MET:HG2	1:K:434:ALA:HA	1.79	0.64
2:J:76:ASP:HB2	6:J:2016:HOH:O	1.97	0.64
1:C:309:LEU:HD12	1:C:316:VAL:HG11	1.80	0.63
1:I:413:MET:HE2	1:I:435:GLU:HG3	1.80	0.63
2:H:58:MET:HE2	2:H:81:HIS:CB	2.29	0.63
1:A:356:THR:HG23	2:B:79:LEU:HD11	1.81	0.61
1:K:319:MET:HG2	6:K:2048:HOH:O	2.00	0.61
1:I:283:SER:O	1:I:287:VAL:HG23	2.00	0.61
1:A:244:LEU:HD13	1:A:253:LEU:HG	1.82	0.61
2:B:113:LEU:HD21	2:D:113:LEU:HD23	1.82	0.61
2:J:49:LEU:HD21	2:J:163:LEU:HD13	1.84	0.60
1:E:412:GLN:O	1:E:415:LEU:HB2	2.02	0.60
1:K:303:GLU:HA	6:K:2057:HOH:O	2.01	0.59
1:C:262:GLY:HA2	1:C:278:VAL:HG23	1.84	0.59
1:I:276:TRP:HB3	1:I:322:GLN:HG3	1.85	0.59
1:K:185:THR:HG22	1:K:459:PRO:HG2	1.84	0.59
1:G:448:MET:HA	1:G:457:LEU:HD11	1.83	0.59
1:K:123:HIS:HB2	3:K:900:FES:S2	2.43	0.59
1:K:309:LEU:HD13	1:K:316:VAL:HG11	1.85	0.58
2:D:40:HIS:CE1	2:F:151:GLU:OE2	2.54	0.58
2:L:44:GLU:HG3	6:L:2011:HOH:O	2.03	0.58
2:H:32:TYR:CD1	2:J:116:ASN:HA	2.39	0.58
2:B:175:ASP:OD2	2:F:111:ARG:HB2	2.04	0.58
1:G:229:SER:HB2	1:G:437:ALA:HB3	1.86	0.57
2:F:168:ALA:O	2:F:169:LYS:HG2	2.04	0.57
1:I:123:HIS:HB2	3:I:900:FES:S2	2.43	0.57
1:C:287:VAL:HG12	1:C:288:MET:CE	2.33	0.56
2:L:54:ILE:HA	2:L:168:ALA:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:239:HIS:HB3	6:I:2040:HOH:O	2.04	0.56
1:E:287:VAL:HG12	1:E:288:MET:CE	2.36	0.56
1:G:120:CYS:SG	6:G:2023:HOH:O	2.58	0.56
2:H:70:GLU:H	2:H:70:GLU:CD	2.14	0.55
2:B:58:MET:CE	2:B:174:LEU:HD22	2.36	0.55
1:A:288:MET:HE3	1:A:336:MET:HB3	1.88	0.55
1:K:182:ASP:HB3	6:K:2031:HOH:O	2.06	0.55
2:H:56:TYR:HB3	2:H:84:GLU:HB2	1.89	0.55
1:G:262:GLY:HA2	1:G:278:VAL:HG23	1.89	0.55
1:A:283:SER:O	1:A:287:VAL:HG23	2.06	0.54
1:I:287:VAL:HG12	1:I:288:MET:CE	2.37	0.54
1:G:276:TRP:HB3	1:G:322:GLN:HG3	1.89	0.54
1:G:251:MET:HG3	1:G:255:GLN:HB2	1.89	0.54
1:G:413:MET:HE2	1:G:435:GLU:HG3	1.90	0.54
1:I:201:THR:HG22	1:I:304:LEU:HD23	1.89	0.54
1:E:340:ARG:HD3	1:E:342:TRP:CH2	2.43	0.53
1:K:36:ASP:O	1:K:39:ILE:HG12	2.08	0.53
1:I:417:ARG:HH21	1:K:143:PHE:C	2.17	0.53
1:G:102:HIS:HB3	6:G:2019:HOH:O	2.09	0.53
1:C:414:GLY:HA2	1:C:417:ARG:HD2	1.90	0.53
1:E:309:LEU:HD13	1:E:316:VAL:HG11	1.90	0.53
