



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:38 PM UTC

PDB ID : 2YFI / pdb_00002yfi
Title : Crystal Structure of Biphenyl dioxygenase variant RR41 (BPDO-RR41)
Authors : Kumar, P.; Bolin, J.T.
Deposited on : 2011-04-06
Resolution : 2.15 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

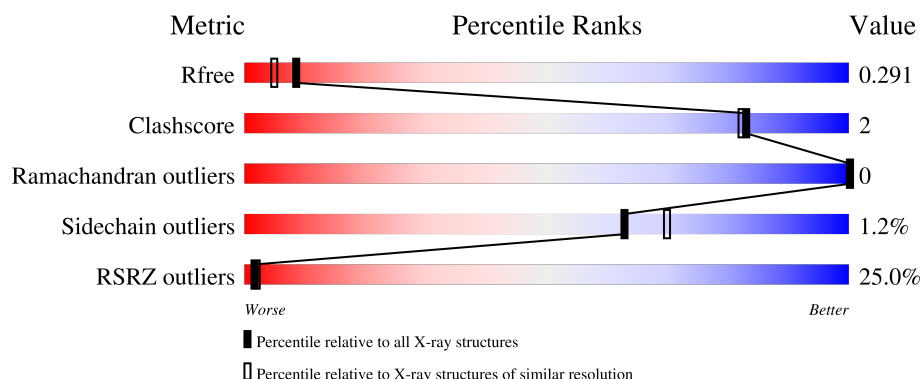
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	18% 87% 7% 6%
1	C	459	19% 88% 6% 6%
1	E	459	17% 88% 6% 6%
1	G	459	33% 87% 7% 6%
1	I	459	41% 88% 6% 6%

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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	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30799 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BIPHENYL DIOXYGENASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			
1	C	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			
1	E	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			
1	G	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			
1	I	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			
1	K	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	ALA	THR	engineered mutation	UNP P37333
A	336	MET	PHE	engineered mutation	UNP P37333
A	338	GLN	ASN	engineered mutation	UNP P37333
A	341	VAL	ILE	engineered mutation	UNP P37333
A	409	PHE	LEU	engineered mutation	UNP P37333
C	335	ALA	THR	engineered mutation	UNP P37333
C	336	MET	PHE	engineered mutation	UNP P37333
C	338	GLN	ASN	engineered mutation	UNP P37333
C	341	VAL	ILE	engineered mutation	UNP P37333
C	409	PHE	LEU	engineered mutation	UNP P37333
E	335	ALA	THR	engineered mutation	UNP P37333
E	336	MET	PHE	engineered mutation	UNP P37333
E	338	GLN	ASN	engineered mutation	UNP P37333
E	341	VAL	ILE	engineered mutation	UNP P37333
E	409	PHE	LEU	engineered mutation	UNP P37333
G	335	ALA	THR	engineered mutation	UNP P37333
G	336	MET	PHE	engineered mutation	UNP P37333

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Chain	Residue	Modelled	Actual	Comment	Reference
G	338	GLN	ASN	engineered mutation	UNP P37333
G	341	VAL	ILE	engineered mutation	UNP P37333
G	409	PHE	LEU	engineered mutation	UNP P37333
I	335	ALA	THR	engineered mutation	UNP P37333
I	336	MET	PHE	engineered mutation	UNP P37333
I	338	GLN	ASN	engineered mutation	UNP P37333
I	341	VAL	ILE	engineered mutation	UNP P37333
I	409	PHE	LEU	engineered mutation	UNP P37333
K	335	ALA	THR	engineered mutation	UNP P37333
K	336	MET	PHE	engineered mutation	UNP P37333
K	338	GLN	ASN	engineered mutation	UNP P37333
K	341	VAL	ILE	engineered mutation	UNP P37333
K	409	PHE	LEU	engineered mutation	UNP P37333

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

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

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

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

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

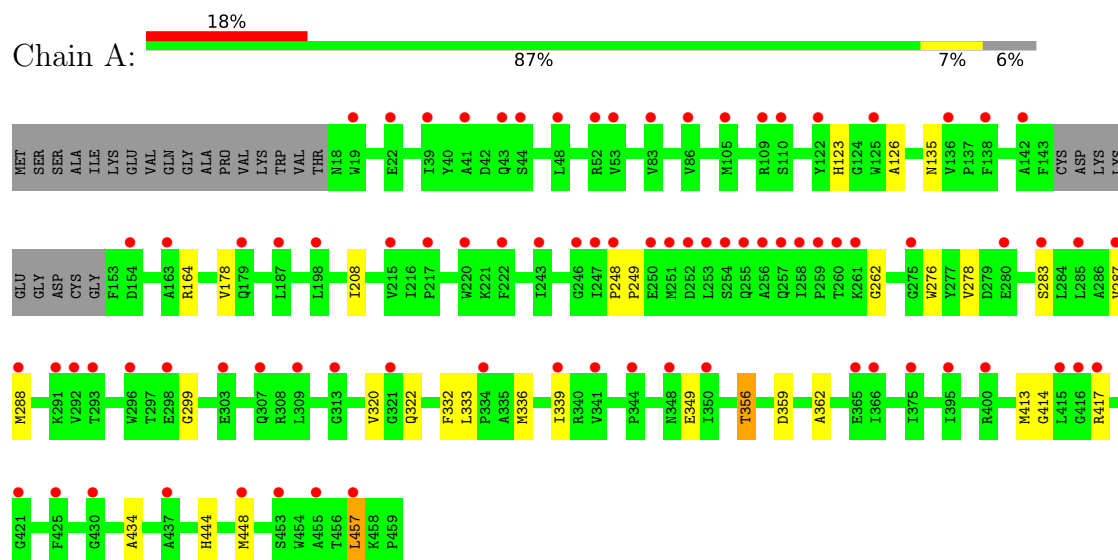
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	210	Total 210	O 210	0	0
5	B	94	Total 94	O 94	0	0
5	C	212	Total 212	O 212	0	0
5	D	99	Total 99	O 99	0	0
5	E	152	Total 152	O 152	0	0
5	F	94	Total 94	O 94	0	0
5	G	73	Total 73	O 73	0	0
5	H	79	Total 79	O 79	0	0
5	I	47	Total 47	O 47	0	0
5	J	46	Total 46	O 46	0	0
5	K	53	Total 53	O 53	0	0
5	L	54	Total 54	O 54	0	0

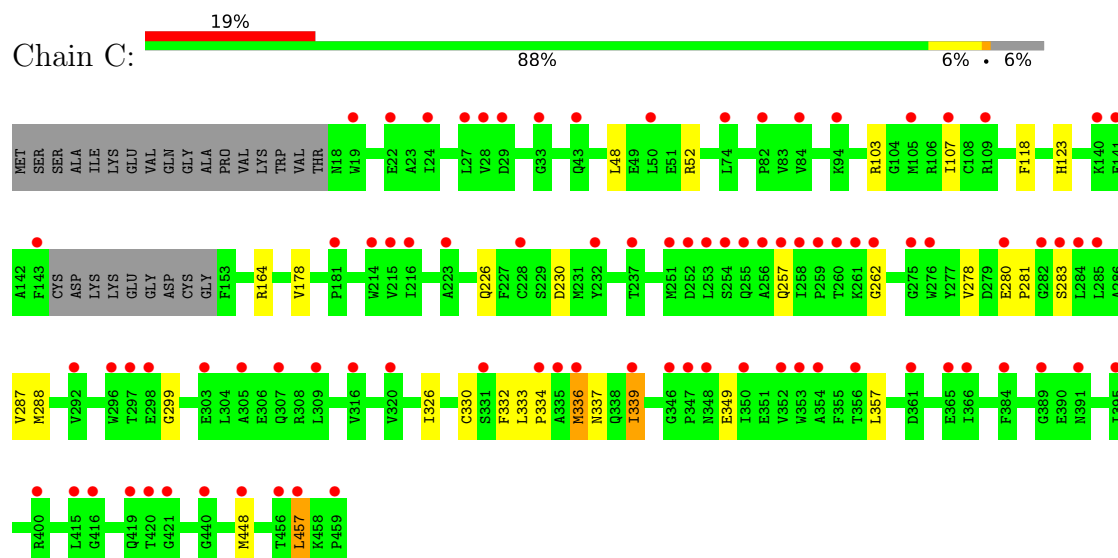
3 Residue-property plots [i](#)

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.

