Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 09:06 pm GMT

PDB ID	:	2YFL
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 (i) 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 (i)) were used in the production of this report:

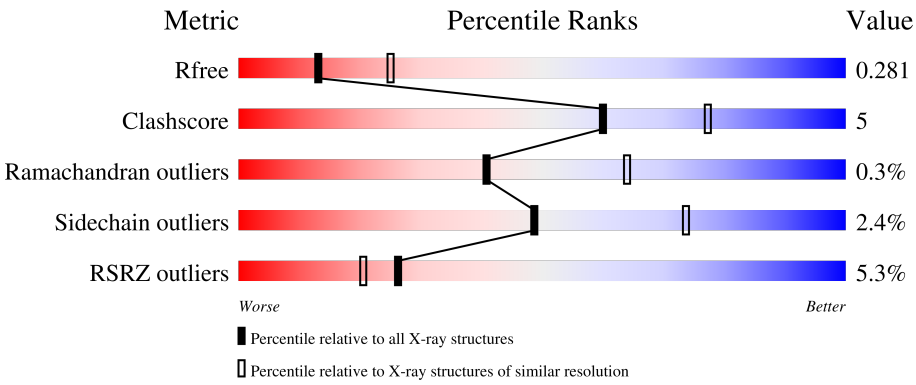
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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%, 83%, 11%, • 6%
1	C	459	3%, 81%, 13%, • 6%
1	E	459	%, 80%, 14%, 6%
1	G	459	12%, 83%, 10%, • 6%
1	I	459	10%, 83%, 11%, 6%

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Mol	Chain	Length	Quality of chain
1	K	459	11% 83% 10% 6%
2	B	188	84% 11%
2	D	188	78% 18%
2	F	188	82% 14%
2	H	188	82% 14%
2	J	188	86% 10%
2	L	188	87% 8%

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	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	433	3430	2182	602	622	24	0	0	0
1	C	433	3430	2182	602	622	24	0	0	0
1	E	433	3430	2182	602	622	24	0	0	0
1	G	433	3430	2182	602	622	24	0	0	0
1	I	433	3430	2182	602	622	24	0	0	0
1	K	433	3430	2182	602	622	24	0	0	0

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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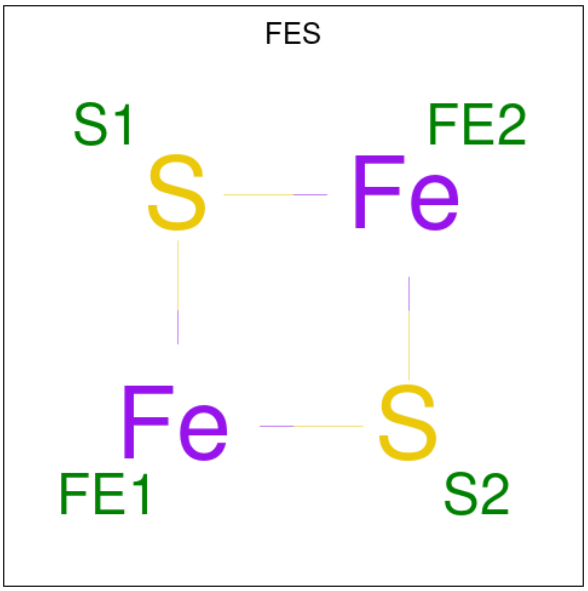
Chain	Residue	Modelled	Actual	Comment	Reference
G	338	GLN	ASN	engineered mutation	UNP P37333
G	341	VAL	ILE	engineered mutation	UNP P37333
G	409	PHE	LEU	engineered mutation	UNP P37333
I	335	ALA	THR	engineered mutation	UNP P37333
I	336	MET	PHE	engineered mutation	UNP P37333
I	338	GLN	ASN	engineered mutation	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
			Total	C	N	O	S			
2	B	180	1496	948	265	279	4	0	0	0
2	D	180	1496	948	265	279	4	0	0	0
2	F	180	1496	948	265	279	4	0	0	0
2	H	180	1496	948	265	279	4	0	0	0
2	J	180	1496	948	265	279	4	0	0	0
2	L	180	1496	948	265	279	4	0	0	0

