



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 09:26 AM EDT

PDB ID : 2YFJ / pdb_00002yfq
Title : Crystal structure of Biphenyl dioxygenase variant RR41 with dibenzofuran
Authors : Kumar, P.; Sylvestre, M.; 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:

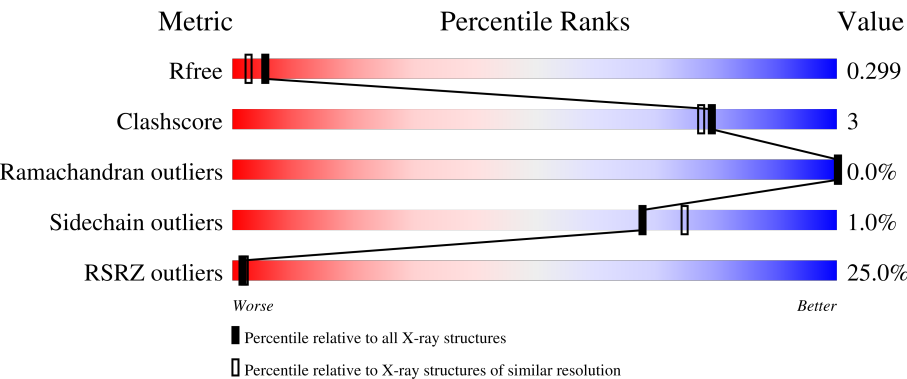
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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	23% 88% 6% 6%
1	C	459	25% 90% • • 6%
1	E	459	20% 86% 8% 6%
1	G	459	30% 87% 7% 6%
1	I	459	31% 87% 8% 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 6 unique types of molecules in this entry. The entry contains 30277 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 30 discrepancies between the modelled and reference sequences:

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

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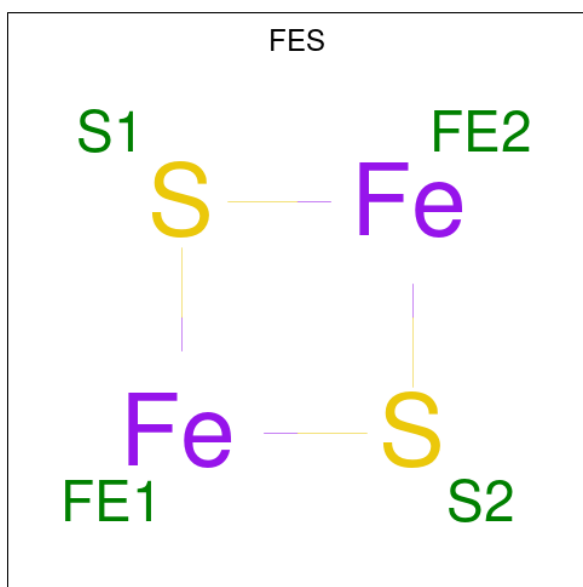
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Chain	Residue	Modelled	Actual	Comment	Reference
G	338	GLN	ASN	engineered mutation	UNP P37333
G	341	VAL	ILE	engineered mutation	UNP P37333
G	409	PHE	LEU	engineered mutation	UNP P37333
I	335	ALA	THR	engineered mutation	UNP P37333
I	336	MET	PHE	engineered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

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

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

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

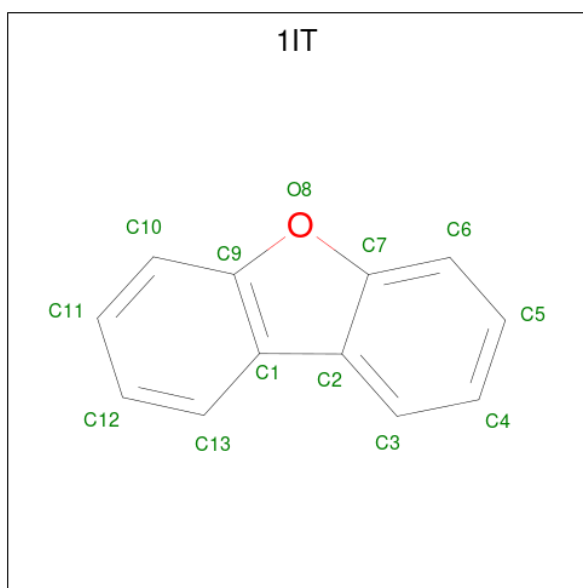


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	I	1	Total	Fe	S	0	0
			4	2	2		
3	K	1	Total	Fe	S	0	0
			4	2	2		

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

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

- Molecule 5 is DIBENZOFURAN (CCD ID: 1IT) (formula: C₁₂H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	12	1		
5	C	1	Total	C	O	0	0
			13	12	1		
5	E	1	Total	C	O	0	0
			13	12	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total	O	0	0
			128	128		
6	B	53	Total	O	0	0
			53	53		
6	C	129	Total	O	0	0
			129	129		
6	D	66	Total	O	0	0
			66	66		
6	E	88	Total	O	0	0
			88	88		
6	F	46	Total	O	0	0
			46	46		
6	G	23	Total	O	0	0
			23	23		
6	H	19	Total	O	0	0
			19	19		

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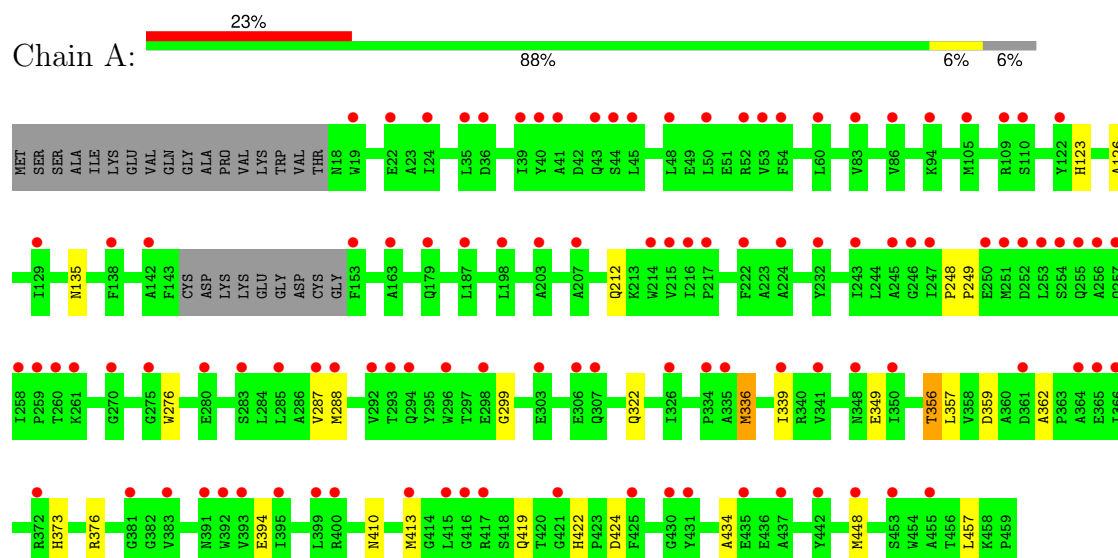
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	29	Total 29	O 29	0	0
6	J	31	Total 31	O 31	0	0
6	K	23	Total 23	O 23	0	0
6	L	17	Total 17	O 17	0	0

