



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:39 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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

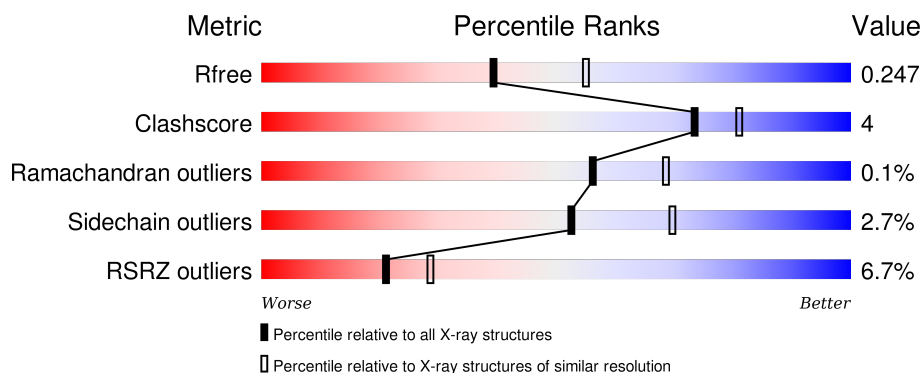
1 Overall quality at a glance

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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. 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	<div> <div>2%</div> <div>86%</div> <div>8%</div> <div>6%</div> </div>
1	C	459	<div> <div>3%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
1	E	459	<div> <div>4%</div> <div>83%</div> <div>10%</div> <div>6%</div> </div>
1	G	459	<div> <div>12%</div> <div>83%</div> <div>10%</div> <div>6%</div> </div>
1	I	459	<div> <div>13%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
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, 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
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 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			

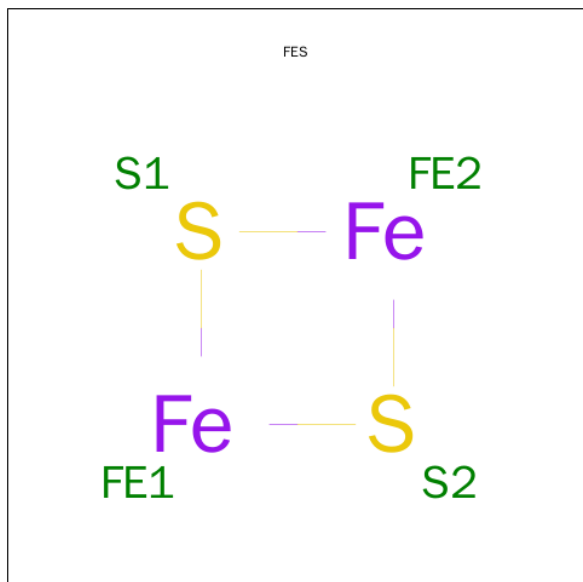
There are 12 discrepancies between the modelled and reference sequences:

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 (three-letter code: FES) (formula: Fe₂S₂).

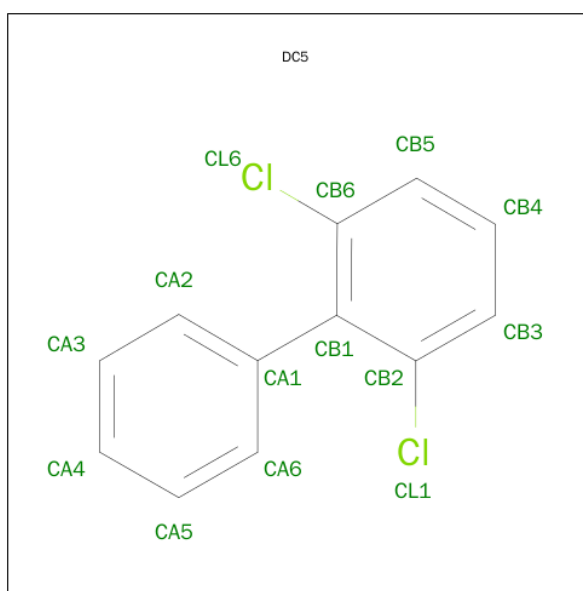


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	I	1	Total	Fe	S	0	0
			4	2	2		
3	K	1	Total	Fe	S	0	0
			4	2	2		

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

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

- Molecule 5 is 2,6-DICHLOROBIPHENYL (three-letter code: 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		

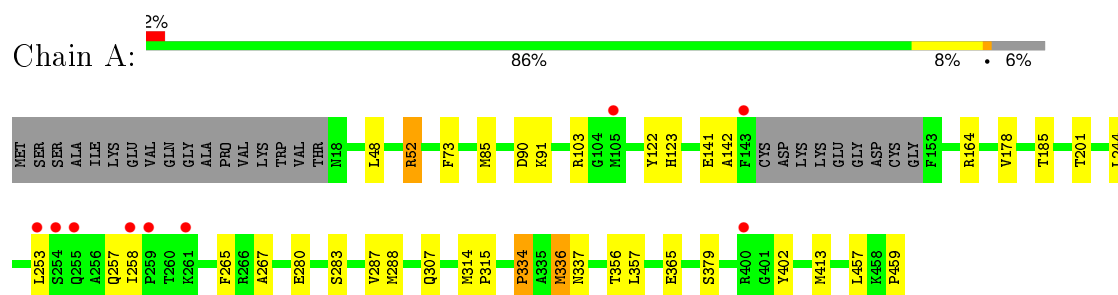
- Molecule 6 is water.