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

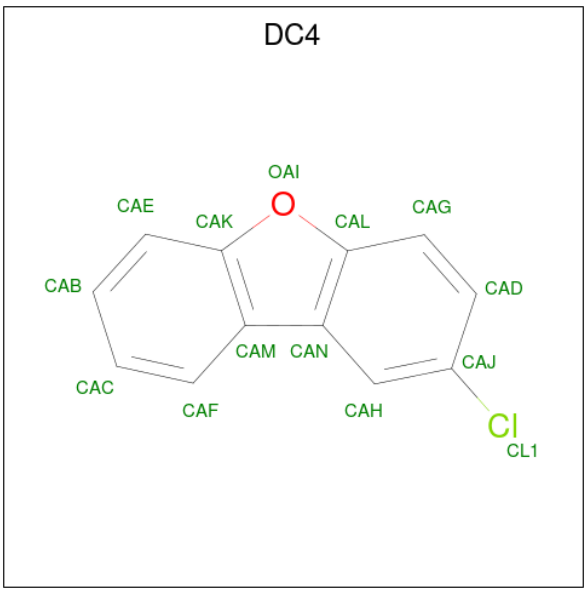


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	4	2	2	0	0
3	C	1	4	2	2	0	0
3	E	1	4	2	2	0	0
3	G	1	4	2	2	0	0
3	I	1	4	2	2	0	0
3	K	1	4	2	2	0	0

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

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

- Molecule 5 is 2-CHLORODIBENZOFURAN (three-letter code: DC4) (formula: $C_{12}H_7ClO$).



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

- Molecule 6 is water.

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

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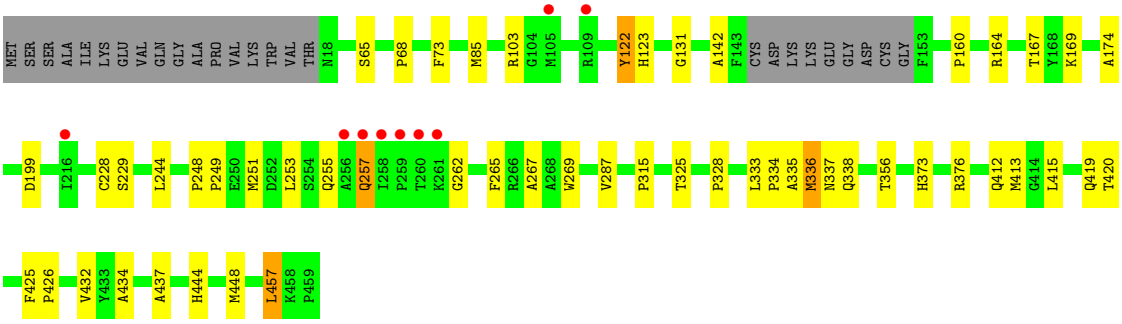
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	J	11	11	11	0	0
			Total	O		
6	K	20	20	20	0	0
			Total	O		
6	L	15	15	15	0	0

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.

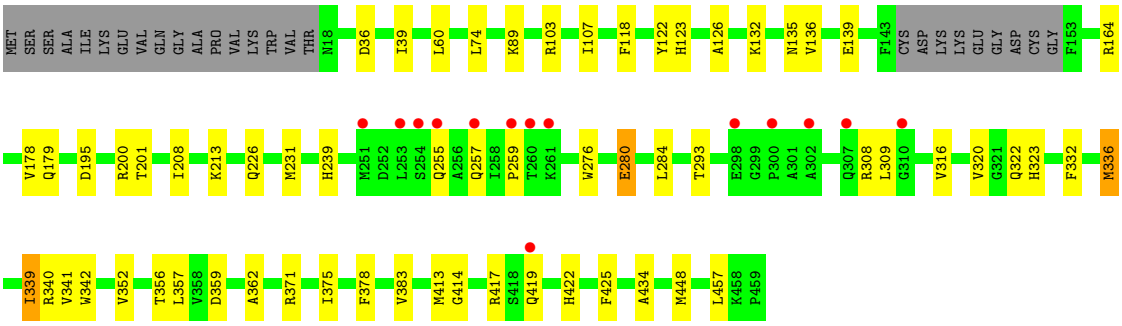
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain A: 2% 83% 11% • 6%



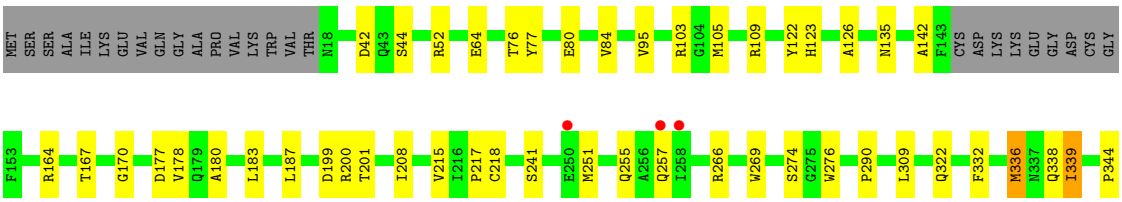
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