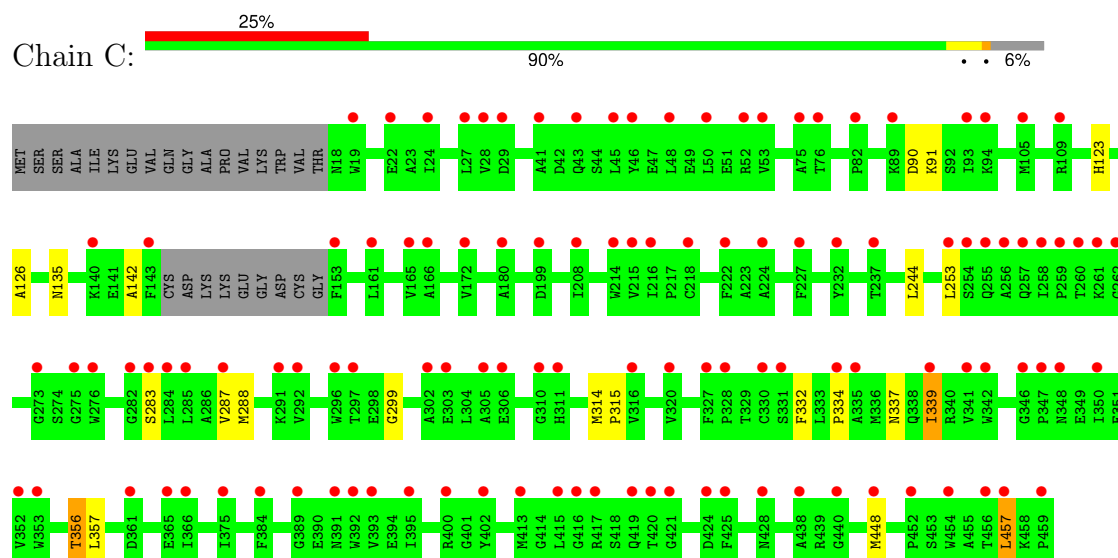
3 Residue-property plots [i](#)

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.

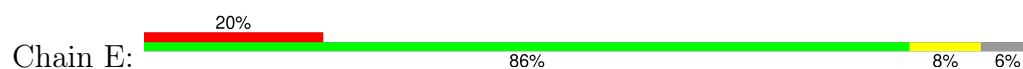
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

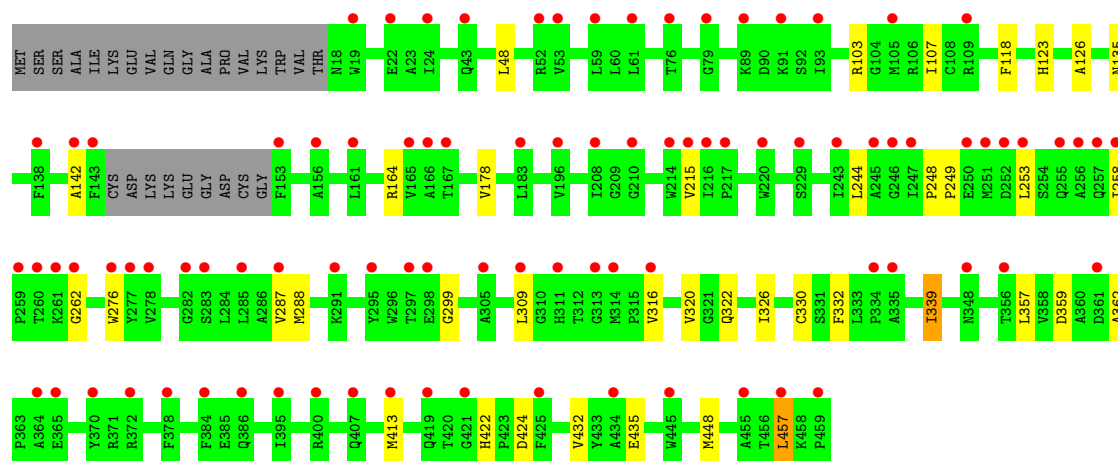


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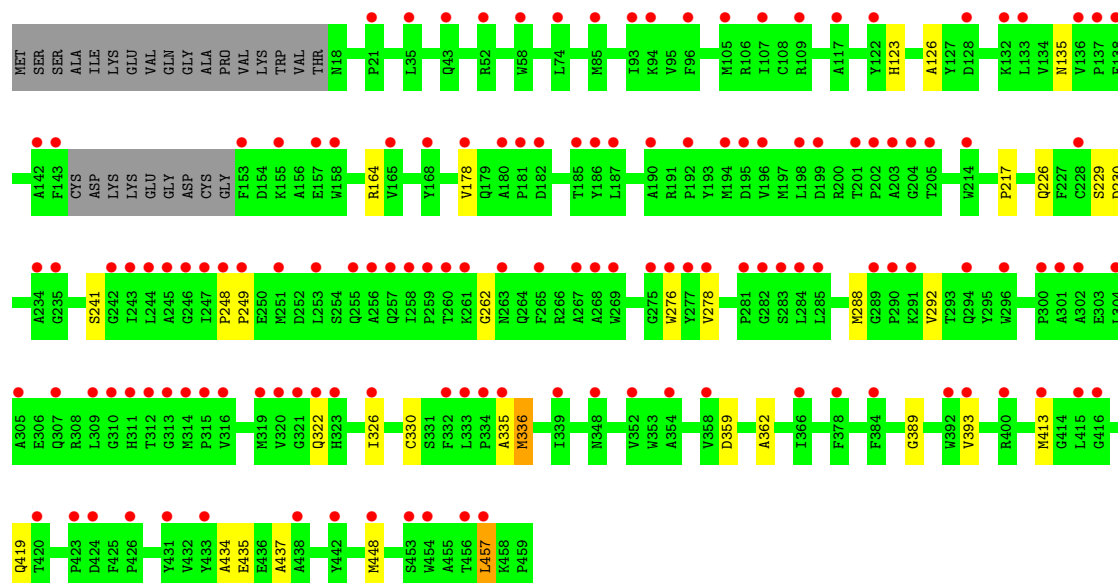
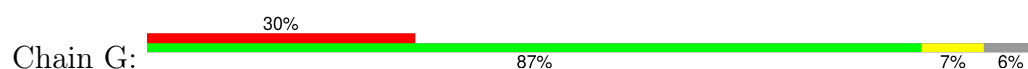