1:I:340:ARG:HD3	1:I:342:TRP:CH2	2.44	0.53
1:G:265:PHE:CZ	1:G:267:ALA:HA	2.43	0.52
1:I:287:VAL:HG12	1:I:288:MET:HE3	1.91	0.52
1:E:333:LEU:CB	1:E:336:MET:HG3	2.39	0.52
1:G:340:ARG:HD3	1:G:342:TRP:CH2	2.44	0.52
1:K:197:MET:HB2	1:K:334:PRO:HB3	1.90	0.52
1:A:413:MET:HG3	1:C:142:ALA:HB1	1.93	0.51
1:G:126:ALA:HB3	1:G:135:ASN:HB3	1.92	0.51
2:D:36:GLN:NE2	2:F:12:PHE:H	2.06	0.51
1:K:266:ARG:NH1	1:K:436:GLU:OE1	2.42	0.51
2:F:58:MET:HE2	2:F:81:HIS:HB3	1.88	0.51
2:J:73:TYR:CE1	2:J:173:LEU:HD22	2.46	0.51
2:B:58:MET:HE2	2:B:81:HIS:CG	2.46	0.50
2:D:32:TYR:CD1	2:F:116:ASN:HA	2.46	0.50
1:K:394:GLU:OE1	2:L:141:LEU:HD13	2.12	0.50
2:D:145:VAL:HG21	2:F:180:LEU:HD11	1.94	0.49
1:A:52:ARG:HD3	6:A:2135:HOH:O	2.11	0.49
1:G:332:PHE:HB3	1:G:339:ILE:HG13	1.94	0.49
1:K:241:SER:HB2	2:L:95:LYS:HG3	1.93	0.49
1:I:183:LEU:O	1:I:187:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:44:SER:O	1:I:48:LEU:HD23	2.13	0.49
2:H:58:MET:HE2	2:H:81:HIS:HB2	1.95	0.48
2:F:124:THR:HB	2:F:127:THR:HB	1.94	0.48
1:A:52:ARG:HD2	6:A:2017:HOH:O	2.14	0.48
1:C:123:HIS:HB2	3:C:900:FES:S2	2.54	0.48
2:L:55:HIS:NE2	2:L:83:ASP:OD2	2.46	0.48
1:I:332:PHE:HB2	6:I:2064:HOH:O	2.13	0.48
1:K:44:SER:O	1:K:48:LEU:HD23	2.14	0.48
1:K:244:LEU:HG	2:L:94:ARG:HG2	1.96	0.48
1:E:287:VAL:HG12	1:E:288:MET:HE3	1.96	0.48
2:B:168:ALA:O	2:B:169:LYS:HG2	2.14	0.47
1:A:211:MET:HE3	1:A:353:TRP:CE3	2.49	0.47
2:F:26:GLU:OE1	2:F:158:ARG:NH2	2.42	0.47
1:E:333:LEU:HB3	1:E:336:MET:HG3	1.96	0.47
2:J:111:ARG:HB2	2:L:175:ASP:OD2	2.14	0.47
1:A:142:ALA:HB1	1:E:413:MET:HG3	1.97	0.47
2:L:49:LEU:HD21	2:L:163:LEU:HD13	1.95	0.47
2:L:140:ARG:HG3	2:L:141:LEU:HG	1.96	0.47
1:K:340:ARG:HD3	1:K:342:TRP:CH2	2.50	0.47
1:K:262:GLY:HA2	1:K:278:VAL:HG23	1.97	0.47
1:C:241:SER:HB2	2:D:95:LYS:HG3	1.97	0.46
1:C:413:MET:HE2	1:C:435:GLU:HG3	1.97	0.46
2:D:67:ARG:NE	2:D:67:ARG:HA	2.31	0.46
1:A:365:GLU:H	1:A:365:GLU:CD	2.22	0.46
1:G:403:LYS:HE3	1:I:176:TRP:HB3	1.98	0.46
1:K:448:MET:HA	1:K:457:LEU:HD11	1.97	0.46
1:I:29:ASP:OD1	1:I:32:LYS:HD2	2.16	0.46
2:F:58:MET:HE2	2:F:81:HIS:CG	2.51	0.46
1:G:413:MET:HG3	1:I:142:ALA:HB1	1.98	0.46