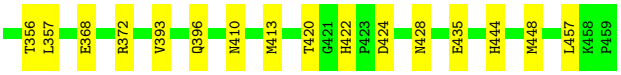
Chain C: 3% 81% 13% • 6%



• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

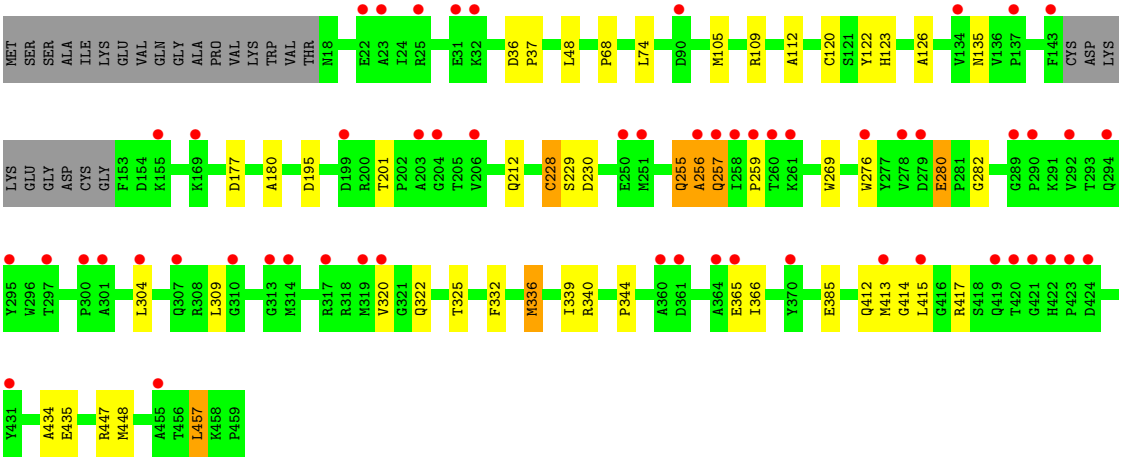
Chain E: % 80% 14% 6%





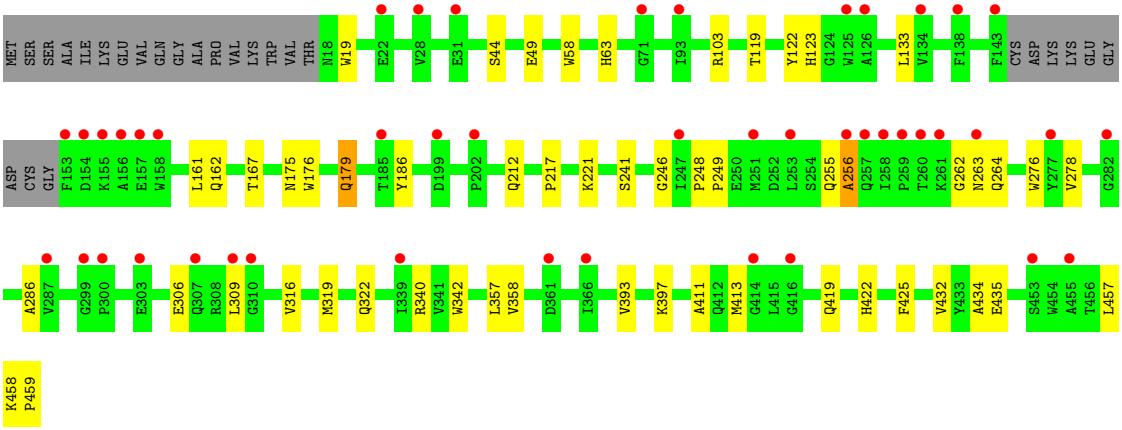
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain G:



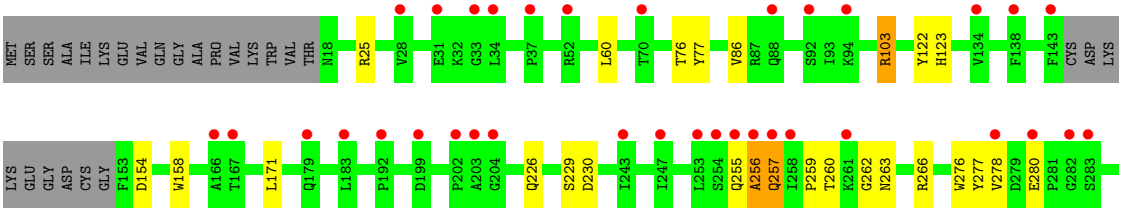
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