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

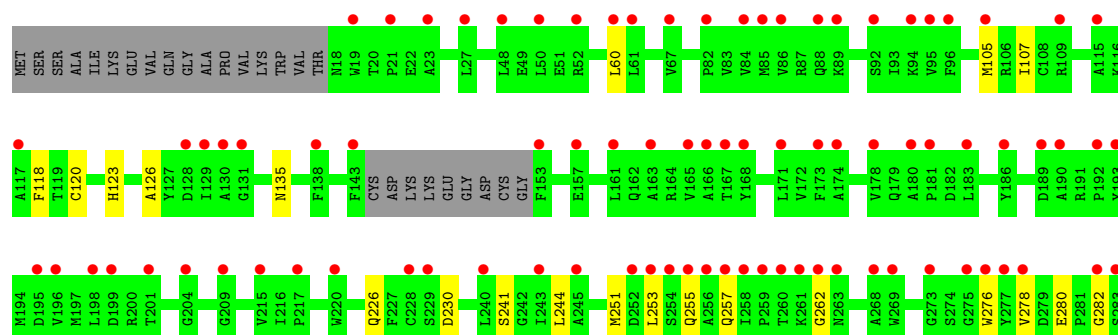
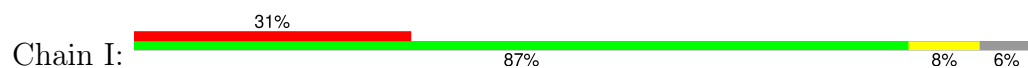


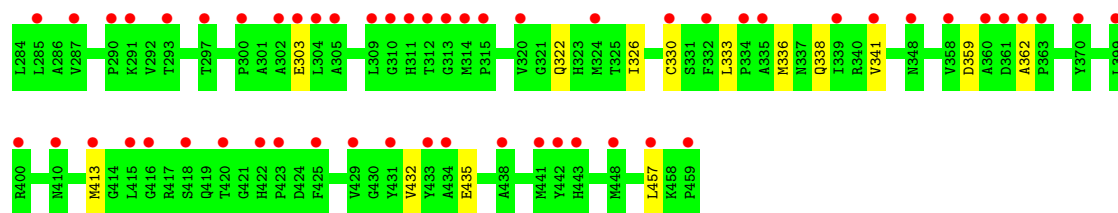


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

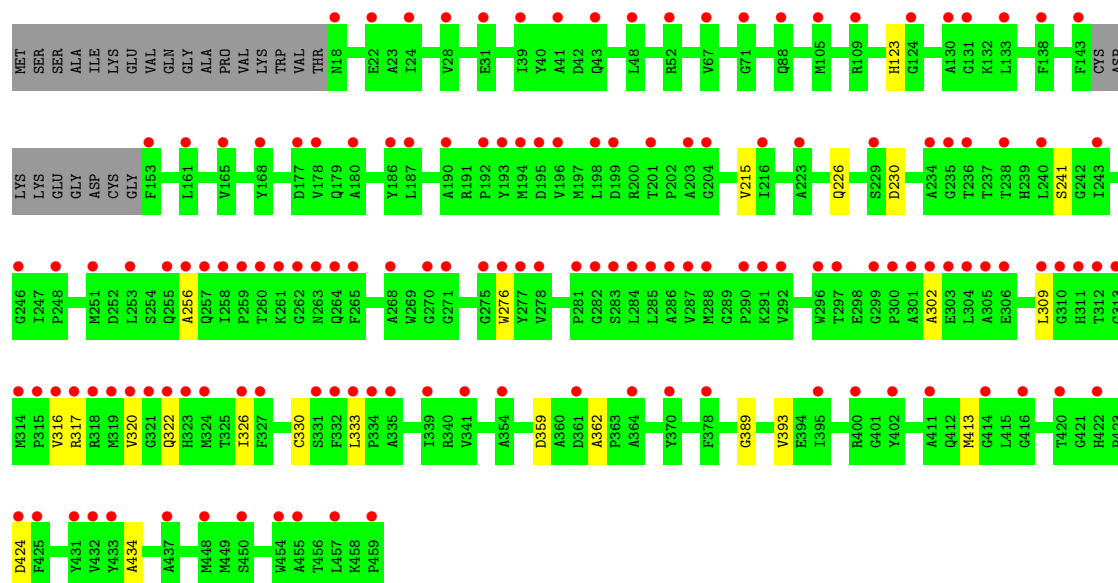
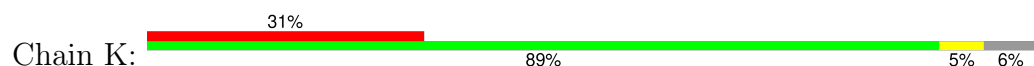


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

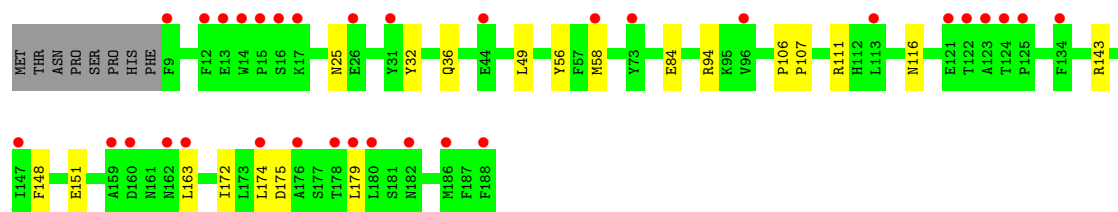
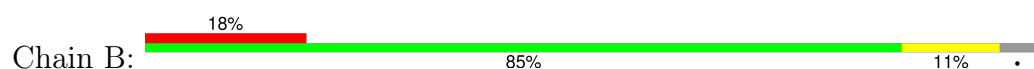




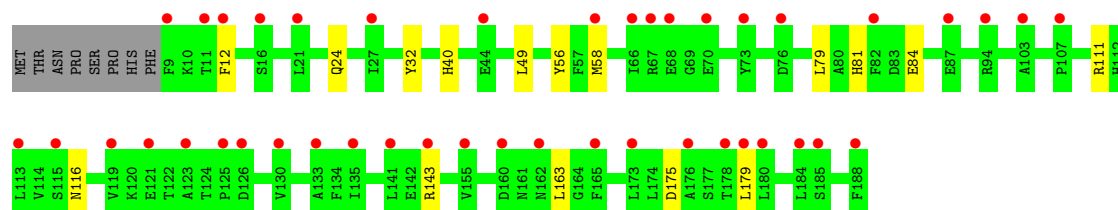
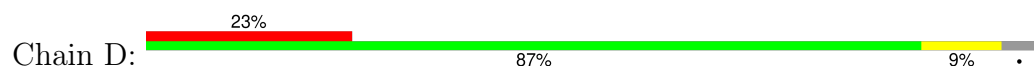
● Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