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

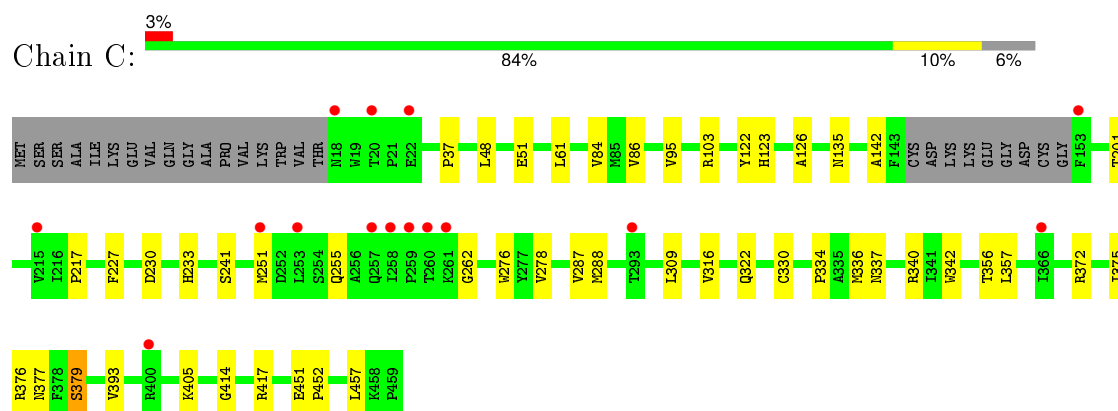
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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.

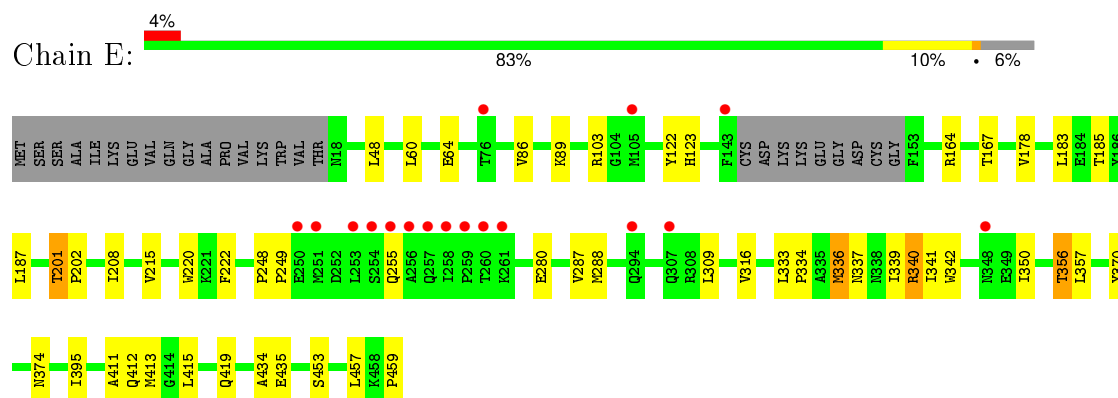
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



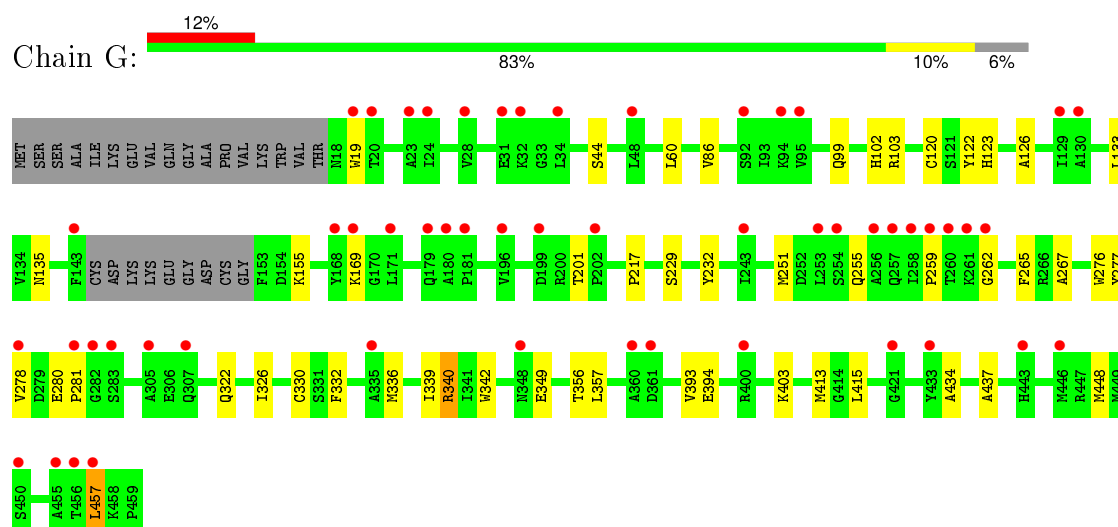
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