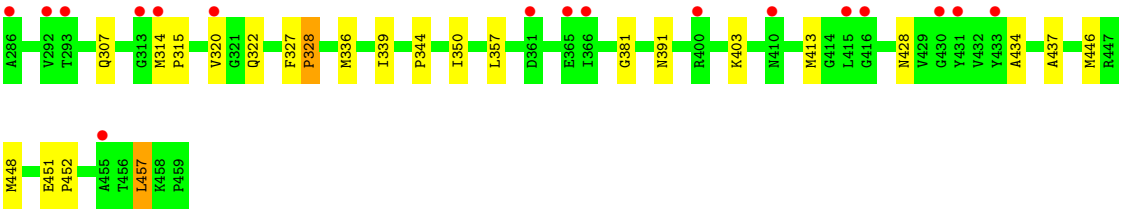
Chain I:



• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain K:



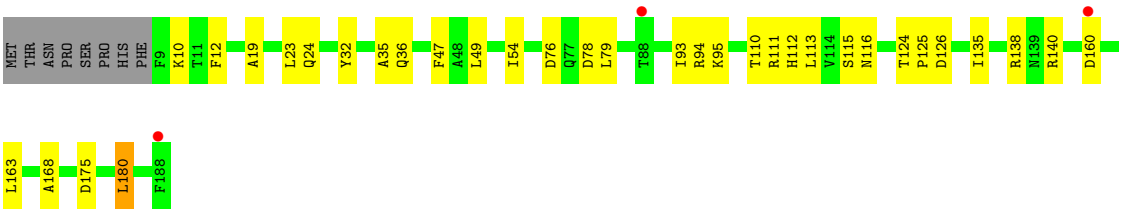


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain B:

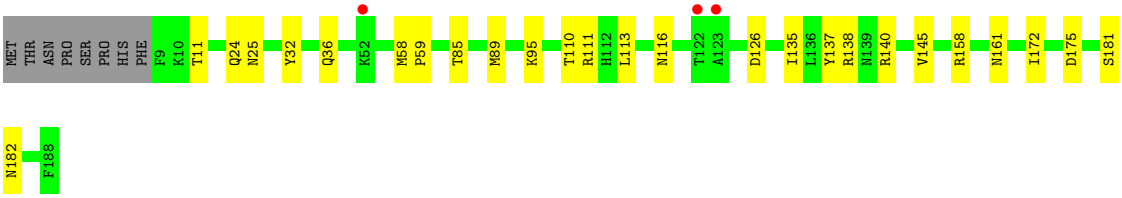
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain D:



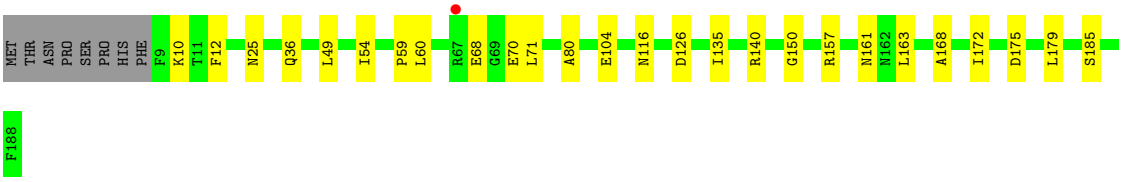
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain F:



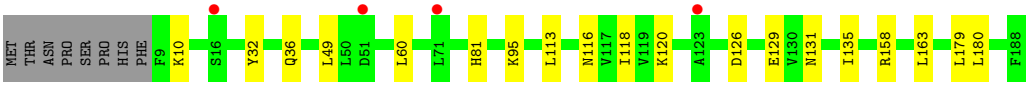
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain H:



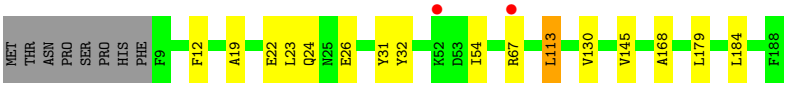
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain J:



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain L:



4 Data and refinement statistics (i)

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 44.82 – 2.54	Depositor EDS
% Data completeness (in resolution range)	77.7 (137.36-2.60) 77.7 (44.82-2.54)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.06%)	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)	0.31 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DC4, FES, FE2

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	0.35	0/3533	0.49	0/4796
1	C	0.34	0/3533	0.49	0/4796
1	E	0.36	0/3533	0.49	0/4796
1	G	0.33	0/3533	0.47	0/4796
1	I	0.32	0/3533	0.47	0/4796
1	K	0.33	0/3533	0.46	0/4796
2	B	0.36	0/1530	0.51	0/2068
2	D	0.35	0/1530	0.51	0/2068
2	F	0.37	0/1530	0.51	0/2068
2	H	0.34	0/1530	0.49	0/2068
2	J	0.33	0/1530	0.47	0/2068
2	L	0.34	0/1530	0.48	0/2068
All	All	0.34	0/30378	0.48	0/41184

There are no bond length outliers.