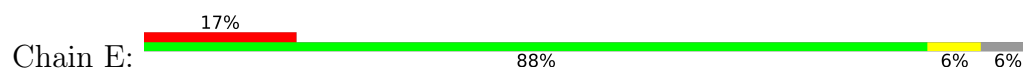
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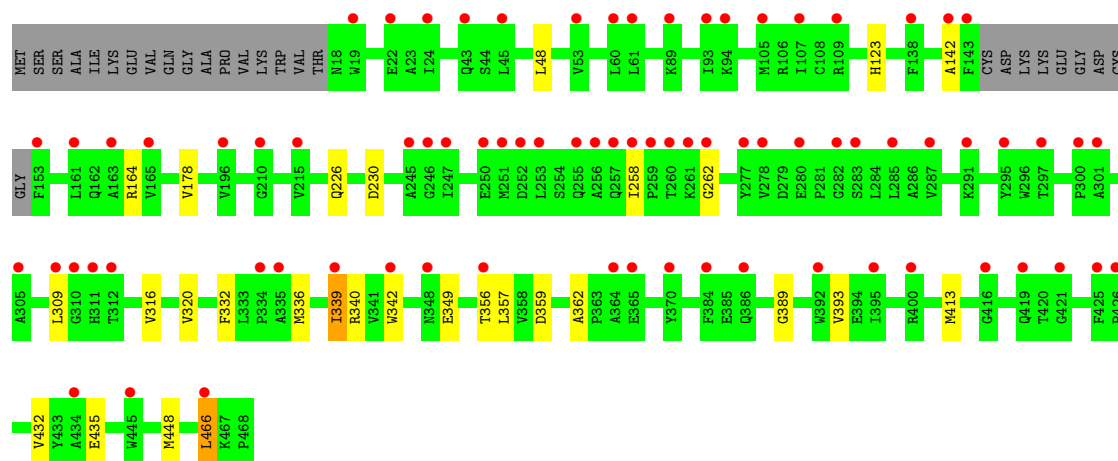


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

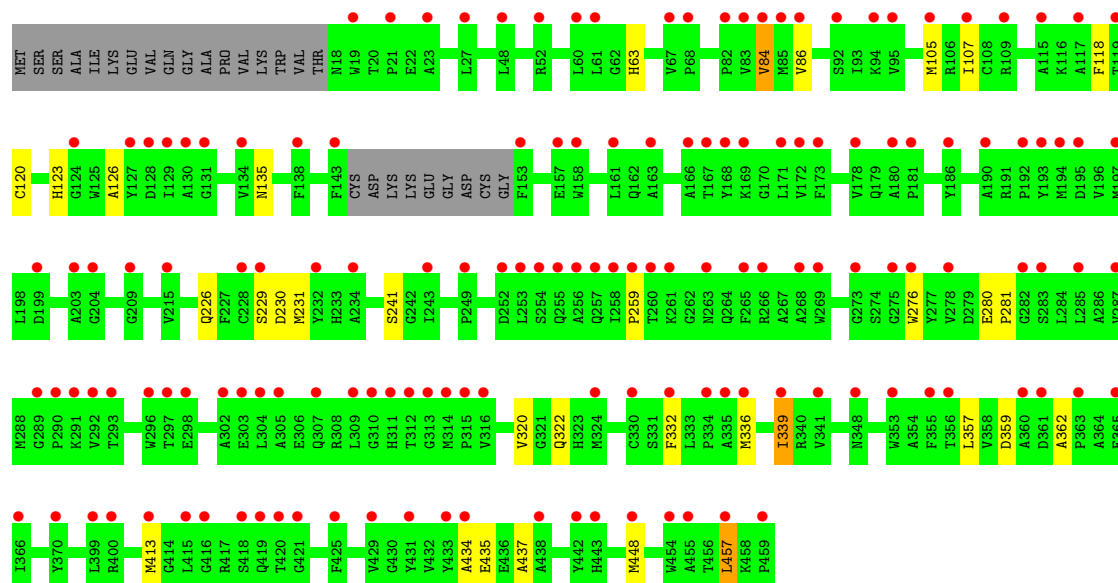
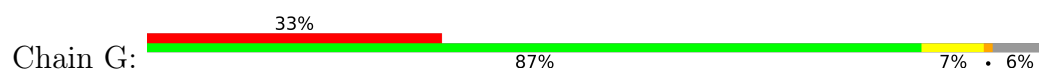


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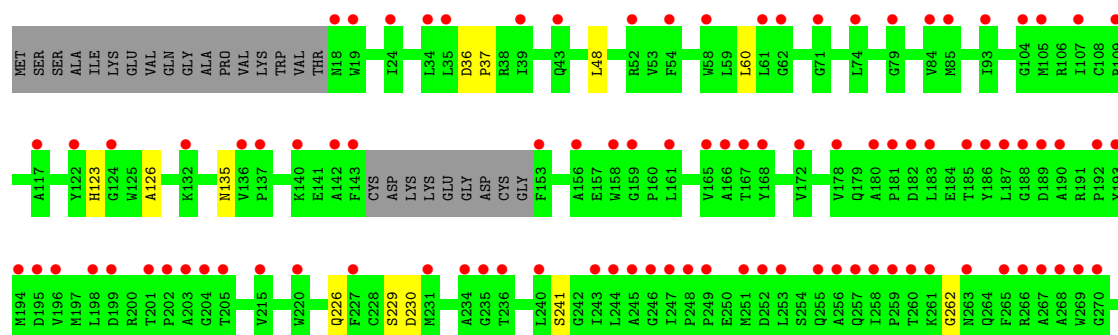
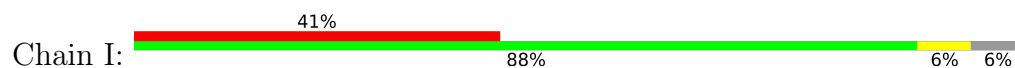


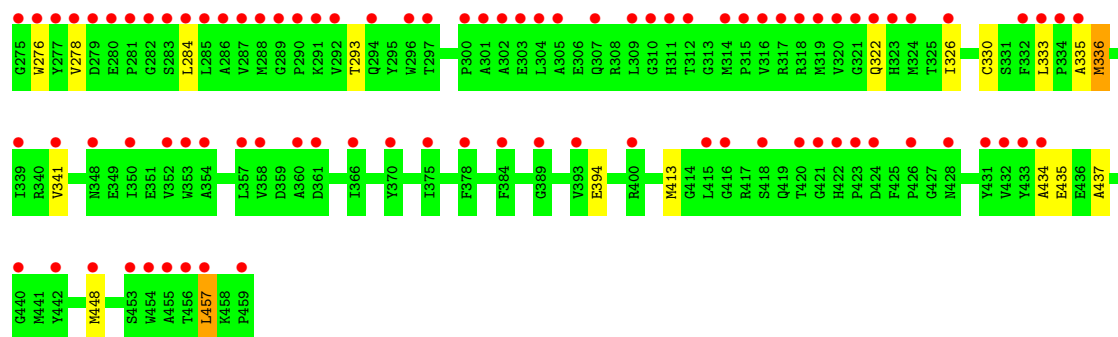


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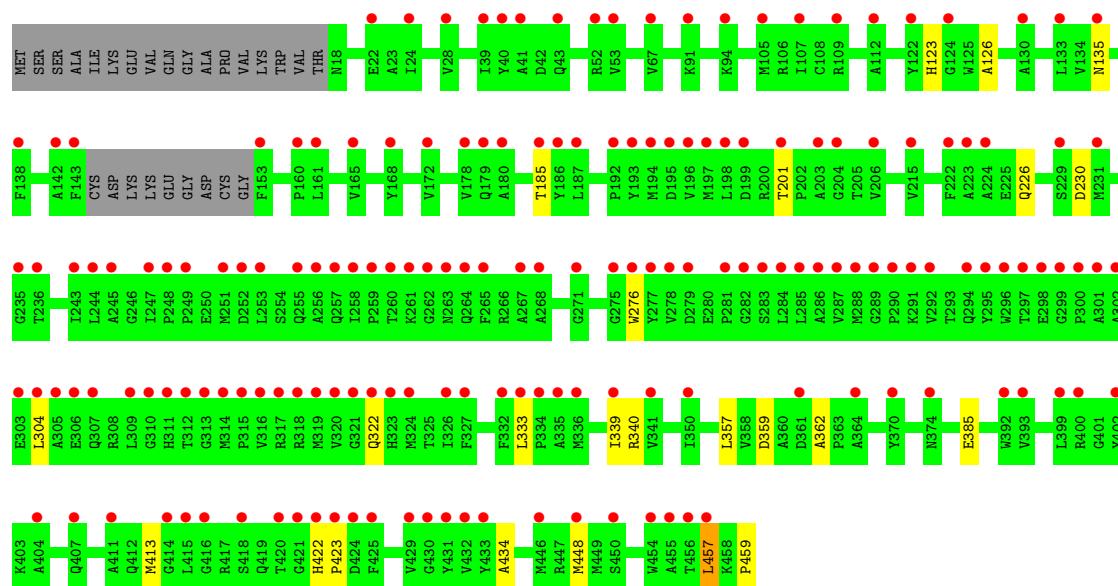
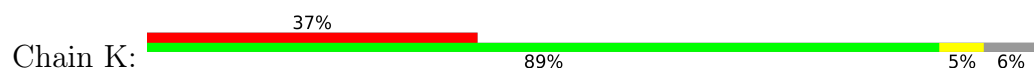


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

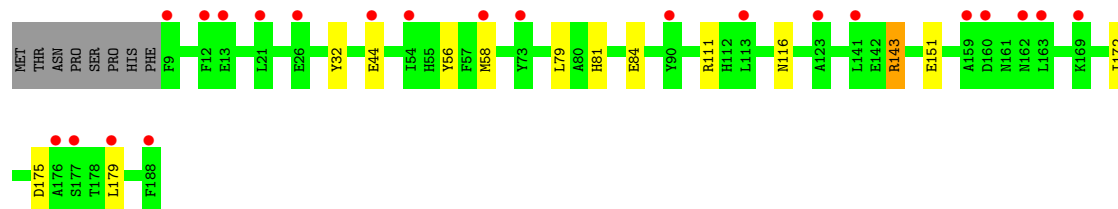
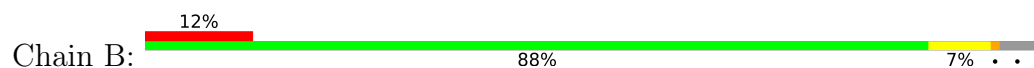