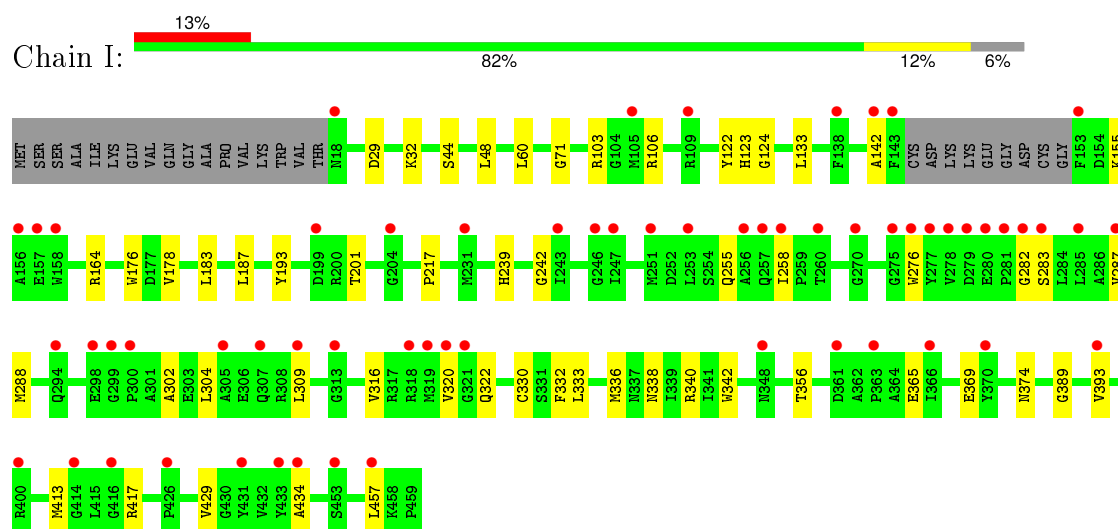
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



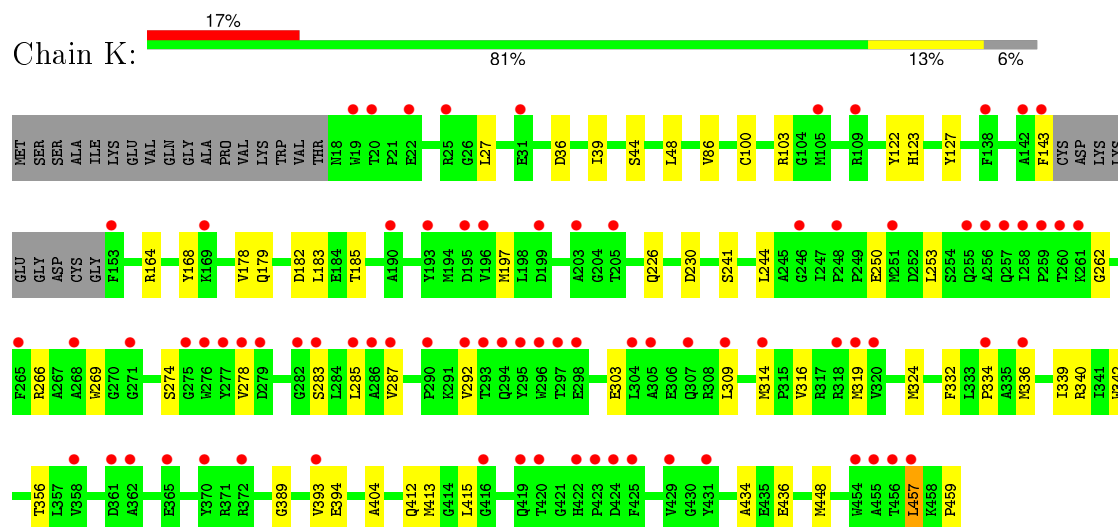
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



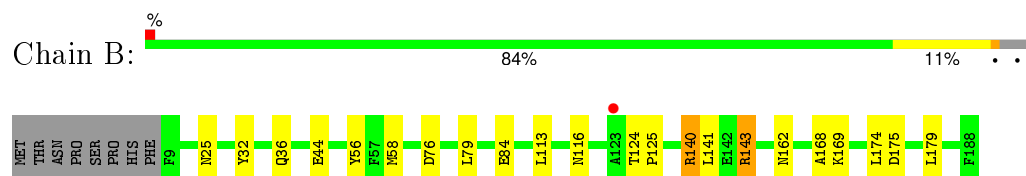
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



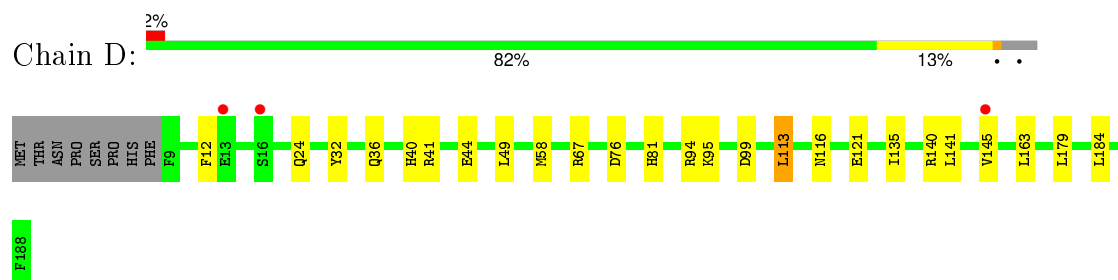
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