There are no bond angle outliers.

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	3430	0	3274	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3430	0	3274	42	0
1	E	3430	0	3274	34	0
1	G	3430	0	3274	32	0
1	I	3430	0	3274	33	0
1	K	3430	0	3274	33	0
2	B	1496	0	1447	16	0
2	D	1496	0	1447	21	0
2	F	1496	0	1447	22	0
2	H	1496	0	1447	18	0
2	J	1496	0	1447	16	0
2	L	1496	0	1447	13	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
6	H	19	0	0	1	0
6	I	35	0	0	9	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	268	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 (268) 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:K:255:GLN:O	1:K:257:GLN:N	1.70	1.24
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:K:256:ALA:O	1:K:257:GLN:O	1.77	1.02
1:K:255:GLN:C	1:K:257:GLN:H	1.65	1.00
1:I:255:GLN:O	1:I:256:ALA:O	1.89	0.91
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:G:255:GLN:O	1:G:257:GLN:N	2.12	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:K:255:GLN:C	1:K:257:GLN:N	2.30	0.74
1:G:126:ALA:HB3	1:G:135:ASN:HB3	1.69	0.74
1:G:255:GLN:C	1:G:257:GLN:H	1.92	0.73
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:G:256:ALA:O	1:G:257:GLN:O	2.13	0.67
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:G:255:GLN:C	1:G:257:GLN:N	2.50	0.64
1:K:256:ALA:O	1:K:257:GLN:C	2.36	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:J:49:LEU:HD21	2:J:163:LEU:HD13	1.79	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:K:255:GLN:O	1:K:256:ALA:C	2.45	0.54
1:I:422:HIS:HB2	6:I:2033:HOH:O	2.09	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:257:GLN:HE21	1:C:259:PRO:N	2.10	0.48
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
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
2:H:36:GLN:HE21	2:L:12:PHE:H	1.62	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:A:262:GLY:C	1:A:432:VAL:HB	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:F:85:THR:O	2:F:89:MET:HG2	2.16	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
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:49:GLU:OE2	1:I:221:LYS:NZ	2.44	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
2:D:116:ASN:HA	2:F:32:TYR:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:257:GLN:HE21	1:C:259:PRO:CA	2.31	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
1:G:269:TRP:HZ2	1:G:457:LEU:HD22	1.84	0.43
1:I:262:GLY:C	1:I:432:VAL:HB	2.39	0.43
1:A:335:ALA:HB3	1:A:336:MET:HE1	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:340:ARG:HH12	1:G:385:GLU:CD	2.23	0.42
2:H:60:LEU:HG	2:H:80:ALA:HA	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: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
1:G:105:MET:HE2	1:G:109:ARG:HD2	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
1:I:306:GLU:C	6:I:2025:HOH:O	2.58	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
1:I:212:GLN:HE21	1:I:212:GLN:HB2	1.62	0.41
1:I:397:LYS:NZ	6:I:2031:HOH:O	2.51	0.41
1:I:458:LYS:HA	1:I:459:PRO:HD3	1.92	0.41
1:C:257:GLN:HE21	1:C:259:PRO:HA	1.85	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:105:MET:CE	1:G:109:ARG:HD2	2.50	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
1:E:105:MET:CE	1:E:109:ARG:HD2	2.51	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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	429/459 (94%)	405 (94%)	23 (5%)	1 (0%)	47 71
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%)	13 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	429/459 (94%)	400 (93%)	28 (6%)	1 (0%)	47	71
1	K	429/459 (94%)	394 (92%)	32 (8%)	3 (1%)	22	43
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%)	41	64

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 (i)

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%)	340 (97%)	10 (3%)	42	68
1	C	350/372 (94%)	339 (97%)	11 (3%)	40	66
1	E	350/372 (94%)	339 (97%)	11 (3%)	40	66
1	G	350/372 (94%)	342 (98%)	8 (2%)	50	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	350/372 (94%)	342 (98%)	8 (2%)	50	75
1	K	350/372 (94%)	344 (98%)	6 (2%)	60	81
2	B	159/167 (95%)	157 (99%)	2 (1%)	69	86
2	D	159/167 (95%)	151 (95%)	8 (5%)	24	47
2	F	159/167 (95%)	158 (99%)	1 (1%)	86	95
2	H	159/167 (95%)	155 (98%)	4 (2%)	47	73
2	J	159/167 (95%)	158 (99%)	1 (1%)	86	95
2	L	159/167 (95%)	157 (99%)	2 (1%)	69	86
All	All	3054/3234 (94%)	2982 (98%)	72 (2%)	49	74