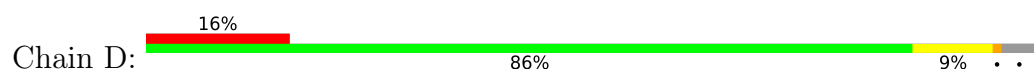
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

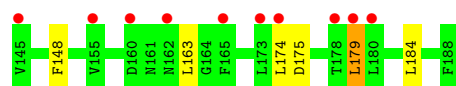


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

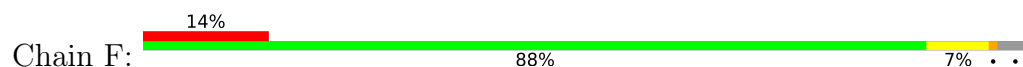


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

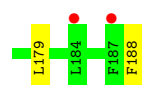
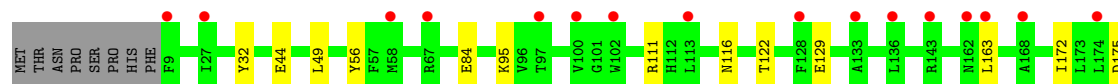




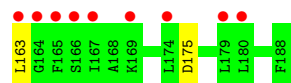
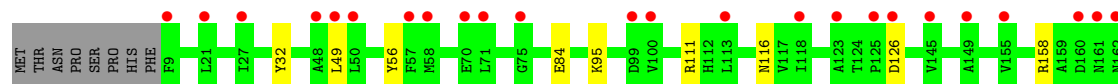
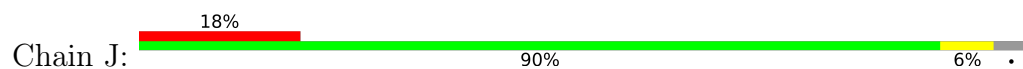
● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



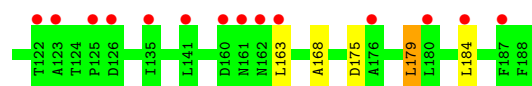
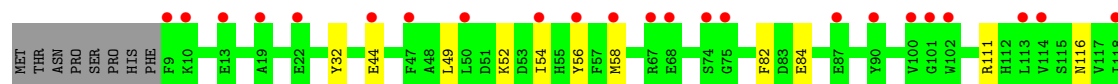
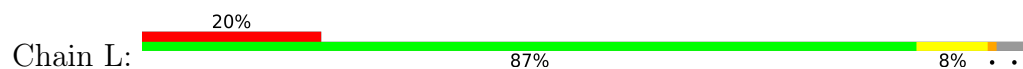
● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



● 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	86.97Å 277.81Å 92.93Å 90.00° 117.61° 90.00°	Depositor
Resolution (Å)	138.68 – 2.15 138.68 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (138.68-2.15) 99.0 (138.68-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.232 0.271 , 0.291	Depositor DCC
R_{free} test set	10445 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	30799	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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

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	0.45	0/3533	0.78	4/4796 (0.1%)
1	C	0.44	0/3533	0.77	2/4796 (0.0%)
1	E	0.43	0/3533	0.76	0/4796
1	G	0.41	0/3533	0.75	1/4796 (0.0%)
1	I	0.41	0/3533	0.73	0/4796
1	K	0.41	0/3533	0.75	2/4796 (0.0%)
2	B	0.39	0/1530	0.68	0/2068
2	D	0.40	0/1530	0.68	0/2068
2	F	0.38	0/1530	0.67	0/2068
2	H	0.38	0/1530	0.67	0/2068
2	J	0.37	0/1530	0.68	0/2068
2	L	0.38	0/1530	0.67	0/2068
All	All	0.41	0/30378	0.73	9/41184 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	299	GLY	CA-C-N	6.30	125.79	119.24
1	C	299	GLY	C-N-CA	6.30	125.79	119.24
1	A	299	GLY	CA-C-N	5.38	125.45	119.32
1	A	299	GLY	C-N-CA	5.38	125.45	119.32
1	A	333	LEU	CA-C-N	5.33	126.50	119.84
1	A	333	LEU	C-N-CA	5.33	126.50	119.84
1	G	231	MET	N-CA-C	-5.19	106.79	113.23
1	K	333	LEU	CA-C-N	5.18	125.23	119.32
1	K	333	LEU	C-N-CA	5.18	125.23	119.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3430	0	3274	19	0
1	C	3430	0	3274	17	0
1	E	3430	0	3274	16	0
1	G	3430	0	3274	18	0
1	I	3430	0	3274	16	0
1	K	3430	0	3274	12	0
2	B	1496	0	1447	12	0
2	D	1496	0	1447	14	0
2	F	1496	0	1447	11	0
2	H	1496	0	1447	11	0
2	J	1496	0	1447	8	0
2	L	1496	0	1447	10	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	210	0	0	1	0
5	B	94	0	0	0	0
5	C	212	0	0	1	0
5	D	99	0	0	0	0
5	E	152	0	0	0	0
5	F	94	0	0	0	0
5	G	73	0	0	2	0
5	H	79	0	0	0	0
5	I	47	0	0	0	0
5	J	46	0	0	0	0
5	K	53	0	0	0	0
5	L	54	0	0	0	0
All	All	30799	0	28326	140	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 2.