1:E:185:THR:HG22	1:E:459:PRO:HG2	1.98	0.46
1:A:185:THR:HG22	1:A:459:PRO:HG2	1.98	0.46
2:B:25:ASN:HD21	2:D:24:GLN:HG2	1.81	0.46
2:H:122:THR:HG22	2:H:129:GLU:HG3	1.97	0.46
2:H:155:VAL:HB	2:H:169:LYS:HB2	1.98	0.46
1:K:340:ARG:CD	1:K:342:TRP:CH2	2.99	0.45
1:I:71:GLY:HA3	6:I:2013:HOH:O	2.17	0.45
1:E:208:ILE:HD12	1:E:356:THR:OG1	2.15	0.45
1:G:280:GLU:HA	1:G:281:PRO:HD3	1.79	0.45
1:A:265:PHE:CZ	1:A:267:ALA:HA	2.52	0.45
1:K:250:GLU:CD	1:K:250:GLU:H	2.24	0.45
2:B:36:GLN:HE21	2:D:12:PHE:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:140:ARG:HG3	2:D:141:LEU:HG	1.98	0.45
2:F:148:PHE:HB3	2:F:174:LEU:HD11	1.98	0.45
1:I:333:LEU:HD12	1:I:338:ASN:HB3	1.98	0.45
1:I:413:MET:HG2	1:I:434:ALA:HA	1.99	0.45
1:G:217:PRO:HG2	1:G:393:VAL:HG22	1.99	0.45
2:D:36:GLN:HB3	2:F:11:THR:HG23	1.99	0.45
1:E:339:ILE:CD1	1:E:357:LEU:HG	2.47	0.45
1:G:19:TRP:HE1	1:G:44:SER:HB2	1.81	0.45
1:I:123:HIS:N	6:I:2025:HOH:O	2.31	0.44
1:I:193:TYR:CE2	1:I:276:TRP:CH2	3.05	0.44
1:A:90:ASP:O	1:A:91:LYS:HB2	2.18	0.44
1:E:339:ILE:HD13	1:E:357:LEU:HG	1.99	0.44
1:E:411:ALA:HA	1:E:435:GLU:OE2	2.18	0.44
2:F:126:ASP:HB3	2:F:158:ARG:HB2	1.99	0.44
1:K:100:CYS:SG	1:K:127:TYR:OH	2.71	0.44
1:A:123:HIS:HB2	3:A:900:FES:S2	2.58	0.44
1:C:251:MET:HG3	1:C:255:GLN:HB2	1.99	0.44
1:E:287:VAL:HG12	1:E:288:MET:HE2	1.98	0.44
1:E:333:LEU:HB2	1:E:336:MET:HG3	2.00	0.44
1:E:183:LEU:O	1:E:187:LEU:HG	2.18	0.44
1:E:333:LEU:O	1:E:337:ASN:N	2.44	0.44
1:I:124:GLY:N	6:I:2025:HOH:O	2.49	0.44
1:C:227:PHE:CZ	1:C:340:ARG:HD2	2.53	0.44
1:E:356:THR:HG23	2:F:79:LEU:HD11	2.00	0.43
1:G:349:GLU:OE2	2:L:143:ARG:NH2	2.42	0.43
2:H:175:ASP:OD2	2:L:111:ARG:HB2	2.18	0.43
1:I:164:ARG:HD2	1:I:178:VAL:HA	1.99	0.43
2:B:56:TYR:HB3	2:B:84:GLU:HB2	2.00	0.43
2:B:113:LEU:HD22	2:D:135:ILE:HD12	2.00	0.43
1:K:283:SER:O	1:K:287:VAL:HG23	2.17	0.43
1:E:164:ARG:HD2	1:E:178:VAL:HA	2.00	0.43
2:J:120:LYS:HB3	2:J:129:GLU:HB2	2.00	0.43
1:G:60:LEU:HD22	1:G:330:CYS:SG	2.59	0.43
1:G:259:PRO:HB2	1:G:277:TYR:CD2	2.54	0.43
1:C:84:VAL:O	1:C:95:VAL:HA	2.18	0.43
2:B:58:MET:HE2	2:B:81:HIS:CB	2.48	0.43
2:B:140:ARG:HG3	2:B:141:LEU:HG	2.01	0.43