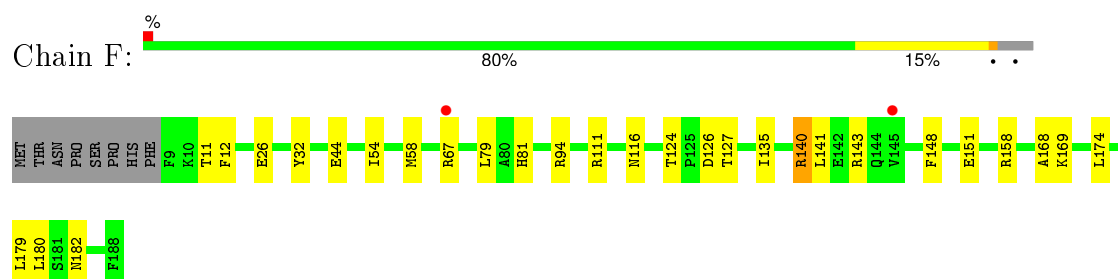
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



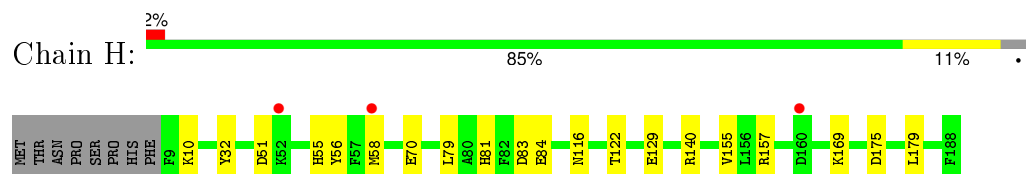
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



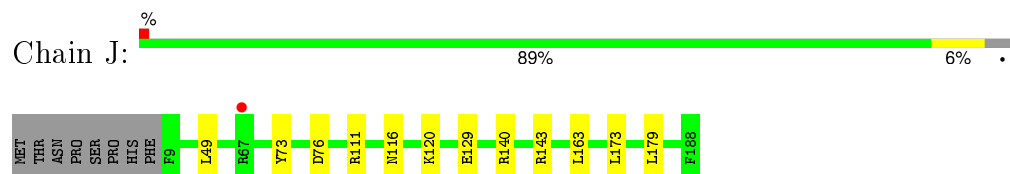
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



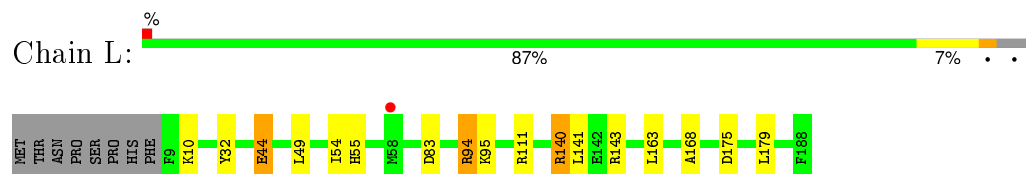
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