All (140) 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:A:413:MET:HG3	1:E:142:ALA:HB1	1.69	0.74
1:C:339:ILE:HD11	1:C:357:LEU:HG	1.78	0.66
1:G:86:VAL:HB	5:G:2017:HOH:O	1.97	0.64
1:K:123:HIS:HB2	3:K:900:FES:S2	2.38	0.63
1:A:123:HIS:HB2	3:A:900:FES:S2	2.40	0.61
1:C:339:ILE:CD1	1:C:357:LEU:HG	2.30	0.60
1:E:123:HIS:HB2	3:E:900:FES:S2	2.42	0.60
1:G:259:PRO:HA	1:G:280:GLU:HG2	1.85	0.59
1:C:123:HIS:HB2	3:C:900:FES:S2	2.44	0.57
2:B:58:MET:HG3	2:B:172:ILE:HB	1.87	0.57
1:I:123:HIS:HB2	3:I:900:FES:S2	2.45	0.57
1:C:52:ARG:HD3	5:C:2205:HOH:O	2.05	0.56
1:G:123:HIS:HB2	3:G:900:FES:S2	2.45	0.56
2:H:175:ASP:OD2	2:L:111:ARG:HB2	2.06	0.55
1:C:448:MET:HA	1:C:457:LEU:HD11	1.89	0.55
1:C:287:VAL:HG12	1:C:288:MET:HE2	1.89	0.55
1:E:339:ILE:HD11	1:E:357:LEU:HG	1.90	0.54
1:K:448:MET:HA	1:K:457:LEU:HD11	1.88	0.54
2:H:56:TYR:HB3	2:H:84:GLU:HB2	1.89	0.54
1:E:413:MET:HE2	1:E:435:GLU:HG3	1.89	0.54
1:K:226:GLN:HA	1:K:230:ASP:HB3	1.90	0.54
2:L:54:ILE:HA	2:L:168:ALA:O	2.07	0.54
1:A:414:GLY:HA2	1:A:417:ARG:HD2	1.89	0.53
1:G:332:PHE:HB3	1:G:339:ILE:HG23	1.90	0.53
2:B:56:TYR:HB3	2:B:84:GLU:HB2	1.89	0.53
1:I:335:ALA:HB3	1:I:336:MET:HE2	1.91	0.53
1:A:287:VAL:HG12	1:A:288:MET:HE3	1.91	0.53
1:G:84:VAL:HG12	5:G:2017:HOH:O	2.08	0.53
2:H:32:TYR:CD1	2:J:116:ASN:HA	2.44	0.53
2:B:143:ARG:NH2	1:E:349:GLU:OE2	2.35	0.52
2:D:116:ASN:HA	2:F:32:TYR:CD1	2.45	0.52
1:C:333:LEU:HB2	1:C:336:MET:HG3	1.92	0.52
1:A:287:VAL:HG12	1:A:288:MET:CE	2.38	0.52
1:I:276:TRP:HB3	1:I:322:GLN:HG3	1.92	0.52
1:K:413:MET:HG2	1:K:434:ALA:HA	1.91	0.51
2:D:175:ASP:OD2	2:F:111:ARG:HB2	2.10	0.51
2:B:175:ASP:OD2	2:D:111:ARG:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:413:MET:HE2	1:I:435:GLU:HG3	1.93	0.51
2:D:49:LEU:HD21	2:D:163:LEU:HD13	1.93	0.51
1:G:126:ALA:HB3	1:G:135:ASN:HB3	1.93	0.51
2:F:49:LEU:HD21	2:F:163:LEU:HD13	1.93	0.50
2:J:49:LEU:HD21	2:J:163:LEU:HD13	1.94	0.50
1:A:332:PHE:HB3	1:A:339:ILE:HG13	1.93	0.49
1:G:276:TRP:HB3	1:G:322:GLN:HG3	1.93	0.49
1:G:413:MET:HE2	1:G:435:GLU:HG3	1.94	0.49
1:G:226:GLN:HA	1:G:230:ASP:HB3	1.93	0.49
1:A:349:GLU:OE2	2:D:143:ARG:NH2	2.41	0.49
2:J:32:TYR:CD1	2:L:116:ASN:HA	2.47	0.49
2:D:12:PHE:H	2:F:36:GLN:HE21	1.61	0.48
1:I:126:ALA:HB3	1:I:135:ASN:HB3	1.96	0.48
1:E:309:LEU:HD13	1:E:316:VAL:HG11	1.95	0.48
1:K:339:ILE:HD13	1:K:357:LEU:HG	1.96	0.48
2:B:151:GLU:OE2	2:D:40:HIS:NE2	2.47	0.48
2:H:49:LEU:HD21	2:H:163:LEU:HD13	1.96	0.47
1:G:359:ASP:HB2	1:G:362:ALA:HB2	1.95	0.47
1:E:332:PHE:HB3	1:E:339:ILE:HG23	1.96	0.47
1:K:185:THR:HG22	1:K:459:PRO:HG2	1.97	0.47
1:E:339:ILE:CD1	1:E:357:LEU:HG	2.45	0.47
1:K:276:TRP:HB3	1:K:322:GLN:HG3	1.97	0.47
1:K:340:ARG:HH12	1:K:385:GLU:CD	2.22	0.47
1:E:448:MET:HA	1:E:466:LEU:HD11	1.96	0.47
1:I:226:GLN:HA	1:I:230:ASP:HB3	1.97	0.47
1:K:126:ALA:HB3	1:K:135:ASN:HB3	1.96	0.47
1:A:276:TRP:HB3	1:A:322:GLN:HG3	1.97	0.46
1:A:356:THR:HG23	2:B:79:LEU:HD11	1.96	0.46
2:D:58:MET:HE2	2:D:81:HIS:CB	2.46	0.46
1:I:262:GLY:HA2	1:I:278:VAL:HG23	1.98	0.46
1:K:359:ASP:HB2	1:K:362:ALA:HB2	1.97	0.46
1:A:283:SER:O	1:A:287:VAL:HG23	2.16	0.46
2:B:116:ASN:HA	2:D:32:TYR:CD1	2.51	0.46
2:L:49:LEU:HD21	2:L:163:LEU:HD13	1.97	0.46
2:B:116:ASN:HA	2:D:32:TYR:CG	2.51	0.46
1:C:332:PHE:HB3	1:C:339:ILE:HG23	1.98	0.46
1:I:448:MET:HA	1:I:457:LEU:HD11	1.97	0.46
1:C:226:GLN:HA	1:C:230:ASP:HB3	1.98	0.46
1:C:107:ILE:HG22	1:C:118:PHE:HB3	1.97	0.46
2:B:111:ARG:HB2	2:F:175:ASP:OD2	2.16	0.45
2:J:126:ASP:HB3	2:J:158:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:ARG:HD2	1:E:178:VAL:HA	1.98	0.45
1:A:164:ARG:HD2	1:A:178:VAL:HA	1.99	0.45
2:B:58:MET:HE2	2:B:81:HIS:CB	2.47	0.45
1:G:63:HIS:CD2	1:G:357:LEU:HD21	2.52	0.45
1:G:107:ILE:HG22	1:G:118:PHE:HB3	1.98	0.45
1:A:444:HIS:HE1	5:A:2103:HOH:O	2.00	0.45
1:C:334:PRO:O	1:C:337:ASN:OD1	2.34	0.45
2:F:179:LEU:HD21	2:F:184:LEU:HD11	1.99	0.44
2:H:172:ILE:HD13	2:H:188:PHE:HB2	1.99	0.44
2:D:56:TYR:HB3	2:D:84:GLU:HB2	1.99	0.44
1:E:340:ARG:HD3	1:E:342:TRP:CH2	2.52	0.44
2:H:116:ASN:HA	2:L:32:TYR:CG	2.53	0.44
1:C:262:GLY:HA2	1:C:278:VAL:HG23	1.99	0.44
1:A:359:ASP:HB2	1:A:362:ALA:HB2	2.00	0.43
2:L:56:TYR:HB3	2:L:84:GLU:HB2	1.99	0.43
2:D:58:MET:HE2	2:D:81:HIS:CG	2.54	0.43
2:F:58:MET:HE2	2:F:81:HIS:CD2	2.53	0.43
2:H:116:ASN:HA	2:L:32:TYR:CD1	2.53	0.43
1:A:448:MET:HA	1:A:457:LEU:HD11	1.99	0.43
2:J:56:TYR:HB3	2:J:84:GLU:HB2	2.00	0.43
1:A:248:PRO:HA	1:A:249:PRO:HD3	1.95	0.43
1:K:422:HIS:HA	1:K:423:PRO:HD3	1.85	0.43
1:G:105:MET:HB3	1:G:120:CYS:SG	2.58	0.43
2:H:111:ARG:HB2	2:J:175:ASP:OD2	2.19	0.42
1:I:229:SER:HB2	1:I:437:ALA:HB3	2.00	0.42
1:I:326:ILE:HB	1:I:330:CYS:HB3	2.01	0.42
2:D:148:PHE:HB3	2:D:174:LEU:HD11	2.01	0.42
2:H:49:LEU:HD11	2:H:163:LEU:HD22	2.01	0.42
2:L:58:MET:HE2	2:L:82:PHE:HD2	1.84	0.42
1:C:164:ARG:HD2	1:C:178:VAL:HA	2.01	0.42
1:E:356:THR:HG23	2:F:79:LEU:HD11	2.02	0.42
1:G:413:MET:HG2	1:G:434:ALA:HA	2.02	0.42
1:I:284:LEU:HD23	1:I:293:THR:HG23	2.00	0.42
1:I:241:SER:HB2	2:J:95:LYS:HG3	2.02	0.42
2:L:179:LEU:HD21	2:L:184:LEU:HD11	2.02	0.42
2:H:122:THR:HG22	2:H:129:GLU:HG3	2.02	0.42
1:E:359:ASP:HB2	1:E:362:ALA:HB2	2.02	0.42
2:F:148:PHE:HB3	2:F:174:LEU:HD11	2.02	0.42
2:B:32:TYR:CD1	2:F:116:ASN:HA	2.55	0.42
1:I:60:LEU:HD23	1:I:341:VAL:HG22	2.02	0.42
1:C:280:GLU:HA	1:C:281:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:MET:HG2	1:A:434:ALA:HA	2.02	0.41
1:A:126:ALA:HB3	1:A:135:ASN:HB3	2.02	0.41
1:G:280:GLU:HA	1:G:281:PRO:HD3	1.94	0.41
1:K:201:THR:HG22	1:K:304:LEU:HD23	2.02	0.41
1:A:208:ILE:HD12	1:A:356:THR:OG1	2.21	0.41
2:B:58:MET:HE2	2:B:81:HIS:HB2	2.01	0.41
1:C:326:ILE:HB	1:C:330:CYS:HB3	2.03	0.41
1:E:262:GLY:C	1:E:432:VAL:HB	2.46	0.41
1:G:241:SER:HB2	2:H:95:LYS:HG3	2.02	0.41
1:C:349:GLU:OE2	2:F:143:ARG:NH2	2.44	0.41
1:E:226:GLN:HA	1:E:230:ASP:HB3	2.02	0.41
1:G:448:MET:HA	1:G:457:LEU:HD11	2.03	0.41
2:J:111:ARG:HB2	2:L:175:ASP:OD2	2.21	0.41
2:D:179:LEU:HD21	2:D:184:LEU:HD11	2.03	0.41
1:I:333:LEU:HB3	1:I:336:MET:HE3	2.02	0.40
1:A:262:GLY:HA2	1:A:278:VAL:HG23	2.02	0.40
1:E:389:GLY:O	1:E:393:VAL:HG23	2.21	0.40
1:I:36:ASP:HA	1:I:37:PRO:HD3	1.96	0.40
1:G:229:SER:HB2	1:G:437:ALA:HB3	2.03	0.40
1:C:283:SER:O	1:C:287:VAL:HG23	2.22	0.40
1:I:413:MET:HG2	1:I:434:ALA:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/459 (94%)	417 (97%)	12 (3%)	0	100	100
1	C	429/459 (94%)	411 (96%)	18 (4%)	0	100	100
1	E	429/459 (94%)	414 (96%)	15 (4%)	0	100	100
1	G	429/459 (94%)	411 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	429/459 (94%)	412 (96%)	17 (4%)	0	100	100
1	K	429/459 (94%)	409 (95%)	20 (5%)	0	100	100
2	B	178/188 (95%)	174 (98%)	4 (2%)	0	100	100
2	D	178/188 (95%)	172 (97%)	6 (3%)	0	100	100
2	F	178/188 (95%)	173 (97%)	5 (3%)	0	100	100
2	H	178/188 (95%)	172 (97%)	6 (3%)	0	100	100
2	J	178/188 (95%)	173 (97%)	5 (3%)	0	100	100
2	L	178/188 (95%)	173 (97%)	5 (3%)	0	100	100
All	All	3642/3882 (94%)	3511 (96%)	131 (4%)	0	100	100

There are no Ramachandran outliers to report.