1:E:222:PHE:CZ	1:E:395:ILE:HG21	2.53	0.43
1:C:37:PRO:HG2	1:C:405:LYS:HA	2.01	0.43
1:C:276:TRP:HB3	1:C:322:GLN:HG3	2.00	0.43
1:E:413:MET:HG2	1:E:434:ALA:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:332:PHE:HB3	1:K:339:ILE:HA	2.00	0.43
1:A:141:GLU:OE1	1:A:141:GLU:N	2.52	0.43
1:C:372:ARG:HD2	6:C:2105:HOH:O	2.18	0.43
2:D:49:LEU:HD21	2:D:163:LEU:HD13	1.99	0.43
1:G:394:GLU:OE2	1:I:106:ARG:NE	2.52	0.43
1:I:217:PRO:HG2	1:I:393:VAL:HG22	1.99	0.43
1:K:164:ARG:HD2	1:K:178:VAL:HA	2.01	0.43
1:C:376:ARG:NH2	1:C:377:ASN:HD21	2.17	0.42
1:K:412:GLN:O	1:K:415:LEU:HB2	2.19	0.42
1:E:64:GLU:OE1	1:E:167:THR:HG21	2.19	0.42
1:K:168:TYR:HB2	1:K:183:LEU:HD21	2.01	0.42
1:A:314:MET:HA	1:A:315:PRO:HD3	1.90	0.42
1:G:99:GLN:NE2	1:K:404:ALA:HB1	2.35	0.42
1:I:322:GLN:CD	1:I:334:PRO:HG2	2.45	0.42
1:A:402:TYR:CZ	1:C:51:GLU:HG3	2.54	0.42
1:E:215:VAL:O	2:F:182:ASN:HA	2.20	0.42
1:E:337:ASN:HB3	1:E:357:LEU:O	2.20	0.42
1:K:27:LEU:HD13	1:K:39:ILE:HG22	2.01	0.42
1:I:356:THR:HG21	1:I:374:ASN:HB3	2.00	0.42
1:A:73:PHE:HA	1:A:85:MET:O	2.19	0.42
1:A:164:ARG:HD2	1:A:178:VAL:HA	1.99	0.42
1:I:365:GLU:O	1:I:369:GLU:HG2	2.19	0.42
1:K:244:LEU:HD13	1:K:253:LEU:HG	2.01	0.42
1:K:269:TRP:NE1	1:K:457:LEU:O	2.53	0.42
1:C:375:ILE:O	1:C:379:SER:HB3	2.20	0.42
1:I:60:LEU:HD22	1:I:330:CYS:SG	2.59	0.42
1:I:242:GLY:HA3	6:I:2040:HOH:O	2.19	0.42
1:A:337:ASN:HB3	1:A:357:LEU:O	2.20	0.42
2:D:113:LEU:HD22	2:F:135:ILE:HD12	2.02	0.42
1:K:274:SER:HB2	1:K:324:MET:HG3	2.01	0.42
1:C:340:ARG:HD3	1:C:342:TRP:CH2	2.54	0.42
1:G:133:LEU:HG	1:G:155:LYS:HD2	2.01	0.42
2:H:116:ASN:HA	2:L:32:TYR:CD1	2.55	0.42
1:A:379:SER:HB2	6:B:2045:HOH:O	2.20	0.42
2:D:58:MET:HE3	2:D:81:HIS:CB	2.50	0.42
1:K:226:GLN:HA	1:K:230:ASP:HB2	2.00	0.42
2:B:113:LEU:CD2	2:D:135:ILE:HD12	2.50	0.41
1:C:262:GLY:C	1:C:432:VAL:HB	2.45	0.41
1:G:356:THR:HG23	2:H:79:LEU:HD11	2.01	0.41
2:B:32:TYR:CG	2:D:116:ASN:HA	2.55	0.41
2:D:99:ASP:OD1	2:F:67:ARG:NE	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:322:GLN:CD	1:E:334:PRO:HG2	2.46	0.41
1:C:337:ASN:HB3	1:C:357:LEU:O	2.20	0.41
1:I:429:VAL:HG13	6:I:2045:HOH:O	2.20	0.41