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	122	TYR
1	A	167	THR
1	A	257	GLN
1	A	315	PRO
1	A	336	MET
1	A	356	THR
1	A	419	GLN
1	A	420	THR
1	A	457	LEU
2	B	10	LYS
2	B	113	LEU
1	C	74	LEU
1	C	89	LYS
1	C	103	ARG
1	C	122	TYR
1	C	132	LYS
1	C	179	GLN
1	C	201	THR
1	C	255	GLN
1	C	280	GLU
1	C	336	MET
1	C	339	ILE
2	D	10	LYS
2	D	76	ASP
2	D	94	ARG

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Mol	Chain	Res	Type
2	D	115	SER
2	D	124	THR
2	D	140	ARG
2	D	160	ASP
2	D	180	LEU
1	E	103	ARG
1	E	122	TYR
1	E	167	THR
1	E	201	THR
1	E	274	SER
1	E	336	MET
1	E	338	GLN
1	E	339	ILE
1	E	410	ASN
1	E	420	THR
1	E	457	LEU
2	F	140	ARG
1	G	48	LEU
1	G	122	TYR
1	G	228	CYS
1	G	229	SER
1	G	280	GLU
1	G	336	MET
1	G	365	GLU
1	G	457	LEU
2	H	10	LYS
2	H	70	GLU
2	H	140	ARG
2	H	179	LEU
1	I	103	ARG
1	I	119	THR
1	I	122	TYR
1	I	167	THR
1	I	179	GLN
1	I	358	VAL
1	I	419	GLN
1	I	457	LEU
2	J	10	LYS
1	K	86	VAL
1	K	103	ARG
1	K	122	TYR
1	K	260	THR

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Mol	Chain	Res	Type
1	K	336	MET
1	K	457	LEU
2	L	67	ARG
2	L	113	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	226	GLN
1	A	263	ASN
1	A	373	HIS
1	A	391	ASN
1	A	410	ASN
1	A	444	HIS
2	B	25	ASN
2	B	36	GLN
2	B	77	GLN
2	B	131	ASN
1	C	179	GLN
1	C	212	GLN
1	C	226	GLN
1	C	257	GLN
1	C	373	HIS
1	C	391	ASN
1	C	410	ASN
1	C	422	HIS
2	D	25	ASN
2	D	36	GLN
2	D	81	HIS
2	D	131	ASN
1	E	179	GLN
1	E	212	GLN
1	E	226	GLN
1	E	338	GLN
1	E	373	HIS
1	E	391	ASN
1	E	410	ASN
1	E	422	HIS
1	E	428	ASN
1	E	444	HIS
2	F	25	ASN

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Mol	Chain	Res	Type
2	F	36	GLN
2	F	131	ASN
1	G	212	GLN
1	G	226	GLN
1	G	419	GLN
1	G	444	HIS
2	H	25	ASN
2	H	36	GLN
2	H	131	ASN
1	I	179	GLN
1	I	212	GLN
1	I	419	GLN
1	I	422	HIS
1	I	444	HIS
2	J	25	ASN
2	J	36	GLN
2	J	131	ASN
1	K	307	GLN
1	K	343	HIS
1	K	348	ASN
1	K	391	ASN
1	K	396	GLN
1	K	410	ASN
2	L	25	ASN
2	L	36	GLN
2	L	131	ASN

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 monosaccharides 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	$\#\|Z\| > 2$
5	DC4	C	1460	-	12,16,16	1.36	1 (8%)	13,23,23	1.05	1 (7%)
3	FES	C	900	1	0,4,4	-	-	-		
3	FES	A	900	1	0,4,4	-	-	-		
3	FES	K	900	1	0,4,4	-	-	-		
3	FES	G	900	6,1	0,4,4	-	-	-		
5	DC4	A	1460	-	12,16,16	1.34	1 (8%)	13,23,23	0.74	0
3	FES	E	900	1	0,4,4	-	-	-		
3	FES	I	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	DC4	C	1460	-	-	-	0/3/3/3
3	FES	C	900	1	-	-	0/1/1/1
3	FES	A	900	1	-	-	0/1/1/1
3	FES	K	900	1	-	-	0/1/1/1
3	FES	G	900	6,1	-	-	0/1/1/1
5	DC4	A	1460	-	-	-	0/3/3/3
3	FES	E	900	1	-	-	0/1/1/1
3	FES	I	900	1	-	-	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	-2.49	1.38	1.45
5	A	1460	DC4	CAM-CAN	-2.12	1.39	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1460	DC4	CAD-CAJ-CAH	-2.19	119.39	121.99