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%)	346 (99%)	4 (1%)	65	72
1	C	350/372 (94%)	344 (98%)	6 (2%)	53	60
1	E	350/372 (94%)	344 (98%)	6 (2%)	53	60
1	G	350/372 (94%)	345 (99%)	5 (1%)	59	66
1	I	350/372 (94%)	346 (99%)	4 (1%)	65	72
1	K	350/372 (94%)	349 (100%)	1 (0%)	86	91
2	B	159/167 (95%)	156 (98%)	3 (2%)	50	56
2	D	159/167 (95%)	157 (99%)	2 (1%)	61	68
2	F	159/167 (95%)	158 (99%)	1 (1%)	78	84
2	H	159/167 (95%)	157 (99%)	2 (1%)	61	68
2	J	159/167 (95%)	159 (100%)	0	100	100
2	L	159/167 (95%)	156 (98%)	3 (2%)	50	56
All	All	3054/3234 (94%)	3017 (99%)	37 (1%)	63	70

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	VAL
1	A	336	MET
1	A	356	THR
1	A	457	LEU
2	B	44	GLU
2	B	143	ARG
2	B	179	LEU
1	C	48	LEU
1	C	103	ARG
1	C	257	GLN
1	C	336	MET
1	C	339	ILE
1	C	457	LEU
2	D	94	ARG
2	D	179	LEU
1	E	48	LEU
1	E	258	ILE
1	E	320	VAL
1	E	336	MET
1	E	339	ILE
1	E	466	LEU
2	F	179	LEU
1	G	84	VAL
1	G	320	VAL
1	G	336	MET
1	G	339	ILE
1	G	457	LEU
2	H	44	GLU
2	H	179	LEU
1	I	48	LEU
1	I	336	MET
1	I	394	GLU
1	I	457	LEU
1	K	457	LEU
2	L	44	GLU
2	L	52	LYS
2	L	179	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	264	GLN
1	A	322	GLN
1	A	377	ASN
1	A	386	GLN
1	A	443	HIS
2	B	77	GLN
1	C	88	GLN
1	C	99	GLN
1	C	226	GLN
1	C	377	ASN
1	C	386	GLN
1	C	391	ASN
1	C	443	HIS
2	D	131	ASN
1	E	18	ASN
1	E	43	GLN
1	E	88	GLN
1	E	255	GLN
1	E	307	GLN
1	E	322	GLN
1	E	377	ASN
1	E	443	HIS
2	F	36	GLN
2	F	77	GLN
2	F	131	ASN
1	G	88	GLN
1	G	99	GLN
1	G	322	GLN
1	G	337	ASN
1	G	343	HIS
1	G	377	ASN
1	G	443	HIS
2	H	144	GLN
1	I	43	GLN
1	I	88	GLN
1	I	322	GLN
1	I	377	ASN
1	I	386	GLN
1	I	407	GLN
1	I	443	HIS
1	K	43	GLN
1	K	88	GLN

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Mol	Chain	Res	Type
1	K	264	GLN
1	K	338	GLN
1	K	374	ASN
1	K	391	ASN
1	K	407	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	K	900	1	0,4,4	-	-	-		
3	FES	E	900	1	0,4,4	-	-	-		
3	FES	G	900	1	0,4,4	-	-	-		
3	FES	A	900	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
3	FES	K	900	1	-	-	0/1/1/1
3	FES	E	900	1	-	-	0/1/1/1
3	FES	G	900	1	-	-	0/1/1/1
3	FES	A	900	1	-	-	0/1/1/1
3	FES	I	900	1	-	-	0/1/1/1
3	FES	C	900	1	-	-	0/1/1/1

There are no bond length outliers.

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	K	900	FES	1	0
3	E	900	FES	1	0
3	G	900	FES	1	0
3	A	900	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%)	1.38	82 (18%) 3 4	25, 41, 49, 56	18 (4%)
1	C	433/459 (94%)	1.46	87 (20%) 3 3	24, 42, 49, 57	18 (4%)
1	E	433/459 (94%)	1.34	78 (18%) 3 4	26, 43, 54, 59	18 (4%)
1	G	433/459 (94%)	1.78	150 (34%) 1 1	26, 47, 50, 59	18 (4%)
1	I	433/459 (94%)	1.96	186 (42%) 0 1	26, 47, 53, 63	18 (4%)
1	K	433/459 (94%)	1.93	170 (39%) 1 1	27, 48, 54, 60	18 (4%)
2	B	180/188 (95%)	1.28	22 (12%) 8 9	31, 42, 49, 52	4 (2%)
2	D	180/188 (95%)	1.35	30 (16%) 4 5	32, 43, 49, 52	4 (2%)
2	F	180/188 (95%)	1.36	27 (15%) 5 6	33, 44, 48, 49	4 (2%)
2	H	180/188 (95%)	1.13	18 (10%) 12 14	34, 46, 50, 51	4 (2%)
2	J	180/188 (95%)	1.43	33 (18%) 3 4	35, 47, 51, 54	4 (2%)
2	L	180/188 (95%)	1.42	37 (20%) 2 3	34, 46, 50, 53	4 (2%)
All	All	3678/3882 (94%)	1.55	920 (25%) 2 2	24, 45, 52, 63	132 (3%)