2:B:124:THR:HA	2:B:125:PRO:HD3	1.96	0.41
2:F:54:ILE:HA	2:F:168:ALA:O	2.20	0.41
1:A:336:MET:H	1:A:336:MET:HG2	1.60	0.41
1:C:217:PRO:HG2	1:C:393:VAL:HG22	2.02	0.41
1:C:376:ARG:HD2	6:D:2048:HOH:O	2.21	0.41
1:E:89:LYS:HE3	1:E:89:LYS:HB2	1.82	0.41
1:E:201:THR:HG22	1:E:202:PRO:HD2	2.03	0.41
2:F:140:ARG:HG3	2:F:141:LEU:HG	2.01	0.41
1:G:413:MET:HG2	1:G:434:ALA:HA	2.02	0.41
2:H:55:HIS:NE2	2:H:83:ASP:OD2	2.39	0.41
1:E:211:MET:HE3	1:E:353:TRP:CE3	2.56	0.41
1:K:57:SER:OG	1:K:448:MET:HE1	2.20	0.41
1:E:60:LEU:HD23	1:E:341:ILE:HG12	2.02	0.41
1:E:370:TYR:O	1:E:374:ASN:HB2	2.21	0.41
2:H:51:ASP:OD2	2:H:157:ARG:HD2	2.20	0.41
1:C:230:ASP:O	1:C:233:HIS:ND1	2.46	0.41
1:C:334:PRO:O	1:C:337:ASN:OD1	2.39	0.41
1:E:248:PRO:HA	1:E:249:PRO:HD3	1.98	0.41
2:B:116:ASN:HA	2:F:32:TYR:CD1	2.56	0.40
1:C:451:GLU:HA	1:C:452:PRO:HD2	1.93	0.40
1:C:413:MET:HE3	1:C:434:ALA:N	2.36	0.40
2:H:58:MET:HE2	2:H:81:HIS:CG	2.56	0.40
1:E:220:TRP:HA	1:E:350:ILE:HG21	2.04	0.40
1:E:262:GLY:C	1:E:432:VAL:HB	2.46	0.40
1:C:61:LEU:HD12	1:C:95:VAL:HG21	2.03	0.40
1:C:126:ALA:HB3	1:C:135:ASN:HB3	2.04	0.40
1:G:326:ILE:HB	1:G:330:CYS:HB3	2.02	0.40
1:I:389:GLY:O	1:I:393:VAL:HG23	2.21	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%)	43	55
1	I	429/459 (94%)	403 (94%)	25 (6%)	1 (0%)	43	55
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%)	48	60

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%)	32	49
1	C	350/372 (94%)	342 (98%)	8 (2%)	44	63
1	E	350/372 (94%)	336 (96%)	14 (4%)	28	42
1	G	350/372 (94%)	341 (97%)	9 (3%)	40	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	350/372 (94%)	344 (98%)	6 (2%)	53	72
1	K	350/372 (94%)	343 (98%)	7 (2%)	48	67
2	B	159/167 (95%)	155 (98%)	4 (2%)	42	60
2	D	159/167 (95%)	152 (96%)	7 (4%)	25	38
2	F	159/167 (95%)	154 (97%)	5 (3%)	35	52
2	H	159/167 (95%)	157 (99%)	2 (1%)	61	77
2	J	159/167 (95%)	156 (98%)	3 (2%)	50	69
2	L	159/167 (95%)	155 (98%)	4 (2%)	42	60
All	All	3054/3234 (94%)	2973 (97%)	81 (3%)	39	58

All (81) 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	201	THR
1	A	257	GLN
1	A	258	ILE
1	A	278	VAL
1	A	280	GLU
1	A	307	GLN
1	A	334	PRO