- 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 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 0.188 , 0.247	Depositor DCC
R_{free} test set	7629 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)	0.31 , 44.1	EDS
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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	3427	0	3276	24	0
1	C	3427	0	3276	28	0
1	E	3427	0	3276	32	0
1	G	3427	0	3276	28	0
1	I	3427	0	3276	34	0
1	K	3427	0	3276	35	0
2	B	1496	0	1447	16	0
2	D	1496	0	1447	26	0
2	F	1496	0	1447	24	0
2	H	1496	0	1447	11	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
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	238	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 (238) 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	1.33	1.06
2:D:58:MET:HE2	2:D:81:HIS:CB	2.01	0.90
1:I:155:LYS:HD2	6:I:2029:HOH:O	1.81	0.81
1:I:133:LEU:HG	6:I:2029:HOH:O	1.83	0.78
1:I:302:ALA:HB3	6:I:2055:HOH:O	1.84	0.77
1:C:201:THR:HB	6:C:2100:HOH:O	1.86	0.75
2:F:58:MET:HE2	2:F:81:HIS:CB	2.18	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
1:E:123:HIS:HB2	3:E:901:FES:S2	2.29	0.72
2:D:58:MET:CE	2:D:81:HIS:HB2	2.17	0.71
2:D:36:GLN:HE21	2:F:12:PHE:H	1.38	0.71
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:A:287:VAL:HG12	1:A:288:MET:CE	2.22	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: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:D:41:ARG:HD3	6:D:2019:HOH:O	1.96	0.66
1:A:287:VAL:HG12	1:A:288:MET:HE3	1.78	0.65
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:K:319:MET:HG2	6:K:2048:HOH:O	2.00	0.61
1:A:356:THR:HG23	2:B:79:LEU:HD11	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:287:VAL:HG12	1:C:288:MET:CE	2.33	0.58
2:H:32:TYR:CD1	2:J:116:ASN:HA	2.39	0.58
2:B:58:MET:HE1	2:B:174:LEU:HD22	1.85	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
2:F:58:MET:HE2	2:F:81:HIS:HB3	1.85	0.57
1:I:123:HIS:HB2	3:I:900:FES:S2	2.43	0.57
2:L:54:ILE:HA	2:L:168:ALA:O	2.06	0.56
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
1:I:287:VAL:HG12	1:I:288:MET:HE3	1.87	0.55
2:B:58:MET:CE	2:B:174:LEU:HD22	2.36	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
2:D:58:MET:HE1	2:D:184:LEU:HD13	1.90	0.54
1:G:251:MET:HG3	1:G:255:GLN:HB2	1.89	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
2:F:58:MET:HE2	2:F:81:HIS:HB2	1.90	0.53
1:G:102:HIS:HB3	6:G:2019:HOH:O	2.09	0.53
2:H:58:MET:HE2	2:H:81:HIS:CB	2.39	0.53
1:C:414:GLY:HA2	1:C:417:ARG:HD2	1.90	0.53
1:I:340:ARG:HD3	1:I:342:TRP:CH2	2.44	0.53
1:E:309:LEU:HD13	1:E:316:VAL:HG11	1.90	0.53
1:G:265:PHE:CZ	1:G:267:ALA:HA	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:73:TYR:CE1	2:J:173:LEU:HD22	2.46	0.51
2:H:70:GLU:H	2:H:70:GLU:CD	2.14	0.51
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
1:I:44:SER:O	1:I:48:LEU:HD23	2.13	0.49
2:F:58:MET:HE3	2:F:81:HIS:CD2	2.47	0.48
1:I:417:ARG:HH21	1:K:143:PHE:C	2.17	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
2:L:55:HIS:NE2	2:L:83:ASP:OD2	2.46	0.48
1:C:123:HIS:HB2	3:C:900:FES:S2	2.54	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:C:287:VAL:HG12	1:C:288:MET:HE2	1.95	0.47
2:F:26:GLU:OE1	2:F:158:ARG:NH2	2.42	0.47
1:A:287:VAL:HG12	1:A:288:MET:HE2	1.96	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
2:L:49:LEU:HD21	2:L:163:LEU:HD13	1.95	0.47
1:A:142:ALA:HB1	1:E:413:MET:HG3	1.97	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
2:D:67:ARG:NE	2:D:67:ARG:HA	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:VAL:HG12	1:C:288:MET:HE3	1.97	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:G:280:GLU:HA	1:G:281:PRO:HD3	1.79	0.45
1:E:208:ILE:HD12	1:E:356:THR:OG1	2.15	0.45
1:A:265:PHE:CZ	1:A:267:ALA:HA	2.52	0.45
1:I:333:LEU:HD12	1:I:338:ASN:HB3	1.98	0.45
2:D:140:ARG:HG3	2:D:141:LEU:HG	1.98	0.45
2:B:36:GLN:HE21	2:D:12:PHE:H	1.64	0.45
2:F:148:PHE:HB3	2:F:174:LEU:HD11	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:193:TYR:CE2	1:I:276:TRP:CH2	3.05	0.44
1:I:123:HIS:N	6:I:2025:HOH:O	2.31	0.44
1:E:339:ILE:HD13	1:E:357:LEU:HG	1.99	0.44
1:A:90:ASP:O	1:A:91:LYS:HB2	2.18	0.44
2:F:126:ASP:HB3	2:F:158:ARG:HB2	1.99	0.44
1:E:411:ALA:HA	1:E:435:GLU:OE2	2.18	0.44
1:K:100:CYS:SG	1:K:127:TYR:OH	2.71	0.44
1:E:333:LEU:HB2	1:E:336:MET:HG3	2.00	0.44
1:E:287:VAL:HG12	1:E:288:MET:HE2	1.98	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: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
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
1:G:349:GLU:OE2	2:L:143:ARG:NH2	2.42	0.43
2:B:113:LEU:HD22	2:D:135:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:TYR:HB3	2:B:84:GLU:HB2	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
1:E:222:PHE:CZ	1:E:395:ILE:HG21	2.53	0.43
2:B:140:ARG:HG3	2:B:141:LEU:HG	2.01	0.43
1:E:413:MET:HG2	1:E:434:ALA:HA	1.99	0.43
1:C:276:TRP:HB3	1:C:322:GLN:HG3	2.00	0.43
1:K:332:PHE:HB3	1:K:339:ILE:HA	2.00	0.43
1:C:37:PRO:HG2	1:C:405:LYS:HA	2.01	0.43
1:G:394:GLU:OE2	1:I:106:ARG:NE	2.52	0.43
2:D:49:LEU:HD21	2:D:163:LEU:HD13	1.99	0.43
1:A:141:GLU:N	1:A:141:GLU:OE1	2.52	0.43
1:A:365:GLU:CD	1:A:365:GLU:H	2.22	0.43
1:I:217:PRO:HG2	1:I:393:VAL:HG22	1.99	0.43
1:C:372:ARG:HD2	6:C:2105:HOH:O	2.18	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: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: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:I:356:THR:HG21	1:I:374:ASN:HB3	2.00	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: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:A:73:PHE:HA	1:A:85:MET:O	2.19	0.42
1:I:242:GLY:HA3	6:I:2040:HOH:O	2.19	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:116:ASN:HA	2:L:32:TYR:CD1	2.55	0.42
1:G:133:LEU:HG	1:G:155:LYS:HD2	2.01	0.42
1:A:379:SER:HB2	6:B:2045:HOH:O	2.20	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:G:356:THR:HG23	2:H:79:LEU:HD11	2.01	0.41
2:D:99:ASP:OD1	2:F:67:ARG:NE	2.52	0.41
2:B:32:TYR:CG	2:D:116:ASN:HA	2.55	0.41
1:I:429:VAL:HG13	6:I:2045:HOH:O	2.20	0.41
1:C:337:ASN:HB3	1:C:357:LEU:O	2.20	0.41
2:F:54:ILE:HA	2:F:168:ALA:O	2.20	0.41
2:B:124:THR:HA	2:B:125:PRO:HD3	1.96	0.41
1:A:336:MET:HG2	1:A:336:MET:H	1.60	0.41
1:C:217:PRO:HG2	1:C:393:VAL:HG22	2.02	0.41
2:D:58:MET:HE2	2:D:81:HIS:CG	2.53	0.41
1:G:413:MET:HG2	1:G:434:ALA:HA	2.02	0.41
1:C:376:ARG:HD2	6:D:2048:HOH:O	2.21	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:K:250:GLU:CD	1:K:250:GLU:H	2.24	0.41
1:E:89:LYS:HB2	1:E:89:LYS:HE3	1.82	0.41
2:H:55:HIS:NE2	2:H:83:ASP:OD2	2.39	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:334:PRO:O	1:C:337:ASN:OD1	2.39	0.41
1:C:230:ASP:O	1:C:233:HIS:ND1	2.46	0.41
1:E:248:PRO:HA	1:E:249:PRO:HD3	1.98	0.41
1:C:451:GLU:HA	1:C:452:PRO:HD2	1.93	0.40
2:B:116:ASN:HA	2:F:32:TYR:CD1	2.56	0.40
1:E:220:TRP:HA	1:E:350:ILE:HG21	2.04	0.40
1:G:326:ILE:HB	1:G:330:CYS:HB3	2.02	0.40
1:C:61:LEU:HD12	1:C:95:VAL:HG21	2.03	0.40
1:I:389:GLY:O	1:I:393:VAL:HG23	2.21	0.40
1:C:126:ALA:HB3	1:C:135:ASN:HB3	2.04	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%)	52	64
1	I	429/459 (94%)	403 (94%)	25 (6%)	1 (0%)	52	64
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%)	56	68