All (920) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	256	ALA	8.9
1	I	256	ALA	8.5
1	A	256	ALA	7.5
1	G	256	ALA	7.4
1	G	258	ILE	6.8
1	C	256	ALA	6.4
1	G	257	GLN	6.4
1	C	283	SER	6.3
1	G	259	PRO	6.2
1	C	258	ILE	6.2
1	K	285	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	I	259	PRO	6.0
1	K	259	PRO	5.9
1	A	260	THR	5.9
1	A	259	PRO	5.9
1	I	258	ILE	5.9
1	K	278	VAL	5.6
1	K	257	GLN	5.4
1	E	257	GLN	5.4
1	A	257	GLN	5.4
1	C	257	GLN	5.3
1	I	257	GLN	5.3
1	I	283	SER	5.3
1	I	260	THR	5.2
1	C	261	LYS	5.2
1	K	282	GLY	5.1
1	G	261	LYS	5.1
1	G	260	THR	5.1
1	G	255	GLN	5.1
1	I	320	VAL	5.0
1	C	259	PRO	5.0
1	E	260	THR	5.0
1	K	260	THR	4.9
1	K	261	LYS	4.9
1	E	259	PRO	4.8
1	I	261	LYS	4.8
1	K	370	TYR	4.7
1	K	258	ILE	4.6
1	C	255	GLN	4.5
1	K	276	TRP	4.5
1	I	285	LEU	4.5
1	I	305	ALA	4.5
1	E	256	ALA	4.4
1	A	261	LYS	4.4
1	I	255	GLN	4.4
1	K	422	HIS	4.4
1	I	143	PHE	4.3
1	C	421	GLY	4.3
1	K	431	TYR	4.3
1	G	117	ALA	4.3
1	I	301	ALA	4.3
1	I	309	LEU	4.3
2	J	113	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	K	109	ARG	4.3
1	E	105	MET	4.3
1	A	258	ILE	4.3
1	K	277	TYR	4.3
1	C	260	THR	4.2
1	G	143	PHE	4.2
1	K	143	PHE	4.2
1	K	265	PHE	4.2
1	A	255	GLN	4.2
1	I	335	ALA	4.1
1	C	339	ILE	4.1
1	K	283	SER	4.1
2	F	160	ASP	4.1
1	K	297	THR	4.1
1	E	210	GLY	4.0
1	I	321	GLY	4.0
1	K	291	LYS	4.0
1	E	297	THR	4.0
1	A	416	GLY	4.0
2	F	123	ALA	4.0
1	K	105	MET	4.0
1	E	246	GLY	4.0
2	B	176	ALA	4.0
1	C	143	PHE	4.0
1	I	457	LEU	3.9
1	K	229	SER	3.9
1	I	278	VAL	3.9
1	G	275	GLY	3.9
1	K	335	ALA	3.9
1	A	109	ARG	3.9
1	K	313	GLY	3.9
1	E	253	LEU	3.9
1	G	457	LEU	3.9
1	E	261	LYS	3.9
1	G	425	PHE	3.9
1	I	366	ILE	3.9
1	K	292	VAL	3.8
1	K	319	MET	3.8
1	A	253	LEU	3.8
1	G	94	LYS	3.8
1	A	339	ILE	3.7
1	E	258	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	199	ASP	3.7
1	K	196	VAL	3.7
1	I	276	TRP	3.7
1	K	305	ALA	3.7
1	K	193	TYR	3.7
1	K	255	GLN	3.7
1	C	282	GLY	3.7
1	G	416	GLY	3.7
1	K	310	GLY	3.7
2	L	100	VAL	3.7
1	E	255	GLN	3.7
2	B	58	MET	3.6
1	K	321	GLY	3.6
1	K	433	TYR	3.6
1	A	283	SER	3.6
2	D	113	LEU	3.6
1	K	204	GLY	3.6
2	L	67	ARG	3.6
1	K	320	VAL	3.6
1	C	320	VAL	3.5
1	I	334	PRO	3.5
1	K	41	ALA	3.5
1	G	285	LEU	3.5
1	A	366	ILE	3.5
1	K	332	PHE	3.5
1	I	234	ALA	3.5
2	F	179	LEU	3.5
1	G	273	GLY	3.5
1	I	204	GLY	3.5
1	C	254	SER	3.5
1	I	277	TYR	3.5
2	L	90	TYR	3.5
1	E	278	VAL	3.5
1	I	287	VAL	3.5
2	J	100	VAL	3.5
1	K	201	THR	3.5
1	K	281	PRO	3.4
1	K	315	PRO	3.4
1	G	302	ALA	3.4
1	G	283	SER	3.4
1	A	105	MET	3.4
1	C	280	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	203	ALA	3.4
1	K	454	TRP	3.4
2	F	162	ASN	3.4
1	E	109	ARG	3.4
1	G	109	ARG	3.4
1	K	424	ASP	3.4
2	H	27	ILE	3.4
1	G	153	PHE	3.4
1	I	253	LEU	3.4
1	K	309	LEU	3.4
2	F	67	ARG	3.4
1	I	275	GLY	3.4
1	I	302	ALA	3.4
1	E	419	GLN	3.4
1	I	198	LEU	3.4
2	D	179	LEU	3.4
1	G	314	MET	3.3
2	H	97	THR	3.3
1	I	431	TYR	3.3
1	I	282	GLY	3.3
1	K	316	VAL	3.3
1	K	425	PHE	3.3
1	I	296	TRP	3.3
1	I	433	TYR	3.3
1	G	305	ALA	3.3
1	K	268	ALA	3.3
1	E	309	LEU	3.3
2	F	184	LEU	3.3
1	A	251	MET	3.3
1	I	251	MET	3.3
1	G	181	PRO	3.3
1	K	168	TYR	3.3
1	G	48	LEU	3.3
2	D	76	ASP	3.3
1	E	283	SER	3.2
1	G	418	SER	3.2
1	A	321	GLY	3.2
1	I	289	GLY	3.2
1	G	429	VAL	3.2
1	I	316	VAL	3.2
1	C	105	MET	3.2
1	I	43	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	K	296	TRP	3.2
1	C	253	LEU	3.2
1	I	284	LEU	3.2
1	K	253	LEU	3.2
2	D	180	LEU	3.2
1	E	143	PHE	3.2
1	A	400	ARG	3.2
1	E	421	GLY	3.2
1	K	22	GLU	3.2
1	G	276	TRP	3.2
1	I	105	MET	3.2
1	I	140	LYS	3.2
1	I	84	VAL	3.2
1	E	142	ALA	3.2
2	J	149	ALA	3.2
2	L	123	ALA	3.2
1	K	198	LEU	3.2
2	L	54	ILE	3.2
2	D	160	ASP	3.2
1	C	275	GLY	3.2
1	G	420	THR	3.2
1	K	324	MET	3.2
1	K	448	MET	3.2
1	I	269	TRP	3.1
1	C	252	ASP	3.1
1	A	138	PHE	3.1
1	I	153	PHE	3.1
2	H	9	PHE	3.1
1	K	289	GLY	3.1
2	J	75	GLY	3.1
1	I	249	PRO	3.1
1	I	180	ALA	3.1
1	I	247	ILE	3.1
1	I	339	ILE	3.1
1	K	284	LEU	3.1
2	J	180	LEU	3.1
1	I	168	TYR	3.1
2	D	58	MET	3.1
1	A	334	PRO	3.1
2	L	160	ASP	3.1
1	E	163	ALA	3.1
1	G	130	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	358	VAL	3.1
2	F	13	GLU	3.1
1	C	457	LEU	3.1
1	E	251	MET	3.1
1	G	282	GLY	3.1
1	K	416	GLY	3.1
1	G	138	PHE	3.1
1	A	142	ALA	3.1
1	C	284	LEU	3.1
1	G	171	LEU	3.1
1	K	161	LEU	3.1
2	J	174	LEU	3.1
2	L	102	TRP	3.0
1	E	348	ASN	3.0
1	K	248	PRO	3.0
1	E	245	ALA	3.0
1	I	190	ALA	3.0
1	K	455	ALA	3.0
1	E	215	VAL	3.0
1	I	304	LEU	3.0
1	I	393	VAL	3.0
1	K	39	ILE	3.0
1	G	313	GLY	3.0
1	K	262	GLY	3.0
1	A	298	GLU	3.0
1	K	251	MET	3.0
1	I	294	GLN	3.0
2	B	163	LEU	3.0
2	F	141	LEU	3.0
1	G	107	ILE	3.0
1	G	311	HIS	3.0
1	A	43	GLN	3.0
1	E	400	ARG	3.0
1	G	163	ALA	3.0
1	G	166	ALA	3.0
2	J	50	LEU	3.0
1	I	188	GLY	3.0
1	I	109	ARG	2.9
1	G	434	ALA	2.9
2	H	113	LEU	2.9
1	G	195	ASP	2.9
2	J	58	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	138	PHE	2.9
1	K	153	PHE	2.9
1	I	158	TRP	2.9
1	C	335	ALA	2.9
1	I	117	ALA	2.9
1	I	354	ALA	2.9
1	A	48	LEU	2.9
1	K	457	LEU	2.9
2	D	141	LEU	2.9
1	A	252	ASP	2.9
1	E	247	ILE	2.9
1	I	326	ILE	2.9
1	K	290	PRO	2.9
1	E	250	GLU	2.9
1	G	193	TYR	2.9
1	G	332	PHE	2.9
2	B	12	PHE	2.9
1	C	348	ASN	2.9
1	I	268	ALA	2.9
2	J	179	LEU	2.9
2	L	180	LEU	2.9
1	I	311	HIS	2.9
1	E	287	VAL	2.9
1	G	84	VAL	2.9
1	I	165	VAL	2.9
1	K	361	ASP	2.9
2	B	160	ASP	2.9
1	C	420	THR	2.9
1	G	312	THR	2.9
1	K	312	THR	2.9
1	K	314	MET	2.9
1	G	334	PRO	2.9
1	K	303	GLU	2.9
1	G	291	LYS	2.9
1	E	305	ALA	2.9
1	K	302	ALA	2.9
2	F	18	ALA	2.9
1	G	209	GLY	2.9
1	I	235	GLY	2.9
1	K	299	GLY	2.9
1	G	309	LEU	2.8
1	I	74	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	133	LEU	2.8
2	B	113	LEU	2.8
2	J	99	ASP	2.8
1	A	293	THR	2.8
1	C	297	THR	2.8
1	K	420	THR	2.8
2	L	125	PRO	2.8
2	L	9	PHE	2.8