1	A	336	MET
1	A	457	LEU
2	B	44	GLU
2	B	76	ASP
2	B	140	ARG
2	B	179	LEU
1	C	48	LEU
1	C	86	VAL
1	C	91	LYS
1	C	103	ARG
1	C	336	MET
1	C	356	THR
1	C	379	SER
1	C	457	LEU
2	D	44	GLU
2	D	77	GLN

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Mol	Chain	Res	Type
2	D	94	ARG
2	D	113	LEU
2	D	121	GLU
2	D	143	ARG
2	D	179	LEU
1	E	48	LEU
1	E	86	VAL
1	E	103	ARG
1	E	201	THR
1	E	255	GLN
1	E	258	ILE
1	E	280	GLU
1	E	334	PRO
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
2	F	180	LEU
1	G	86	VAL
1	G	89	LYS
1	G	103	ARG
1	G	201	THR
1	G	285	LEU
1	G	336	MET
1	G	340	ARG
1	G	415	LEU
1	G	457	LEU
2	H	140	ARG
2	H	179	LEU
1	I	103	ARG
1	I	255	GLN
1	I	258	ILE
1	I	278	VAL
1	I	320	VAL
1	I	457	LEU
2	J	140	ARG

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Mol	Chain	Res	Type
2	J	143	ARG
2	J	179	LEU
1	K	86	VAL
1	K	103	ARG
1	K	179	GLN
1	K	285	LEU
1	K	336	MET
1	K	356	THR
1	K	457	LEU
2	L	17	LYS
2	L	44	GLU
2	L	140	ARG
2	L	179	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	88	GLN
1	A	263	ASN
1	A	386	GLN
2	B	25	ASN
2	B	36	GLN
2	B	144	GLN
1	C	88	GLN
1	C	99	GLN
1	C	226	GLN
1	C	263	ASN
1	C	311	HIS
1	C	377	ASN
1	C	386	GLN
1	C	428	ASN
1	C	443	HIS
2	D	25	ASN
2	D	36	GLN
2	D	40	HIS
1	E	43	GLN
1	E	377	ASN
1	E	407	GLN
1	E	419	GLN
1	E	443	HIS
1	G	88	GLN

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Mol	Chain	Res	Type
1	G	99	GLN
1	G	162	GLN
1	G	226	GLN
1	G	255	GLN
1	G	322	GLN
1	G	373	HIS
1	G	377	ASN
1	G	443	HIS
2	H	81	HIS
2	H	86	HIS
2	H	131	ASN
1	I	88	GLN
1	I	263	ASN
1	I	374	ASN
1	I	386	GLN
2	J	77	GLN
1	K	88	GLN
1	K	99	GLN
1	K	255	GLN
1	K	307	GLN
1	K	322	GLN
1	K	386	GLN
1	K	428	ASN
1	K	443	HIS
2	L	81	HIS
2	L	131	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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	$\# Z > 2$
5	DC5	A	902	-	15,15,15	1.35	1 (6%)	18,20,20	0.56	0
5	DC5	E	900	-	15,15,15	1.43	1 (6%)	18,20,20	0.74	1 (5%)
3	FES	G	900	1,6	0,4,4	-	-	-	-	-
5	DC5	C	902	-	15,15,15	1.33	1 (6%)	18,20,20	0.81	0
3	FES	K	900	1	0,4,4	-	-	-	-	-
3	FES	A	900	1	0,4,4	-	-	-	-	-
3	FES	E	901	1	0,4,4	-	-	-	-	-
3	FES	I	900	1	0,4,4	-	-	-	-	-