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%)	44	59
1	C	350/372 (94%)	341 (97%)	9 (3%)	54	71
1	E	350/372 (94%)	337 (96%)	13 (4%)	41	55
1	G	350/372 (94%)	342 (98%)	8 (2%)	58	75
1	I	350/372 (94%)	343 (98%)	7 (2%)	63	79
1	K	350/372 (94%)	342 (98%)	8 (2%)	58	75
2	B	159/167 (95%)	154 (97%)	5 (3%)	47	64
2	D	159/167 (95%)	153 (96%)	6 (4%)	40	54
2	F	159/167 (95%)	155 (98%)	4 (2%)	55	73
2	H	159/167 (95%)	156 (98%)	3 (2%)	65	81
2	J	159/167 (95%)	156 (98%)	3 (2%)	65	81
2	L	159/167 (95%)	154 (97%)	5 (3%)	47	64
All	All	3054/3234 (94%)	2971 (97%)	83 (3%)	52	70

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
2	B	25	ASN
2	B	36	GLN
1	C	377	ASN
1	C	428	ASN
2	D	25	ASN
2	D	36	GLN
2	D	40	HIS
2	D	131	ASN
1	G	373	HIS
2	H	81	HIS
2	H	86	HIS
1	I	419	GLN
1	K	294	GLN
1	K	307	GLN
2	L	81	HIS

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 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	1.30	1 (6%)	20,20,20	0.55	0
3	FES	C	900	1	0,4,4	0.00	-	0,4,4	0.00	-
5	DC5	C	902	-	15,15,15	1.26	1 (6%)	20,20,20	0.81	0
5	DC5	E	900	-	15,15,15	1.37	1 (6%)	20,20,20	0.84	0
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	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DC5	A	902	-	-	0/4/4/4	0/2/2/2
3	FES	C	900	1	-	0/0/4/4	0/1/1/1
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	0/1/1/1
3	FES	G	900	1,6	-	0/0/4/4	0/1/1/1
3	FES	I	900	1	-	0/0/4/4	0/1/1/1
3	FES	K	900	1	-	0/0/4/4	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	-5.04	1.40	1.50
5	A	902	DC5	CB1-CA1	-4.50	1.41	1.50
5	C	902	DC5	CB1-CA1	-4.38	1.41	1.50

There are no bond angle outliers.