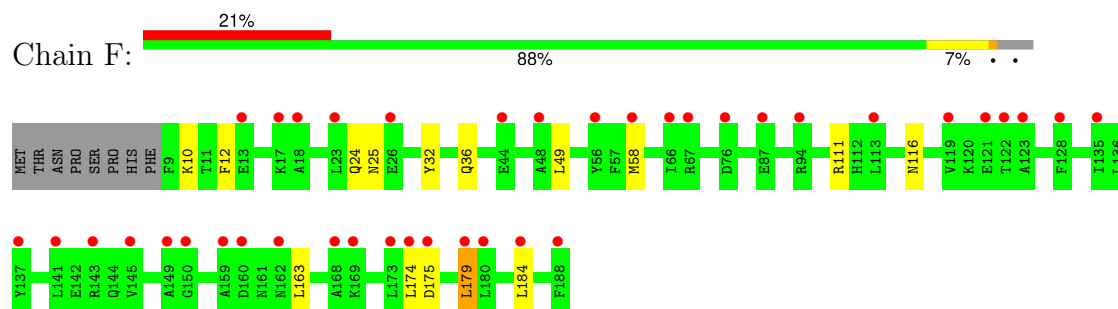
● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



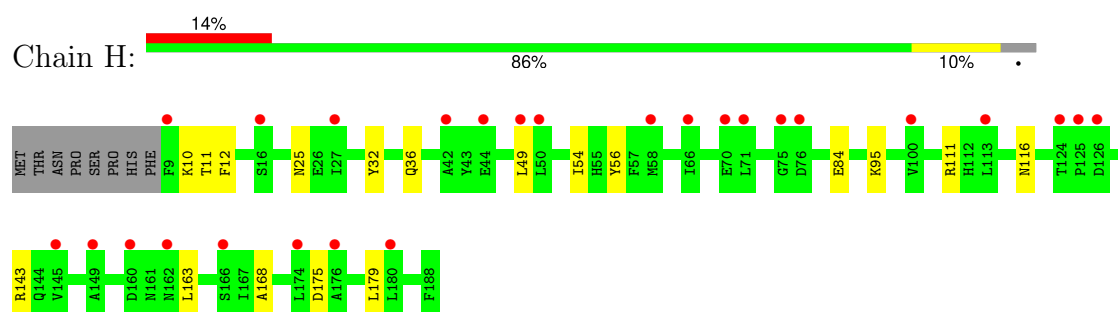
● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



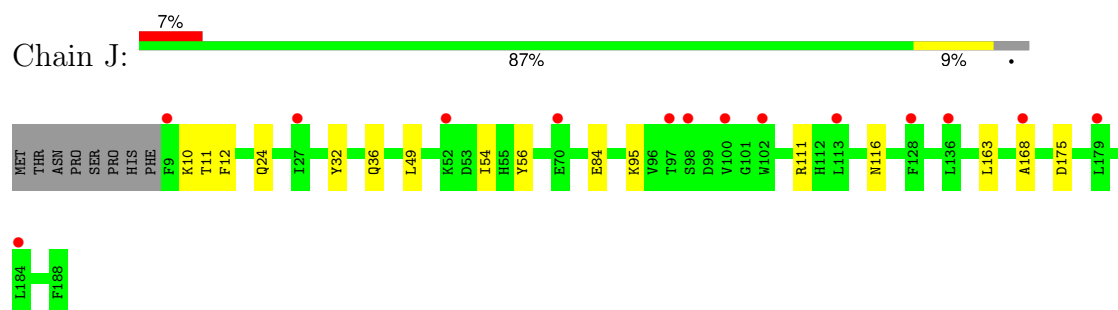
● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



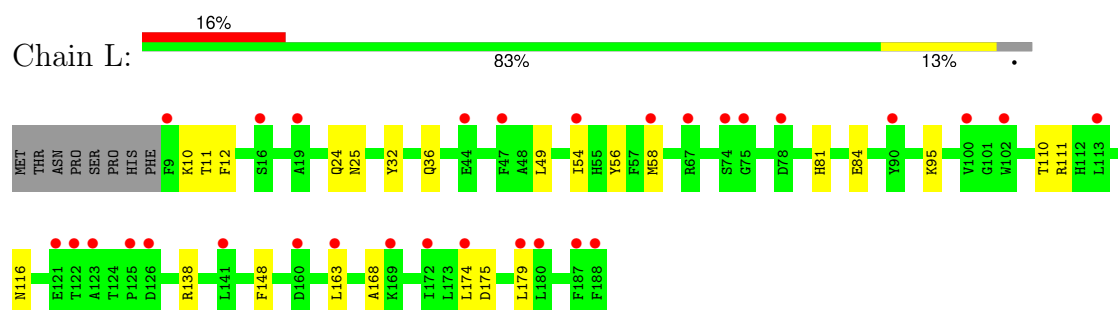
● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



● 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	86.98Å 278.12Å 92.96Å 90.00° 117.65° 90.00°	Depositor
Resolution (Å)	138.68 – 2.15 138.68 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.9 (138.68-2.15) 93.1 (138.68-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.204 , 0.233 0.281 , 0.299	Depositor DCC
R_{free} test set	9876 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	30277	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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, IIT, FES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/3533	0.77	2/4796 (0.0%)
1	C	0.43	0/3533	0.76	2/4796 (0.0%)
1	E	0.43	0/3533	0.76	2/4796 (0.0%)
1	G	0.41	0/3533	0.75	0/4796
1	I	0.41	0/3533	0.74	0/4796
1	K	0.40	0/3533	0.74	2/4796 (0.0%)
2	B	0.39	0/1530	0.68	0/2068
2	D	0.39	0/1530	0.67	0/2068
2	F	0.38	0/1530	0.69	0/2068
2	H	0.36	0/1530	0.67	0/2068
2	J	0.37	0/1530	0.66	0/2068
2	L	0.37	0/1530	0.67	0/2068
All	All	0.41	0/30378	0.73	8/41184 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	GLY	CA-C-N	5.91	125.11	118.97
1	A	299	GLY	C-N-CA	5.91	125.11	118.97
1	C	299	GLY	CA-C-N	5.64	125.75	119.32
1	C	299	GLY	C-N-CA	5.64	125.75	119.32
1	K	333	LEU	CA-C-N	5.12	125.16	119.32
1	K	333	LEU	C-N-CA	5.12	125.16	119.32
1	E	299	GLY	CA-C-N	5.04	124.65	119.05
1	E	299	GLY	C-N-CA	5.04	124.65	119.05

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	20	0
1	C	3430	0	3274	16	0
1	E	3430	0	3274	22	0
1	G	3430	0	3274	18	0
1	I	3430	0	3274	17	0
1	K	3430	0	3274	11	0
2	B	1496	0	1447	15	0
2	D	1496	0	1447	14	0
2	F	1496	0	1447	12	0
2	H	1496	0	1447	14	0
2	J	1496	0	1447	14	0
2	L	1496	0	1447	19	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	13	0	8	0	0
5	C	13	0	8	0	0
5	E	13	0	8	0	0
6	A	128	0	0	0	0
6	B	53	0	0	0	0
6	C	129	0	0	0	0
6	D	66	0	0	0	0
6	E	88	0	0	0	0
6	F	46	0	0	0	0
6	G	23	0	0	0	0
6	H	19	0	0	0	0
6	I	29	0	0	0	0
6	J	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	23	0	0	0	0
6	L	17	0	0	0	0
All	All	30277	0	28350	156	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 3.