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
5	C	1460	DC4	8	0
3	C	900	FES	1	0
3	A	900	FES	1	0
3	K	900	FES	1	0
3	G	900	FES	2	0
5	A	1460	DC4	1	0
3	E	900	FES	1	0
3	I	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.17	9 (2%)	63	58	35, 49, 66, 74	18 (4%)
1	C	433/459 (94%)	-0.08	14 (3%)	47	40	36, 56, 79, 88	18 (4%)
1	E	433/459 (94%)	-0.10	3 (0%)	87	86	36, 52, 72, 81	18 (4%)
1	G	433/459 (94%)	0.65	57 (13%)	3	2	50, 94, 141, 162	18 (4%)
1	I	433/459 (94%)	0.63	45 (10%)	6	4	53, 94, 140, 162	18 (4%)
1	K	433/459 (94%)	0.71	52 (12%)	4	2	56, 95, 137, 156	18 (4%)
2	B	180/188 (95%)	-0.20	2 (1%)	80	78	32, 46, 61, 68	4 (2%)
2	D	180/188 (95%)	-0.16	3 (1%)	70	66	34, 49, 62, 70	4 (2%)
2	F	180/188 (95%)	-0.09	3 (1%)	70	66	35, 48, 67, 74	4 (2%)
2	H	180/188 (95%)	-0.11	1 (0%)	89	88	43, 62, 84, 95	4 (2%)
2	J	180/188 (95%)	0.02	4 (2%)	62	56	40, 64, 84, 94	4 (2%)
2	L	180/188 (95%)	-0.09	2 (1%)	80	78	41, 61, 81, 91	4 (2%)
All	All	3678/3882 (94%)	0.16	195 (5%)	26	20	32, 62, 121, 162	132 (3%)