3	FES	C	900	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	DC5	A	902	-	-	0/4/4/4	0/2/2/2
5	DC5	E	900	-	-	0/4/4/4	0/2/2/2
5	DC5	C	902	-	-	0/4/4/4	0/2/2/2
3	FES	G	900	1,6	-	-	0/1/1/1
3	FES	K	900	1	-	-	0/1/1/1
3	FES	A	900	1	-	-	0/1/1/1
3	FES	E	901	1	-	-	0/1/1/1
3	FES	I	900	1	-	-	0/1/1/1
3	FES	C	900	1	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	900	DC5	CB1-CA1	-5.24	1.40	1.50
5	A	902	DC5	CB1-CA1	-4.68	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	902	DC5	CB1-CA1	-4.55	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	2.11	118.22	116.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	900	FES	1	0
3	K	900	FES	1	0
3	A	900	FES	1	0
3	E	901	FES	1	0
3	I	900	FES	1	0
3	C	900	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	433/459 (94%)	-0.23	9 (2%) 63 65	19, 38, 53, 70	18 (4%)
1	C	433/459 (94%)	-0.16	7 (1%) 70 72	20, 41, 60, 76	18 (4%)
1	E	433/459 (94%)	-0.11	8 (1%) 67 69	21, 43, 67, 78	18 (4%)
1	G	433/459 (94%)	0.62	23 (5%) 32 34	38, 80, 116, 130	18 (4%)
1	I	433/459 (94%)	0.67	25 (5%) 29 31	31, 82, 136, 162	18 (4%)
1	K	433/459 (94%)	0.73	30 (6%) 23 25	38, 86, 151, 175	18 (4%)
2	B	180/188 (95%)	-0.42	0 100 100	23, 36, 57, 65	4 (2%)
2	D	180/188 (95%)	-0.32	1 (0%) 85 86	26, 39, 58, 62	4 (2%)
2	F	180/188 (95%)	-0.39	1 (0%) 85 86	26, 38, 56, 62	4 (2%)
2	H	180/188 (95%)	-0.20	0 100 100	30, 49, 67, 79	4 (2%)
2	J	180/188 (95%)	-0.04	0 100 100	31, 55, 76, 83	4 (2%)
2	L	180/188 (95%)	-0.03	0 100 100	29, 53, 76, 87	4 (2%)
All	All	3678/3882 (94%)	0.11	104 (2%) 55 57	19, 51, 112, 175	132 (3%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	257	GLN	8.2
1	G	256	ALA	7.7
1	C	259	PRO	7.6
1	A	256	ALA	7.6
1	K	256	ALA	7.5
1	C	256	ALA	7.1
1	G	258	ILE	7.0
1	I	257	GLN	7.0
1	A	258	ILE	6.8
1	E	256	ALA	6.4
1	A	257	GLN	5.6

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Mol	Chain	Res	Type	RSRZ
1	I	256	ALA	5.6
1	G	259	PRO	5.6
1	E	257	GLN	5.6
1	E	260	THR	5.6
1	K	257	GLN	5.4
1	K	260	THR	5.3
1	G	260	THR	5.3
1	E	259	PRO	5.2
1	I	259	PRO	5.1
1	E	258	ILE	5.0
1	K	259	PRO	4.9
1	K	258	ILE	4.7
1	A	259	PRO	4.5
1	E	255	GLN	4.5
1	I	258	ILE	4.5