All (156) 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	1.59	0.84
1:C:339:ILE:HD11	1:C:357:LEU:HG	1.72	0.72
1:I:262:GLY:HA2	1:I:278:VAL:HG23	1.75	0.67
1:A:123:HIS:HB2	3:A:900:FES:S2	2.35	0.66
1:C:339:ILE:CD1	1:C:357:LEU:HG	2.25	0.66
1:A:422:HIS:HD2	1:A:424:ASP:H	1.44	0.63
1:C:287:VAL:HG12	1:C:288:MET:HE3	1.82	0.62
1:A:287:VAL:HG12	1:A:288:MET:HE3	1.81	0.62
1:K:123:HIS:HB2	3:K:900:FES:S2	2.40	0.61
1:C:123:HIS:HB2	3:C:900:FES:S2	2.41	0.61
1:G:123:HIS:HB2	3:G:900:FES:S2	2.40	0.61
1:A:339:ILE:HD11	1:A:357:LEU:HG	1.83	0.59
1:G:217:PRO:HD2	1:G:393:VAL:HG22	1.83	0.59
1:A:373:HIS:HD2	1:A:376:ARG:HE	1.49	0.59
1:C:287:VAL:HG12	1:C:288:MET:CE	2.33	0.58
1:E:123:HIS:HB2	3:E:900:FES:S2	2.43	0.58
1:I:123:HIS:HB2	3:I:900:FES:S2	2.44	0.58
2:B:36:GLN:HE21	2:F:12:PHE:H	1.53	0.57
1:A:413:MET:HG2	1:A:434:ALA:HA	1.88	0.56
1:E:164:ARG:HD2	1:E:178:VAL:HA	1.88	0.55
1:I:276:TRP:HB3	1:I:322:GLN:HG3	1.87	0.55
2:H:10:LYS:HG3	2:H:11:THR:H	1.70	0.55
1:A:287:VAL:HG12	1:A:288:MET:CE	2.37	0.54
1:E:332:PHE:HB3	1:E:339:ILE:HG23	1.90	0.54
2:J:56:TYR:HB3	2:J:84:GLU:HB2	1.89	0.54
1:C:356:THR:CG2	2:D:79:LEU:HD21	2.38	0.54
2:F:49:LEU:HD21	2:F:163:LEU:HD13	1.91	0.53
1:E:339:ILE:HD11	1:E:357:LEU:HG	1.90	0.53
2:B:56:TYR:HB3	2:B:84:GLU:HB2	1.90	0.53
1:K:276:TRP:HB3	1:K:322:GLN:HG3	1.91	0.52
1:G:413:MET:HE2	1:G:435:GLU:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:PRO:O	1:C:337:ASN:OD1	2.28	0.52
2:J:49:LEU:HD21	2:J:163:LEU:HD13	1.92	0.52
1:C:332:PHE:HB3	1:C:339:ILE:HG23	1.92	0.51
1:G:276:TRP:HB3	1:G:322:GLN:HG3	1.92	0.51
1:K:241:SER:HB2	2:L:95:LYS:HG3	1.93	0.51
1:I:244:LEU:HD13	1:I:253:LEU:HG	1.93	0.51
1:E:126:ALA:HB3	1:E:135:ASN:HB3	1.92	0.50
1:E:448:MET:HA	1:E:457:LEU:HD11	1.94	0.50
2:B:175:ASP:OD2	2:D:111:ARG:HB2	2.11	0.50
2:H:116:ASN:HA	2:J:32:TYR:CD1	2.47	0.50
2:B:32:TYR:CD1	2:F:116:ASN:HA	2.47	0.49
1:K:309:LEU:HD13	1:K:316:VAL:HG11	1.94	0.49
1:K:359:ASP:HB2	1:K:362:ALA:HB2	1.95	0.49
2:D:58:MET:HE2	2:D:81:HIS:CB	2.42	0.49
2:J:10:LYS:HG3	2:J:11:THR:H	1.76	0.49
1:E:309:LEU:HD13	1:E:316:VAL:HG11	1.93	0.49
2:D:12:PHE:H	2:F:36:GLN:HE21	1.60	0.48
2:B:143:ARG:HD3	1:E:215:VAL:HG21	1.94	0.48
1:A:339:ILE:CD1	1:A:357:LEU:HG	2.43	0.48
1:G:413:MET:HG2	1:G:434:ALA:HA	1.95	0.48
1:A:349:GLU:OE2	2:D:143:ARG:NH2	2.42	0.48
2:D:24:GLN:HG2	2:F:25:ASN:HD21	1.78	0.48
1:I:413:MET:HE2	1:I:435:GLU:HG3	1.94	0.48
2:B:116:ASN:HA	2:D:32:TYR:CD1	2.48	0.48
2:H:36:GLN:HE21	2:L:12:PHE:H	1.61	0.48
2:J:175:ASP:OD2	2:L:111:ARG:HB2	2.12	0.48
1:G:359:ASP:HB2	1:G:362:ALA:HB2	1.96	0.48
1:G:448:MET:HA	1:G:457:LEU:HD11	1.95	0.47
2:D:175:ASP:OD2	2:F:111:ARG:HB2	2.14	0.47
1:I:126:ALA:HB3	1:I:135:ASN:HB3	1.96	0.47
1:I:257:GLN:HB3	1:I:282:GLY:HA3	1.97	0.47
2:H:49:LEU:HD21	2:H:163:LEU:HD13	1.96	0.47
2:H:175:ASP:OD2	2:J:111:ARG:HB2	2.15	0.47
2:J:10:LYS:HG3	2:J:11:THR:N	2.30	0.46
2:L:56:TYR:HB3	2:L:84:GLU:HB2	1.96	0.46
2:D:56:TYR:HB3	2:D:84:GLU:HB2	1.97	0.46
1:K:226:GLN:HA	1:K:230:ASP:HB3	1.97	0.46
2:B:58:MET:HG3	2:B:172:ILE:HB	1.96	0.46
2:H:32:TYR:CD1	2:L:116:ASN:HA	2.50	0.46
2:J:12:PHE:H	2:L:36:GLN:HE21	1.64	0.46
1:A:336:MET:H	1:A:336:MET:HG2	1.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:HIS:CD2	1:A:424:ASP:H	2.31	0.45
1:I:226:GLN:HA	1:I:230:ASP:HB3	1.96	0.45
2:D:49:LEU:HD21	2:D:163:LEU:HD13	1.98	0.45
1:E:244:LEU:HD13	1:E:253:LEU:HG	1.99	0.45
1:E:339:ILE:CD1	1:E:357:LEU:HG	2.47	0.45
1:K:413:MET:HG2	1:K:434:ALA:HA	1.99	0.45
1:A:448:MET:HA	1:A:457:LEU:HD11	1.99	0.45
2:L:54:ILE:HA	2:L:168:ALA:O	2.17	0.45
2:B:111:ARG:HB2	2:F:175:ASP:OD2	2.17	0.45
2:B:32:TYR:CG	2:F:116:ASN:HA	2.52	0.44
1:A:212:GLN:HE21	1:A:212:GLN:HB2	1.63	0.44
1:G:241:SER:HB2	2:H:95:LYS:HG3	1.98	0.44
2:B:25:ASN:HD21	2:F:24:GLN:HG2	1.82	0.44
2:B:148:PHE:HB3	2:B:174:LEU:HD11	1.99	0.44