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	361	ASP	8.9
1	K	258	ILE	8.4
1	G	292	VAL	6.5
1	K	199	ASP	6.0
1	K	34	LEU	5.5
1	I	157	GLU	5.5
1	G	259	PRO	5.4
1	G	256	ALA	5.4
1	I	300	PRO	5.2
1	K	257	GLN	5.2
1	G	143	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	I	257	GLN	5.0
1	K	243	ILE	4.9
1	K	320	VAL	4.8
1	I	158	TRP	4.8
1	I	251	MET	4.7
1	G	257	GLN	4.6
1	G	31	GLU	4.5
1	G	422	HIS	4.4
1	G	423	PRO	4.3
1	I	253	LEU	4.3
1	I	416	GLY	4.3
1	G	260	THR	4.2
1	G	22	GLU	4.2
1	K	94	LYS	4.1
1	I	455	ALA	4.1
1	C	260	THR	4.0
1	G	294	GLN	4.0
1	K	416	GLY	3.8
1	G	300	PRO	3.8
1	I	282	GLY	3.8
1	K	433	TYR	3.7
1	I	143	PHE	3.7
1	I	154	ASP	3.6
1	I	153	PHE	3.6
1	K	202	PRO	3.6
1	K	31	GLU	3.5
1	K	361	ASP	3.5
1	K	192	PRO	3.5
1	E	250	GLU	3.5
1	G	415	LEU	3.5
1	K	286	ALA	3.5
1	K	278	VAL	3.4
1	G	370	TYR	3.4
1	G	314	MET	3.4
2	B	123	ALA	3.4
1	I	93	ILE	3.4
1	G	364	ALA	3.3
1	I	155	LYS	3.3
1	E	257	GLN	3.3
1	G	251	MET	3.3
1	G	455	ALA	3.2
1	K	283	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	K	256	ALA	3.2
1	G	289	GLY	3.2
2	J	16	SER	3.2
1	I	256	ALA	3.1
1	A	105	MET	3.1
1	E	258	ILE	3.1
1	I	258	ILE	3.1
1	G	250	GLU	3.1
1	G	278	VAL	3.0
1	K	415	LEU	3.0
1	I	366	ILE	3.0
1	G	313	GLY	3.0
1	G	261	LYS	3.0
1	K	410	ASN	3.0
1	G	204	GLY	3.0
1	K	255	GLN	2.9
2	F	52	LYS	2.9
1	K	293	THR	2.9
1	I	125	TRP	2.9
1	G	420	THR	2.9
1	K	431	TYR	2.9
1	G	25	ARG	2.9
1	G	295	TYR	2.9
2	D	160	ASP	2.9
1	G	424	ASP	2.9
1	G	307	GLN	2.8
1	K	203	ALA	2.8
1	I	261	LYS	2.8
1	I	310	GLY	2.8
1	C	259	PRO	2.8
1	G	360	ALA	2.8
1	C	298	GLU	2.7
1	K	88	GLN	2.7
1	C	310	GLY	2.7
2	L	67	ARG	2.7
1	C	300	PRO	2.7
1	G	290	PRO	2.7
1	G	320	VAL	2.7
1	K	166	ALA	2.7
1	C	254	SER	2.7
1	K	313	GLY	2.7
1	K	261	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	261	LYS	2.7
1	G	32	LYS	2.7
1	G	206	VAL	2.6
2	D	188	PHE	2.6
1	A	259	PRO	2.6
1	G	297	THR	2.6
1	G	419	GLN	2.6
2	L	52	LYS	2.6
1	K	455	ALA	2.6
1	G	199	ASP	2.6
1	I	134	VAL	2.5
1	G	319	MET	2.5
1	I	202	PRO	2.5
1	G	134	VAL	2.5
1	G	317	ARG	2.5
1	K	292	VAL	2.5
1	G	279	ASP	2.5
1	G	421	GLY	2.5
1	G	304	LEU	2.5
1	I	71	GLY	2.5
1	I	339	ILE	2.5
1	K	430	GLY	2.5
1	G	276	TRP	2.5
1	C	257	GLN	2.4
1	C	302	ALA	2.4
1	G	169	LYS	2.4
1	I	277	TYR	2.4
1	K	280	GLU	2.4
1	G	203	ALA	2.4
2	B	162	ASN	2.4
1	C	251	MET	2.4
1	K	204	GLY	2.4
1	A	258	ILE	2.4
2	J	71	LEU	2.4
1	I	263	ASN	2.4
1	K	282	GLY	2.4
1	I	259	PRO	2.4
1	I	22	GLU	2.4
1	K	254	SER	2.4
1	I	361	ASP	2.4
1	K	138	PHE	2.4
1	G	365	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	258	ILE	2.4
1	G	310	GLY	2.4
2	D	88	THR	2.3
1	I	303	GLU	2.3
1	K	143	PHE	2.3
1	G	431	TYR	2.3
1	I	31	GLU	2.3
1	I	156	ALA	2.3
1	G	301	ALA	2.3
1	I	126	ALA	2.3
1	K	366	ILE	2.3
2	F	123	ALA	2.3
1	K	365	GLU	2.3
1	G	155	LYS	2.3
1	I	247	ILE	2.3
1	I	138	PHE	2.2
1	K	400	ARG	2.2
2	J	123	ALA	2.2
1	C	255	GLN	2.2
1	K	183	LEU	2.2
1	K	52	ARG	2.2
1	I	260	THR	2.2
1	K	33	GLY	2.2
1	I	28	VAL	2.2
1	K	247	ILE	2.2
1	G	137	PRO	2.2
1	I	309	LEU	2.2
1	I	199	ASP	2.2
2	J	51	ASP	2.2
1	A	260	THR	2.1
1	I	307	GLN	2.1
1	I	453	SER	2.1
1	C	419	GLN	2.1
1	I	299	GLY	2.1
1	A	256	ALA	2.1
1	G	23	ALA	2.1
1	I	414	GLY	2.1
1	K	28	VAL	2.1
1	K	167	THR	2.1
1	K	179	GLN	2.1
1	G	90	ASP	2.1
1	K	134	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	70	THR	2.1
1	I	287	VAL	2.1
1	A	109	ARG	2.1
1	G	413	MET	2.1
1	C	261	LYS	2.1
1	K	314	MET	2.1
2	F	122	THR	2.1
1	K	253	LEU	2.0
2	H	67	ARG	2.0
1	K	92	SER	2.0
1	A	257	GLN	2.0
1	C	307	GLN	2.0
1	C	253	LEU	2.0
1	I	185	THR	2.0
1	K	37	PRO	2.0
1	A	216	ILE	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 monosaccharides 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	DC4	C	1460	14/14	0.72	0.61	53,53,53,53	14
5	DC4	A	1460	14/14	0.86	0.40	49,49,49,49	14
3	FES	I	900	4/4	0.96	0.10	76,76,76,77	0
3	FES	K	900	4/4	0.96	0.12	71,72,72,72	0
4	FE2	K	901	1/1	0.97	0.12	76,76,76,76	0
3	FES	E	900	4/4	0.97	0.12	40,40,41,41	0
4	FE2	I	901	1/1	0.97	0.13	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FES	C	900	4/4	0.98	0.11	46,49,49,50	0
3	FES	A	900	4/4	0.98	0.13	46,46,46,48	0
3	FES	G	900	4/4	0.98	0.07	65,67,68,68	0
4	FE2	C	901	1/1	0.99	0.16	57,57,57,57	0
4	FE2	G	901	1/1	0.99	0.15	89,89,89,89	0
4	FE2	A	901	1/1	0.99	0.13	40,40,40,40	0
4	FE2	E	901	1/1	1.00	0.14	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.