1	C	258	ILE	4.3
1	C	255	GLN	4.2
1	C	260	THR	4.2
1	G	255	GLN	4.0
1	A	255	GLN	3.9
1	K	455	ALA	3.7
1	A	261	LYS	3.7
1	G	421	GLY	3.6
1	I	260	THR	3.6
1	I	109	ARG	3.5
1	C	257	GLN	3.5
1	E	261	LYS	3.4
1	K	153	PHE	3.3
1	I	283	SER	3.3
1	K	261	LYS	3.3
1	I	287	VAL	3.3
1	K	255	GLN	3.3
1	I	261	LYS	3.2
1	I	301	ALA	3.1
1	I	255	GLN	3.1
1	A	260	THR	3.1
1	C	261	LYS	3.1
1	E	253	LEU	2.9
1	G	261	LYS	2.9
1	K	326	ILE	2.9
1	I	282	GLY	2.8
1	K	94	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	296	TRP	2.7
2	D	16	SER	2.7
1	K	291	LYS	2.7
1	G	278	VAL	2.7
1	K	143	PHE	2.6
1	I	94	LYS	2.6
1	G	262	GLY	2.6
1	I	143	PHE	2.6
1	G	335	ALA	2.5
1	K	277	TYR	2.5
1	G	243	ILE	2.5
1	K	301	ALA	2.5
1	I	310	GLY	2.5
1	K	290	PRO	2.5
1	G	143	PHE	2.4
1	K	309	LEU	2.4
1	I	296	TRP	2.4
1	I	312	THR	2.4
1	A	143	PHE	2.4
1	K	423	PRO	2.4
2	F	123	ALA	2.4
1	G	291	LYS	2.4
1	G	196	VAL	2.3
1	K	320	VAL	2.3
1	K	283	SER	2.3
1	G	28	VAL	2.3
1	K	292	VAL	2.3
1	G	52	ARG	2.2
1	G	254	SER	2.2
1	I	278	VAL	2.2
1	G	423	PRO	2.2
1	I	270	GLY	2.2
1	K	421	GLY	2.2
1	G	193	TYR	2.2
1	G	433	TYR	2.2
1	I	307	GLN	2.2
1	K	304	LEU	2.1
1	K	300	PRO	2.1
1	K	321	GLY	2.1
1	I	366	ILE	2.1
1	G	283	SER	2.1
1	I	142	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	109	ARG	2.1
1	I	364	ALA	2.1
1	I	309	LEU	2.1
1	G	312	THR	2.0
1	A	365	GLU	2.0
1	K	335	ALA	2.0
1	K	196	VAL	2.0
1	I	202	PRO	2.0
1	K	459	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DC5	C	902	14/14	0.85	0.14	71,73,74,74	0
5	DC5	A	902	14/14	0.86	0.13	54,58,61,61	0
5	DC5	E	900	14/14	0.88	0.14	72,74,76,76	0
4	FE2	G	901	1/1	0.96	0.05	58,58,58,58	0
3	FES	I	900	4/4	0.98	0.05	62,62,64,66	0
3	FES	K	900	4/4	0.98	0.06	56,57,57,59	0
3	FES	G	900	4/4	0.98	0.06	72,73,73,74	0
3	FES	A	900	4/4	0.99	0.04	38,39,39,40	0
4	FE2	I	901	1/1	0.99	0.02	58,58,58,58	0
4	FE2	K	901	1/1	0.99	0.04	74,74,74,74	0
3	FES	C	900	4/4	0.99	0.03	27,31,32,33	0
3	FES	E	901	4/4	0.99	0.04	36,38,38,40	0
4	FE2	A	901	1/1	0.99	0.04	34,34,34,34	0
4	FE2	C	901	1/1	1.00	0.01	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FE2	E	902	1/1	1.00	0.03	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.