1:G:126:ALA:HB3	1:G:135:ASN:HB3	1.99	0.44
1:G:226:GLN:HA	1:G:230:ASP:HB3	2.00	0.44
2:D:116:ASN:HA	2:F:32:TYR:CD1	2.53	0.44
2:H:25:ASN:HD21	2:L:24:GLN:HG2	1.82	0.44
1:I:107:ILE:HG22	1:I:118:PHE:HB3	1.99	0.44
2:J:116:ASN:HA	2:L:32:TYR:CD1	2.52	0.44
2:L:10:LYS:HG3	2:L:11:THR:N	2.32	0.44
2:D:58:MET:HE2	2:D:81:HIS:HB2	2.00	0.43
1:E:359:ASP:HB2	1:E:362:ALA:HB2	2.00	0.43
2:B:116:ASN:HA	2:D:32:TYR:CG	2.53	0.43
1:G:288:MET:HB3	1:G:292:VAL:HB	2.00	0.43
1:A:248:PRO:HA	1:A:249:PRO:HD3	1.93	0.43
1:C:448:MET:HA	1:C:457:LEU:HD11	1.98	0.43
1:I:251:MET:HG3	1:I:255:GLN:HB3	2.00	0.43
2:L:148:PHE:HB3	2:L:174:LEU:HD11	2.01	0.43
1:G:262:GLY:HA2	1:G:278:VAL:HG23	2.00	0.43
2:H:111:ARG:HB2	2:L:175:ASP:OD2	2.18	0.43
1:C:283:SER:O	1:C:287:VAL:HG23	2.17	0.43
1:G:248:PRO:HA	1:G:249:PRO:HD3	1.91	0.43
2:H:36:GLN:NE2	2:L:12:PHE:H	2.17	0.43
1:I:359:ASP:HB2	1:I:362:ALA:HB2	2.01	0.43
1:A:126:ALA:HB3	1:A:135:ASN:HB3	2.00	0.43
1:E:326:ILE:HB	1:E:330:CYS:HB3	2.00	0.43
2:H:54:ILE:HA	2:H:168:ALA:O	2.19	0.43
1:C:142:ALA:HB1	1:E:413:MET:HG3	2.01	0.42
2:L:10:LYS:HG3	2:L:11:THR:H	1.83	0.42
2:B:106:PRO:HA	2:B:107:PRO:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:229:SER:HB2	1:G:437:ALA:HB3	2.02	0.42
2:J:24:GLN:HG2	2:L:25:ASN:HD21	1.84	0.42
1:A:413:MET:CG	1:E:142:ALA:HB1	2.41	0.42
2:J:54:ILE:HA	2:J:168:ALA:O	2.19	0.42
1:K:302:ALA:HB1	1:K:317:ARG:HG2	2.02	0.42
2:B:151:GLU:OE2	2:D:40:HIS:NE2	2.52	0.42
1:I:241:SER:HB2	2:J:95:LYS:HG3	2.00	0.42
1:I:326:ILE:HB	1:I:330:CYS:HB3	2.02	0.42
2:L:110:THR:HG22	2:L:138:ARG:HG2	2.00	0.42
1:A:359:ASP:HB2	1:A:362:ALA:HB2	2.02	0.42
1:E:276:TRP:HB3	1:E:322:GLN:HG3	2.02	0.42
2:H:56:TYR:HB3	2:H:84:GLU:HB2	2.01	0.42
1:A:276:TRP:HB3	1:A:322:GLN:HG3	2.01	0.42
1:C:126:ALA:HB3	1:C:135:ASN:HB3	2.02	0.42
2:F:179:LEU:HD21	2:F:184:LEU:HD11	2.02	0.42
2:B:49:LEU:HD21	2:B:163:LEU:HD13	2.01	0.41
1:A:339:ILE:HD12	1:A:356:THR:HA	2.02	0.41
1:E:248:PRO:HA	1:E:249:PRO:HD3	1.96	0.41
1:E:262:GLY:C	1:E:432:VAL:HB	2.45	0.41
2:L:58:MET:HE2	2:L:81:HIS:CD2	2.55	0.41
1:I:60:LEU:HD23	1:I:341:VAL:HG22	2.02	0.41
1:G:326:ILE:HB	1:G:330:CYS:HB3	2.01	0.41
1:G:335:ALA:HB3	1:G:336:MET:HE2	2.03	0.41
2:H:12:PHE:H	2:J:36:GLN:NE2	2.19	0.41
1:I:262:GLY:C	1:I:432:VAL:HB	2.46	0.41
2:F:58:MET:CE	2:F:174:LEU:HD22	2.50	0.41
1:E:287:VAL:HG12	1:E:288:MET:HE2	2.03	0.41
1:E:422:HIS:CD2	1:E:424:ASP:H	2.39	0.41
1:G:389:GLY:O	1:G:393:VAL:HG23	2.19	0.41
2:H:143:ARG:HD3	1:K:215:VAL:HG21	2.03	0.41
2:J:116:ASN:HA	2:L:32:TYR:CG	2.56	0.41
1:K:326:ILE:HB	1:K:330:CYS:HB3	2.02	0.41
1:K:389:GLY:O	1:K:393:VAL:HG23	2.21	0.41
1:C:90:ASP:O	1:C:91:LYS:HB2	2.20	0.40
1:C:314:MET:HA	1:C:315:PRO:HD3	1.89	0.40
1:C:339:ILE:HD13	1:C:357:LEU:HG	2.02	0.40
1:C:244:LEU:HD13	1:C:253:LEU:HG	2.02	0.40
1:G:164:ARG:HD2	1:G:178:VAL:HA	2.02	0.40
1:I:105:MET:HB3	1:I:120:CYS:SG	2.62	0.40
1:I:333:LEU:HD12	1:I:338:GLN:HB3	2.04	0.40
1:E:413:MET:HE2	1:E:435:GLU:HG3	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:49:LEU:HD21	2:L:163:LEU:HD13	2.03	0.40
1:E:107:ILE:HG22	1:E:118:PHE:HB3	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%)	415 (97%)	14 (3%)	0	100	100
1	C	429/459 (94%)	409 (95%)	20 (5%)	0	100	100
1	E	429/459 (94%)	416 (97%)	13 (3%)	0	100	100
1	G	429/459 (94%)	416 (97%)	13 (3%)	0	100	100
1	I	429/459 (94%)	408 (95%)	21 (5%)	0	100	100
1	K	429/459 (94%)	410 (96%)	18 (4%)	1 (0%)	43	44
2	B	178/188 (95%)	174 (98%)	4 (2%)	0	100	100
2	D	178/188 (95%)	173 (97%)	5 (3%)	0	100	100
2	F	178/188 (95%)	173 (97%)	5 (3%)	0	100	100
2	H	178/188 (95%)	174 (98%)	4 (2%)	0	100	100
2	J	178/188 (95%)	173 (97%)	5 (3%)	0	100	100
2	L	178/188 (95%)	170 (96%)	8 (4%)	0	100	100
All	All	3642/3882 (94%)	3511 (96%)	130 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	256	ALA