1	E	277	TYR	2.8
1	C	419	GLN	2.8
1	A	448	MET	2.8
1	I	267	ALA	2.8
1	I	270	GLY	2.8
1	K	414	GLY	2.8
2	D	103	ALA	2.8
1	C	285	LEU	2.8
1	G	161	LEU	2.8
1	G	303	GLU	2.8
1	I	181	PRO	2.8
1	K	334	PRO	2.8
2	J	167	ILE	2.8
2	B	162	ASN	2.8
2	L	58	MET	2.8
1	I	186	TYR	2.8
1	E	335	ALA	2.8
1	G	190	ALA	2.8
1	G	67	VAL	2.8
1	G	192	PRO	2.8
1	G	316	VAL	2.8
1	A	243	ILE	2.8
1	I	243	ILE	2.8
1	A	348	ASN	2.8
1	I	348	ASN	2.8
1	A	246	GLY	2.8
1	C	416	GLY	2.8
1	K	186	TYR	2.8
1	E	285	LEU	2.8
1	I	201	THR	2.8
2	F	122	THR	2.8
1	K	192	PRO	2.8
1	A	350	ILE	2.8
1	C	400	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	453	SER	2.7
1	C	365	GLU	2.7
2	L	75	GLY	2.7
1	I	286	ALA	2.7
1	K	267	ALA	2.7
2	F	180	LEU	2.7
1	I	167	THR	2.7
1	A	417	ARG	2.7
2	D	143	ARG	2.7
1	C	215	VAL	2.7
1	K	243	ILE	2.7
1	G	269	TRP	2.7
1	I	310	GLY	2.7
1	E	434	ALA	2.7
1	K	142	ALA	2.7
1	I	52	ARG	2.7
1	G	297	THR	2.7
1	G	433	TYR	2.7
1	K	322	GLN	2.7
1	I	263	ASN	2.7
1	A	292	VAL	2.7
1	G	86	VAL	2.7
1	G	105	MET	2.7
1	G	178	VAL	2.7
1	G	278	VAL	2.7
1	I	314	MET	2.7
1	E	24	ILE	2.7
1	A	254	SER	2.7
1	G	330	CYS	2.7
1	A	421	GLY	2.7
1	K	124	GLY	2.7
1	K	112	ALA	2.7
1	K	286	ALA	2.7
1	K	301	ALA	2.7
1	K	411	ALA	2.7
2	L	19	ALA	2.7
1	G	304	LEU	2.7
1	E	426	PRO	2.7
1	I	192	PRO	2.7
1	I	315	PRO	2.7
1	C	336	MET	2.7
1	A	83	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	24	ILE	2.7
1	C	350	ILE	2.7
1	G	243	ILE	2.7
1	G	361	ASP	2.7
1	K	24	ILE	2.7
1	K	279	ASP	2.7
2	J	27	ILE	2.7
1	G	131	GLY	2.7
1	I	416	GLY	2.7
1	G	158	TRP	2.7
1	I	220	TRP	2.7
1	A	307	GLN	2.6
1	E	43	GLN	2.6
1	A	280	GLU	2.6
1	C	305	ALA	2.6
1	A	309	LEU	2.6
1	C	356	THR	2.6
1	I	236	THR	2.6
1	I	288	MET	2.6
2	D	9	PHE	2.6
1	I	281	PRO	2.6
2	D	162	ASN	2.6
1	A	44	SER	2.6
1	A	247	ILE	2.6
1	I	93	ILE	2.6
1	I	432	VAL	2.6
2	H	100	VAL	2.6
1	I	104	GLY	2.6
1	K	235	GLY	2.6
1	K	271	GLY	2.6
1	K	264	GLN	2.6
1	I	454	TRP	2.6
2	D	121	GLU	2.6
1	G	61	LEU	2.6
1	I	195	ASP	2.6
1	G	370	TYR	2.6
1	K	318	ARG	2.6
1	G	292	VAL	2.6
1	K	165	VAL	2.6
1	K	339	ILE	2.6
2	L	114	VAL	2.6
1	A	285	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	300	PRO	2.6
1	E	334	PRO	2.6
1	I	248	PRO	2.6
1	I	291	LYS	2.6
2	B	9	PHE	2.6
1	I	400	ARG	2.6
2	L	74	SER	2.6
1	C	307	GLN	2.6
1	G	95	VAL	2.6
1	G	442	TYR	2.6
1	K	43	GLN	2.6
1	K	326	ILE	2.6
2	B	90	TYR	2.6
2	J	145	VAL	2.6
1	C	346	GLY	2.6
1	K	311	HIS	2.6
1	G	438	ALA	2.6
1	K	195	ASP	2.6
1	K	300	PRO	2.6
1	A	19	TRP	2.6
1	A	110	SER	2.6
1	C	296	TRP	2.6
1	G	254	SER	2.6
1	G	399	LEU	2.6
2	D	16	SER	2.6
1	K	307	GLN	2.5
1	A	22	GLU	2.5
1	E	365	GLU	2.5
1	A	341	VAL	2.5
1	A	395	ILE	2.5
1	C	366	ILE	2.5
1	G	129	ILE	2.5
2	B	54	ILE	2.5
1	C	389	GLY	2.5
1	K	275	GLY	2.5
1	K	446	MET	2.5
1	K	323	HIS	2.5
1	G	348	ASN	2.5
1	I	318	ARG	2.5
1	C	361	ASP	2.5
1	C	456	THR	2.5
1	G	459	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	415	LEU	2.5
1	I	34	LEU	2.5
1	I	244	LEU	2.5
2	F	188	PHE	2.5
2	F	58	MET	2.5
1	E	310	GLY	2.5
1	I	62	GLY	2.5
1	I	178	VAL	2.5
1	K	91	LYS	2.5
2	D	67	ARG	2.5
2	H	67	ARG	2.5
1	E	252	ASP	2.5
2	J	126	ASP	2.5
1	I	185	THR	2.5
1	G	68	PRO	2.5
1	G	115	ALA	2.5
1	G	315	PRO	2.5
1	G	335	ALA	2.5
1	I	300	PRO	2.5
2	B	159	ALA	2.5
1	I	35	LEU	2.5
2	L	141	LEU	2.5
1	I	324	MET	2.5
2	D	12	PHE	2.5
1	C	19	TRP	2.5
1	C	214	TRP	2.5
1	E	19	TRP	2.5
1	G	289	GLY	2.5
1	I	421	GLY	2.5
1	C	84	VAL	2.5
1	C	352	VAL	2.5
1	G	215	VAL	2.5
1	G	263	ASN	2.5
2	L	161	ASN	2.5
1	I	189	ASP	2.5
1	I	279	ASP	2.5
1	K	179	GLN	2.5
1	G	268	ALA	2.5
1	I	156	ALA	2.5
1	I	459	PRO	2.5
1	G	27	LEU	2.5
2	B	179	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	J	71	LEU	2.5
2	L	113	LEU	2.5
1	K	197	MET	2.5
1	K	336	MET	2.5
1	A	222	PHE	2.5
1	C	109	ARG	2.5
1	E	425	PHE	2.5
1	I	227	PHE	2.5
1	I	265	PHE	2.5
1	K	400	ARG	2.5
2	H	128	PHE	2.5
2	J	9	PHE	2.5
1	I	353	TRP	2.5
2	H	102	TRP	2.5
1	C	292	VAL	2.4
1	K	287	VAL	2.4
2	J	118	ILE	2.5
1	A	365	GLU	2.4
1	E	386	GLN	2.4
1	K	294	GLN	2.4
2	J	70	GLU	2.4
1	I	442	TYR	2.4
1	I	426	PRO	2.4
1	G	413	MET	2.4
1	I	85	MET	2.4
1	I	194	MET	2.4
1	C	415	LEU	2.4
1	E	94	LYS	2.4
1	E	466	LEU	2.4
1	I	187	LEU	2.4
1	E	93	ILE	2.4
1	K	67	VAL	2.4
1	K	107	ILE	2.4
1	G	19	TRP	2.4
1	K	172	VAL	2.4
1	K	450	SER	2.4
1	G	23	ALA	2.4
1	E	61	LEU	2.4
2	J	49	LEU	2.4
1	E	262	GLY	2.4
1	I	71	GLY	2.4
1	E	22	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	265	PHE	2.4
2	B	188	PHE	2.4
1	G	128	ASP	2.4
1	G	199	ASP	2.4
1	E	53	VAL	2.4
1	E	107	ILE	2.4
1	I	196	VAL	2.4
1	K	247	ILE	2.4
1	I	231	MET	2.4
1	I	319	MET	2.4
1	K	418	SER	2.4
1	A	122	TYR	2.4
1	E	312	THR	2.4
1	K	185	THR	2.4
1	A	248	PRO	2.4
1	I	202	PRO	2.4
2	B	73	TYR	2.4
1	A	457	LEU	2.4
1	G	60	LEU	2.4
1	I	357	LEU	2.4
1	K	304	LEU	2.4
2	D	174	LEU	2.4
2	L	50	LEU	2.4
2	D	68	GLU	2.4
2	L	44	GLU	2.4
1	I	18	ASN	2.4
1	I	124	GLY	2.4
1	K	263	ASN	2.4
1	I	54	PHE	2.4
1	G	52	ARG	2.4
1	G	134	VAL	2.4
1	I	136	VAL	2.4
1	K	178	VAL	2.4
1	K	215	VAL	2.4
1	A	296	TRP	2.4
1	G	119	THR	2.4
1	C	82	PRO	2.4
1	G	82	PRO	2.4
1	G	443	HIS	2.4
1	I	420	THR	2.4
1	C	303	GLU	2.3
1	G	180	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	130	ALA	2.3
1	K	333	LEU	2.3
2	B	21	LEU	2.3
2	J	21	LEU	2.3
1	I	246	GLY	2.3
2	L	101	GLY	2.3
1	A	425	PHE	2.3
1	G	197	MET	2.3
1	K	288	MET	2.3
1	K	327	PHE	2.3
2	L	10	LYS	2.3
1	C	216	ILE	2.3
1	A	287	VAL	2.3
1	E	196	VAL	2.3
1	G	229	SER	2.3
1	G	366	ILE	2.3
2	D	115	SER	2.3
2	D	130	VAL	2.3
2	J	166	SER	2.3
1	G	21	PRO	2.3
1	G	167	THR	2.3
1	G	356	THR	2.3
1	I	423	PRO	2.3
1	K	160	PRO	2.3
2	D	178	THR	2.3
2	L	122	THR	2.3
1	G	157	GLU	2.3
2	L	13	GLU	2.3
1	G	353	TRP	2.3
1	A	163	ALA	2.3
1	E	364	ALA	2.3
1	G	431	TYR	2.3
1	I	142	ALA	2.3
1	I	245	ALA	2.3
1	K	223	ALA	2.3
1	I	61	LEU	2.3