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	A	900	FES	1	0
3	C	900	FES	1	0
3	E	901	FES	1	0
3	G	900	FES	1	0
3	I	900	FES	1	0
3	K	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%)	-0.31	9 (2%) 67 74	24, 38, 56, 70	18 (4%)
1	C	433/459 (94%)	-0.12	15 (3%) 48 56	27, 41, 61, 76	18 (4%)
1	E	433/459 (94%)	-0.09	17 (3%) 43 52	24, 43, 68, 78	18 (4%)
1	G	433/459 (94%)	0.69	53 (12%) 5 9	43, 82, 116, 130	18 (4%)
1	I	433/459 (94%)	0.81	61 (14%) 4 6	39, 84, 136, 163	18 (4%)
1	K	433/459 (94%)	0.98	80 (18%) 2 2	42, 87, 151, 175	18 (4%)
2	B	180/188 (95%)	-0.28	1 (0%) 90 93	26, 36, 57, 65	4 (2%)
2	D	180/188 (95%)	-0.10	3 (1%) 73 79	28, 40, 58, 62	4 (2%)
2	F	180/188 (95%)	-0.29	2 (1%) 82 86	26, 38, 56, 62	4 (2%)
2	H	180/188 (95%)	-0.21	3 (1%) 73 79	34, 49, 67, 79	4 (2%)
2	J	180/188 (95%)	-0.05	1 (0%) 90 93	35, 56, 76, 83	4 (2%)
2	L	180/188 (95%)	-0.01	1 (0%) 90 93	34, 53, 76, 87	4 (2%)
All	All	3678/3882 (94%)	0.19	246 (6%) 21 29	24, 51, 113, 175	132 (3%)