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%)	345 (99%)	5 (1%)	59	66
1	C	350/372 (94%)	347 (99%)	3 (1%)	70	77
1	E	350/372 (94%)	344 (98%)	6 (2%)	53	60
1	G	350/372 (94%)	347 (99%)	3 (1%)	70	77
1	I	350/372 (94%)	346 (99%)	4 (1%)	65	72
1	K	350/372 (94%)	348 (99%)	2 (1%)	78	84
2	B	159/167 (95%)	157 (99%)	2 (1%)	61	68
2	D	159/167 (95%)	158 (99%)	1 (1%)	78	84
2	F	159/167 (95%)	157 (99%)	2 (1%)	61	68
2	H	159/167 (95%)	158 (99%)	1 (1%)	78	84
2	J	159/167 (95%)	159 (100%)	0	100	100
2	L	159/167 (95%)	158 (99%)	1 (1%)	78	84
All	All	3054/3234 (94%)	3024 (99%)	30 (1%)	68	75

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	MET
1	A	356	THR
1	A	394	GLU
1	A	410	ASN
1	A	419	GLN
2	B	94	ARG
2	B	179	LEU
1	C	339	ILE
1	C	356	THR
1	C	457	LEU
2	D	179	LEU
1	E	48	LEU
1	E	103	ARG
1	E	258	ILE

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Mol	Chain	Res	Type
1	E	320	VAL
1	E	339	ILE
1	E	457	LEU
2	F	10	LYS
2	F	179	LEU
1	G	336	MET
1	G	419	GLN
1	G	457	LEU
2	H	179	LEU
1	I	280	GLU
1	I	303	GLU
1	I	336	MET
1	I	457	LEU
1	K	320	VAL
1	K	424	ASP
2	L	179	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	99	GLN
1	A	212	GLN
1	A	226	GLN
1	A	322	GLN
1	A	373	HIS
1	A	377	ASN
1	A	391	ASN
1	A	410	ASN
1	A	419	GLN
1	A	422	HIS
1	A	443	HIS
1	A	444	HIS
2	B	25	ASN
2	B	36	GLN
1	C	43	GLN
1	C	88	GLN
1	C	99	GLN
1	C	114	ASN
1	C	212	GLN
1	C	226	GLN
1	C	255	GLN

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Mol	Chain	Res	Type
1	C	373	HIS
1	C	391	ASN
1	C	410	ASN
1	C	422	HIS
1	C	443	HIS
1	C	444	HIS
1	E	43	GLN
1	E	179	GLN
1	E	212	GLN
1	E	255	GLN
1	E	264	GLN
1	E	322	GLN
1	E	377	ASN
1	E	391	ASN
1	E	407	GLN
1	E	410	ASN
1	E	422	HIS
1	E	443	HIS
1	E	444	HIS
2	F	25	ASN
2	F	36	GLN
2	F	77	GLN
1	G	43	GLN
1	G	88	GLN
1	G	212	GLN
1	G	311	HIS
1	G	374	ASN
1	G	377	ASN
1	G	386	GLN
1	G	407	GLN
1	G	410	ASN
1	G	422	HIS
1	G	444	HIS
2	H	25	ASN
2	H	36	GLN
2	H	131	ASN
1	I	88	GLN
1	I	212	GLN
1	I	226	GLN
1	I	255	GLN
1	I	264	GLN
1	I	322	GLN

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Mol	Chain	Res	Type
1	I	377	ASN
1	I	391	ASN
1	I	410	ASN
1	I	419	GLN
1	I	443	HIS
1	I	444	HIS
2	J	36	GLN
2	J	86	HIS
2	J	131	ASN
2	J	144	GLN
1	K	43	GLN
1	K	88	GLN
1	K	99	GLN
1	K	212	GLN
1	K	226	GLN
1	K	255	GLN
1	K	264	GLN
1	K	343	HIS
1	K	377	ASN
1	K	386	GLN
1	K	391	ASN
1	K	410	ASN
1	K	428	ASN
1	K	443	HIS
2	L	25	ASN
2	L	36	GLN
2	L	162	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FES	A	900	1	0,4,4	-	-	-		
3	FES	K	900	1	0,4,4	-	-	-		
5	1IT	E	1451	-	15,15,15	1.55	2 (13%)	21,21,21	2.00	8 (38%)
3	FES	E	900	1	0,4,4	-	-	-		
3	FES	C	900	1	0,4,4	-	-	-		
3	FES	G	900	1	0,4,4	-	-	-		
5	1IT	A	1460	-	15,15,15	1.55	2 (13%)	21,21,21	2.02	8 (38%)
3	FES	I	900	1	0,4,4	-	-	-		
5	1IT	C	1451	-	15,15,15	1.53	2 (13%)	21,21,21	2.04	8 (38%)

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	-	-	0/1/1/1
3	FES	K	900	1	-	-	0/1/1/1
5	1IT	E	1451	-	-	-	0/3/3/3
3	FES	E	900	1	-	-	0/1/1/1
3	FES	C	900	1	-	-	0/1/1/1
3	FES	G	900	1	-	-	0/1/1/1
5	1IT	A	1460	-	-	-	0/3/3/3
3	FES	I	900	1	-	-	0/1/1/1
5	1IT	C	1451	-	-	-	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1451	1IT	O8-C9	3.74	1.44	1.38
5	A	1460	1IT	O8-C9	3.74	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1451	1IT	O8-C9	3.73	1.44	1.38
5	E	1451	1IT	O8-C7	3.73	1.44	1.38
5	A	1460	1IT	O8-C7	3.67	1.44	1.38
5	C	1451	1IT	O8-C7	3.65	1.44	1.38