1	I	159	GLY	2.3
1	I	415	LEU	2.3
1	K	415	LEU	2.3
1	I	182	ASP	2.3
1	K	199	ASP	2.3
1	G	400	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	448	MET	2.3
1	E	89	LYS	2.3
1	G	85	MET	2.3
1	E	138	PHE	2.3
2	L	187	PHE	2.3
2	B	177	SER	2.3
1	I	107	ILE	2.3
1	A	86	VAL	2.3
1	G	83	VAL	2.3
1	G	298	GLU	2.3
1	I	172	VAL	2.3
2	B	26	GLU	2.3
1	C	237	THR	2.3
1	C	334	PRO	2.3
1	I	205	THR	2.3
1	I	166	ALA	2.3
1	K	203	ALA	2.3
2	D	80	ALA	2.3
2	J	48	ALA	2.3
1	A	275	GLY	2.3
1	C	262	GLY	2.3
1	C	353	TRP	2.3
1	I	19	TRP	2.3
1	I	424	ASP	2.3
2	L	126	ASP	2.3
2	B	169	LYS	2.3
2	F	17	LYS	2.3
1	I	323	HIS	2.3
1	C	384	PHE	2.3
1	G	173	PHE	2.3
2	B	13	GLU	2.3
1	C	43	GLN	2.3
1	E	339	ILE	2.3
1	A	136	VAL	2.3
1	K	429	VAL	2.3
1	I	312	THR	2.3
1	G	228	CYS	2.3
1	K	317	ARG	2.3
1	A	154	ASP	2.3
1	A	437	ALA	2.3
1	A	455	ALA	2.3
1	E	301	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	455	ALA	2.3
1	K	364	ALA	2.3
1	E	416	GLY	2.3
1	I	440	GLY	2.3
2	D	10	LYS	2.3
1	C	50	LEU	2.3
1	K	194	MET	2.3
2	F	113	LEU	2.3
2	H	174	LEU	2.3
2	J	163	LEU	2.3
2	L	163	LEU	2.3
1	K	295	TYR	2.3
2	F	56	TYR	2.3
1	I	58	TRP	2.3
1	C	22	GLU	2.2
1	K	306	GLU	2.2
2	F	87	GLU	2.2
1	I	307	GLN	2.2
1	E	153	PHE	2.2
2	D	47	PHE	2.2
2	J	57	PHE	2.2
1	A	344	PRO	2.2
1	C	316	VAL	2.2
1	C	459	PRO	2.2
1	K	393	VAL	2.2
1	K	423	PRO	2.2
2	F	143	ARG	2.2
1	C	94	LYS	2.2
1	K	224	ALA	2.2
2	H	58	MET	2.2
1	A	415	LEU	2.2
1	I	183	LEU	2.2
1	K	40	TYR	2.2
2	L	22	GLU	2.2
1	I	384	PHE	2.2
1	K	52	ARG	2.2
2	D	165	PHE	2.2
1	C	140	LYS	2.2
1	G	290	PRO	2.2
1	G	341	VAL	2.2
1	I	132	LYS	2.2
1	I	375	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	J	125	PRO	2.2
2	J	162	ASN	2.2
1	K	432	VAL	2.2
2	J	155	VAL	2.2
1	C	251	MET	2.2
1	I	79	GLY	2.2
1	I	389	GLY	2.2
1	K	180	ALA	2.2
1	A	187	LEU	2.2
1	K	187	LEU	2.2
2	F	174	LEU	2.2
2	H	163	LEU	2.2
1	E	295	TYR	2.2
1	E	370	TYR	2.2
1	I	122	TYR	2.2
1	A	125	TRP	2.2
1	E	392	TRP	2.2
1	I	266	ARG	2.2
2	F	94	ARG	2.2
1	A	291	LYS	2.2
1	K	135	ASN	2.2
2	J	161	ASN	2.2
1	E	384	PHE	2.2
1	I	332	PHE	2.2
1	K	236	THR	2.2
2	D	11	THR	2.2
1	C	29	ASP	2.2
1	I	341	VAL	2.2
1	A	303	GLU	2.2
1	C	141	GLU	2.2
1	G	124	GLY	2.2
1	G	204	GLY	2.2
1	I	322	GLN	2.2
2	F	19	ALA	2.2
2	F	149	ALA	2.2
2	H	133	ALA	2.2
2	J	123	ALA	2.2
1	C	228	CYS	2.2
1	I	161	LEU	2.2
2	B	141	LEU	2.2
2	D	21	LEU	2.2
1	G	92	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	418	SER	2.2
1	I	370	TYR	2.2
2	L	56	TYR	2.2
1	K	94	LYS	2.2
1	E	445	TRP	2.2
1	G	194	MET	2.2
1	G	448	MET	2.2
1	K	392	TRP	2.2
1	G	252	ASP	2.2
1	A	39	ILE	2.1
1	C	395	ILE	2.1
1	E	280	GLU	2.1
1	K	222	PHE	2.1
2	B	44	GLU	2.1
2	F	167	ILE	2.1
1	K	28	VAL	2.1
1	A	313	GLY	2.1
1	G	307	GLN	2.1
1	K	407	GLN	2.1
1	E	311	HIS	2.1
1	I	434	ALA	2.1
1	K	404	ALA	2.1
2	H	168	ALA	2.1
1	A	52	ARG	2.1
1	A	198	LEU	2.1
1	C	309	LEU	2.1
1	G	253	LEU	2.1
2	H	184	LEU	2.1
1	I	428	ASN	2.1
1	K	374	ASN	2.1
2	D	137	TYR	2.1
1	C	298	GLU	2.1
1	K	252	ASP	2.1
1	C	181	PRO	2.1
1	G	249	PRO	2.1
1	C	276	TRP	2.1
1	G	339	ILE	2.1
1	G	355	PHE	2.1
1	I	24	ILE	2.1
1	I	378	PHE	2.1
1	C	33	GLY	2.1
1	E	165	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	421	GLY	2.1
1	K	421	GLY	2.1
2	H	143	ARG	2.1
1	G	203	ALA	2.1
2	L	176	ALA	2.1
1	C	391	ASN	2.1
1	G	336	MET	2.1
1	I	280	GLU	2.1
1	I	303	GLU	2.1
1	K	298	GLU	2.1
2	L	68	GLU	2.1
2	L	87	GLU	2.1
1	I	361	ASP	2.1
2	J	160	ASP	2.1
1	G	168	TYR	2.1
1	G	186	TYR	2.1
1	I	193	TYR	2.1
1	K	122	TYR	2.1
1	E	356	THR	2.1
1	G	293	THR	2.1
1	I	137	PRO	2.1
1	K	249	PRO	2.1
1	K	456	THR	2.1
1	A	375	ILE	2.1
1	C	440	GLY	2.1
1	E	342	TRP	2.1
1	G	454	TRP	2.1
1	A	215	VAL	2.1
1	C	28	VAL	2.1
1	G	172	VAL	2.1
1	I	292	VAL	2.1
1	K	206	VAL	2.1
2	F	145	VAL	2.1
1	E	291	LYS	2.1
1	C	354	ALA	2.1
1	I	360	ALA	2.1
2	B	123	ALA	2.1
1	C	74	LEU	2.1
1	C	331	SER	2.1
1	E	45	LEU	2.1
1	E	161	LEU	2.1
1	I	240	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	333	LEU	2.1
1	A	250	GLU	2.1
1	G	324	MET	2.1
1	G	365	GLU	2.1
1	I	448	MET	2.1
1	K	231	MET	2.1
2	H	162	ASN	2.1
2	L	162	ASN	2.1
1	I	252	ASP	2.1
1	A	179	GLN	2.1
1	G	127	TYR	2.1
1	G	232	TYR	2.1
1	G	363	PRO	2.1
1	G	310	GLY	2.1
1	K	430	GLY	2.1
2	J	164	GLY	2.1
1	C	107	ILE	2.1
1	E	395	ILE	2.1
1	I	39	ILE	2.1
1	K	350	ILE	2.1
2	L	118	ILE	2.1
1	G	287	VAL	2.1
1	I	215	VAL	2.1
1	I	352	VAL	2.1
1	K	53	VAL	2.1
2	F	128	PHE	2.1
2	H	187	PHE	2.1
1	A	41	ALA	2.1
1	A	453	SER	2.1
1	C	223	ALA	2.1
1	G	360	ALA	2.1
1	I	455	ALA	2.1
1	K	245	ALA	2.1
1	C	27	LEU	2.0
1	E	60	LEU	2.0
1	K	244	LEU	2.0
2	H	136	LEU	2.0
2	L	184	LEU	2.0
1	G	419	GLN	2.0
1	G	266	ARG	2.0
1	I	317	ARG	2.0
1	I	422	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	297	THR	2.0
1	K	402	TYR	2.0
2	J	169	LYS	2.0
1	A	430	GLY	2.0
1	E	282	GLY	2.0
1	I	350	ILE	2.0
2	L	135	ILE	2.0
1	A	53	VAL	2.0
1	K	341	VAL	2.0
2	D	145	VAL	2.0
2	D	155	VAL	2.0
2	F	9	PHE	2.0
2	J	165	PHE	2.0
2	L	47	PHE	2.0
1	A	288	MET	2.0
2	F	185	SER	2.0
1	A	220	TRP	2.0
1	G	234	ALA	2.0
1	G	296	TRP	2.0
1	K	399	LEU	2.0
2	D	173	LEU	2.0
1	G	169	LYS	2.0
1	A	217	PRO	2.0
1	C	347	PRO	2.0
1	I	290	PRO	2.0
1	I	456	THR	2.0
1	C	232	TYR	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
4	FE2	I	901	1/1	0.92	0.16	71,71,71,71	0
4	FE2	G	901	1/1	0.94	0.11	56,56,56,56	0
3	FES	I	900	4/4	0.94	0.10	55,55,56,56	0
3	FES	G	900	4/4	0.95	0.10	60,60,60,61	0
3	FES	K	900	4/4	0.97	0.08	60,60,61,62	0
4	FE2	K	901	1/1	0.97	0.09	65,65,65,65	0
4	FE2	A	901	1/1	0.98	0.08	40,40,40,40	0
3	FES	A	900	4/4	0.98	0.05	29,29,30,31	0
3	FES	C	900	4/4	0.98	0.06	33,35,35,35	0
3	FES	E	900	4/4	0.98	0.06	35,35,35,35	0
4	FE2	E	901	1/1	0.99	0.06	44,44,44,44	0
4	FE2	C	901	1/1	0.99	0.07	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.