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	258	ILE	16.0
1	G	257	GLN	9.8
1	K	282	GLY	9.2
1	G	258	ILE	8.3
1	I	282	GLY	8.2
1	G	260	THR	7.8
1	I	278	VAL	7.2
1	K	290	PRO	7.1
1	K	248	PRO	6.2
1	K	257	GLN	6.1
1	K	292	VAL	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	258	ILE	6.1
1	K	320	VAL	6.1
1	G	254	SER	6.0
1	G	259	PRO	5.9
1	C	258	ILE	5.9
1	I	281	PRO	5.9
1	K	22	GLU	5.8
1	I	143	PHE	5.8
1	K	294	GLN	5.8
1	K	455	ALA	5.7
1	K	278	VAL	5.5
1	K	361	ASP	5.5
1	I	258	ILE	5.3
1	K	277	TYR	5.2
1	I	366	ILE	5.2
1	G	253	LEU	5.2
1	K	420	THR	5.1
1	K	370	TYR	4.9
1	K	424	ASP	4.9
1	G	261	LYS	4.9
1	K	305	ALA	4.8
1	I	199	ASP	4.8
1	K	295	TYR	4.8
1	G	256	ALA	4.8
1	K	314	MET	4.8
1	I	142	ALA	4.8
1	K	260	THR	4.6
1	I	305	ALA	4.6
1	G	202	PRO	4.6
1	K	153	PHE	4.5
1	E	260	THR	4.4
1	I	277	TYR	4.2
1	I	280	GLU	4.1
1	K	319	MET	4.0
1	C	257	GLN	4.0
1	K	256	ALA	3.9
1	I	279	ASP	3.9
1	I	270	GLY	3.8
1	K	196	VAL	3.8
1	K	143	PHE	3.8
1	A	254	SER	3.7
1	G	92	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	246	GLY	3.7
1	A	143	PHE	3.7
1	I	276	TRP	3.7
1	I	285	LEU	3.6
1	K	422	HIS	3.6
1	G	196	VAL	3.6
1	K	203	ALA	3.6
1	K	276	TRP	3.6
1	I	253	LEU	3.5
1	K	251	MET	3.5
1	K	138	PHE	3.5
1	K	307	GLN	3.4
1	K	318	ARG	3.4
1	G	305	ALA	3.4
1	K	362	ALA	3.4
1	E	250	GLU	3.4
1	I	416	GLY	3.3
1	I	300	PRO	3.3
1	E	256	ALA	3.3
1	K	457	LEU	3.3
1	I	457	LEU	3.3
1	G	34	LEU	3.2
1	G	457	LEU	3.2
1	G	180	ALA	3.2
1	G	169	LYS	3.2
1	C	22	GLU	3.2
1	G	199	ASP	3.2
1	E	253	LEU	3.2
1	G	48	LEU	3.2
1	I	156	ALA	3.2
1	K	259	PRO	3.2
1	K	285	LEU	3.2
1	K	372	ARG	3.2
1	G	282	GLY	3.1
1	I	361	ASP	3.1
1	K	199	ASP	3.1
1	I	287	VAL	3.1
1	K	429	VAL	3.1
1	K	423	PRO	3.1
1	K	283	SER	3.0
1	G	129	ILE	3.0
1	I	307	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	414	GLY	2.9
1	I	294	GLN	2.9
2	D	145	VAL	2.9
1	K	431	TYR	2.9
1	K	261	LYS	2.9
1	K	297	THR	2.9
1	C	261	LYS	2.9
1	I	243	ILE	2.9
1	C	260	THR	2.9
1	G	433	TYR	2.9
1	I	247	ILE	2.9
1	G	94	LYS	2.9
1	G	283	SER	2.9
1	G	335	ALA	2.9
1	I	320	VAL	2.9
1	C	259	PRO	2.9
1	K	296	TRP	2.9
1	I	153	PHE	2.9
1	K	246	GLY	2.8
1	I	309	LEU	2.8
1	K	304	LEU	2.8
1	G	421	GLY	2.8
1	K	268	ALA	2.8
1	E	259	PRO	2.8
1	E	261	LYS	2.8
1	E	257	GLN	2.8
1	G	400	ARG	2.8
1	I	434	ALA	2.8
1	K	20	THR	2.8
1	G	28	VAL	2.8
1	G	130	ALA	2.8
1	I	453	SER	2.7
1	E	251	MET	2.7
1	G	143	PHE	2.7
1	K	309	LEU	2.7
1	K	205	THR	2.7
1	K	336	MET	2.7
1	G	243	ILE	2.7
1	G	446	MET	2.7
1	K	334	PRO	2.7
1	I	158	TRP	2.7
1	K	286	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	313	GLY	2.7
1	C	366	ILE	2.7
2	D	16	SER	2.7
1	G	20	THR	2.7
1	C	400	ARG	2.6
1	I	318	ARG	2.6
1	A	261	LYS	2.6
1	G	281	PRO	2.6
1	G	361	ASP	2.6
1	G	262	GLY	2.6
1	I	321	GLY	2.6
1	I	393	VAL	2.6
1	I	204	GLY	2.6
1	I	251	MET	2.6
1	I	256	ALA	2.6
1	E	254	SER	2.6
1	K	255	GLN	2.6
1	I	109	ARG	2.6
1	G	168	TYR	2.5
1	I	260	THR	2.5
1	C	251	MET	2.5
1	I	283	SER	2.5
1	K	393	VAL	2.5
1	E	258	ILE	2.5
1	K	31	GLU	2.5
2	H	52	LYS	2.5
1	G	23	ALA	2.5
1	G	450	SER	2.5
1	I	105	MET	2.5
1	K	193	TYR	2.5
1	I	348	ASN	2.5
1	I	363	PRO	2.5
1	K	416	GLY	2.4
1	K	293	THR	2.4
1	G	348	ASN	2.4
1	A	400	ARG	2.4
1	G	179	GLN	2.4
1	K	419	GLN	2.4
1	C	153	PHE	2.4
1	I	18	ASN	2.4
1	G	19	TRP	2.4
1	E	143	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	298	GLU	2.4
1	G	278	VAL	2.4
1	K	358	VAL	2.4
1	K	456	THR	2.4
1	I	431	TYR	2.4
1	G	456	THR	2.4
2	B	123	ALA	2.4
2	J	67	ARG	2.4
1	I	299	GLY	2.3
1	G	24	ILE	2.3
1	G	31	GLU	2.3
1	K	287	VAL	2.3
1	C	253	LEU	2.3
1	K	271	GLY	2.3
1	A	253	LEU	2.3
1	I	433	TYR	2.3
1	G	443	HIS	2.3
1	I	319	MET	2.3
1	I	138	PHE	2.3
1	A	105	MET	2.3
1	E	348	ASN	2.3
1	K	425	PHE	2.2
1	E	76	THR	2.2
1	G	455	ALA	2.2
2	H	58	MET	2.2
1	A	259	PRO	2.2
1	G	181	PRO	2.2
1	K	105	MET	2.2
1	C	20	THR	2.2
1	G	360	ALA	2.2
1	K	365	GLU	2.2
1	A	255	GLN	2.2
1	C	215	VAL	2.2
1	E	294	GLN	2.2
1	G	32	LYS	2.1
1	K	195	ASP	2.1
1	K	25	ARG	2.1
1	I	275	GLY	2.1
2	F	145	VAL	2.1
1	I	157	GLU	2.1
1	C	293	THR	2.1
2	H	160	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	307	GLN	2.1
1	G	95	VAL	2.1
1	K	279	ASP	2.1
2	F	67	ARG	2.1
1	C	18	ASN	2.1
1	G	171	LEU	2.1
1	K	109	ARG	2.1
1	G	307	GLN	2.1
1	K	190	ALA	2.1
1	I	400	ARG	2.1
1	I	257	GLN	2.1
1	I	370	TYR	2.1
2	L	58	MET	2.1
1	K	19	TRP	2.1
1	K	454	TRP	2.1
1	I	298	GLU	2.0
1	K	265	PHE	2.0
1	E	105	MET	2.0
1	E	255	GLN	2.0
1	K	169	LYS	2.0
1	I	426	PRO	2.0
1	K	275	GLY	2.0
2	D	13	GLU	2.0
1	I	231	MET	2.0
1	K	142	ALA	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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DC5	C	902	14/14	0.84	0.24	5.33	71,73,74,74	0
5	DC5	A	902	14/14	0.86	0.17	2.62	54,58,61,61	0
5	DC5	E	900	14/14	0.85	0.16	2.60	72,74,76,76	0
3	FES	E	901	4/4	0.99	0.11	-0.00	36,38,38,40	0
3	FES	A	900	4/4	0.99	0.11	-0.07	38,39,39,40	0
3	FES	C	900	4/4	0.99	0.10	-0.43	27,31,32,33	0
3	FES	G	900	4/4	0.98	0.11	-0.47	72,73,73,74	0
3	FES	I	900	4/4	0.97	0.12	-0.51	62,62,64,66	0
3	FES	K	900	4/4	0.97	0.12	-0.57	56,57,57,59	0
4	FE2	E	902	1/1	1.00	0.12	-	40,40,40,40	0
4	FE2	C	901	1/1	1.00	0.12	-	37,37,37,37	0
4	FE2	K	901	1/1	0.99	0.09	-	74,74,74,74	0
4	FE2	I	901	1/1	0.99	0.09	-	58,58,58,58	0
4	FE2	A	901	1/1	0.99	0.14	-	34,34,34,34	0
4	FE2	G	901	1/1	0.96	0.11	-	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.