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1451	1IT	C3-C2-C7	3.93	122.66	118.53
5	C	1451	1IT	C13-C1-C9	3.86	122.59	118.53
5	E	1451	1IT	C13-C1-C9	3.84	122.56	118.53
5	A	1460	1IT	C3-C2-C7	3.84	122.56	118.53
5	A	1460	1IT	C13-C1-C9	3.83	122.56	118.53
5	E	1451	1IT	C3-C2-C7	3.81	122.53	118.53
5	A	1460	1IT	O8-C9-C10	3.33	128.39	124.12
5	C	1451	1IT	O8-C7-C6	3.33	128.39	124.12
5	E	1451	1IT	O8-C9-C10	3.32	128.37	124.12
5	A	1460	1IT	O8-C7-C6	3.31	128.36	124.12
5	C	1451	1IT	O8-C9-C10	3.29	128.34	124.12
5	E	1451	1IT	O8-C7-C6	3.18	128.19	124.12
5	C	1451	1IT	C6-C7-C2	-2.64	121.14	123.69
5	A	1460	1IT	C10-C9-C1	-2.53	121.24	123.69
5	E	1451	1IT	C10-C9-C1	-2.53	121.24	123.69
5	A	1460	1IT	C6-C7-C2	-2.51	121.26	123.69
5	C	1451	1IT	C10-C9-C1	-2.49	121.29	123.69
5	E	1451	1IT	C6-C7-C2	-2.37	121.40	123.69
5	C	1451	1IT	C12-C13-C1	-2.26	116.48	120.23
5	E	1451	1IT	C4-C3-C2	-2.23	116.54	120.23
5	A	1460	1IT	C4-C3-C2	-2.20	116.58	120.23
5	E	1451	1IT	C12-C13-C1	-2.13	116.70	120.23
5	A	1460	1IT	C12-C13-C1	-2.10	116.74	120.23
5	C	1451	1IT	C4-C3-C2	-2.09	116.76	120.23

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	K	900	FES	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	900	FES	1	0
3	C	900	FES	1	0
3	G	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

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%)	1.58	106 (24%) 2 2	25, 42, 47, 56	18 (4%)
1	C	433/459 (94%)	1.63	116 (26%) 1 1	24, 41, 47, 55	18 (4%)
1	E	433/459 (94%)	1.43	91 (21%) 2 3	24, 42, 50, 58	18 (4%)
1	G	433/459 (94%)	1.72	139 (32%) 1 1	23, 41, 48, 54	18 (4%)
1	I	433/459 (94%)	1.70	141 (32%) 1 1	24, 42, 47, 53	18 (4%)
1	K	433/459 (94%)	1.78	143 (33%) 1 1	23, 42, 48, 53	18 (4%)
2	B	180/188 (95%)	1.43	33 (18%) 3 4	30, 42, 48, 53	4 (2%)
2	D	180/188 (95%)	1.53	43 (23%) 2 2	31, 42, 48, 51	4 (2%)
2	F	180/188 (95%)	1.40	39 (21%) 2 3	33, 43, 47, 49	4 (2%)
2	H	180/188 (95%)	1.31	26 (14%) 6 6	33, 43, 47, 50	4 (2%)
2	J	180/188 (95%)	1.12	14 (7%) 19 21	32, 42, 46, 48	4 (2%)
2	L	180/188 (95%)	1.27	30 (16%) 4 5	31, 41, 45, 47	4 (2%)
All	All	3678/3882 (94%)	1.55	921 (25%) 2 2	23, 42, 48, 58	132 (3%)

All (921) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	256	ALA	9.0
1	C	258	ILE	8.4
1	K	256	ALA	8.4
1	G	256	ALA	8.3
1	A	256	ALA	8.0
1	I	257	GLN	7.1
1	C	256	ALA	7.1
1	C	261	LYS	6.6
1	I	258	ILE	6.6
1	A	260	THR	6.3
1	C	259	PRO	6.3

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Mol	Chain	Res	Type	RSRZ
1	E	256	ALA	6.2
1	A	259	PRO	6.1
1	I	259	PRO	6.0
1	E	257	GLN	6.0
1	G	257	GLN	6.0
1	G	259	PRO	5.9
1	I	255	GLN	5.8
1	K	257	GLN	5.8
1	K	259	PRO	5.8
1	A	258	ILE	5.8
1	K	258	ILE	5.7
1	E	259	PRO	5.5
1	K	255	GLN	5.4
1	I	260	THR	5.4
1	E	260	THR	5.3
2	F	123	ALA	5.3
1	C	257	GLN	5.3
1	K	260	THR	5.2
1	G	260	THR	5.2
1	G	258	ILE	5.0
1	I	261	LYS	4.9
1	K	261	LYS	4.9
1	G	261	LYS	4.8
2	H	44	GLU	4.8
1	G	255	GLN	4.8
1	C	255	GLN	4.7
1	E	258	ILE	4.7
1	G	285	LEU	4.5
1	K	433	TYR	4.5
2	F	160	ASP	4.5
1	A	366	ILE	4.5
1	C	260	THR	4.5
1	K	278	VAL	4.4
1	G	320	VAL	4.4
1	K	276	TRP	4.4
1	E	105	MET	4.3
1	A	257	GLN	4.3
1	A	255	GLN	4.3
1	K	143	PHE	4.3
1	G	199	ASP	4.3
1	I	117	ALA	4.3
1	K	277	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	I	143	PHE	4.2
1	E	261	LYS	4.2
1	K	455	ALA	4.2
1	C	339	ILE	4.1
2	B	44	GLU	4.1
1	G	305	ALA	4.1
1	C	421	GLY	4.1
1	G	278	VAL	4.1
1	E	283	SER	4.1
1	K	285	LEU	4.0
1	K	370	TYR	4.0
1	E	278	VAL	4.0
2	J	97	THR	4.0
1	A	261	LYS	4.0
1	C	143	PHE	4.0
1	G	143	PHE	4.0
1	K	109	ARG	4.0
1	A	416	GLY	4.0
2	L	67	ARG	3.9
2	D	160	ASP	3.9
1	A	105	MET	3.9
1	A	109	ARG	3.8
1	G	277	TYR	3.8
2	B	176	ALA	3.8
1	K	424	ASP	3.8
1	E	255	GLN	3.8
1	K	229	SER	3.8
1	A	253	LEU	3.8
2	J	113	LEU	3.7
1	A	251	MET	3.7
1	K	105	MET	3.7
1	K	282	GLY	3.7
2	B	58	MET	3.7
1	E	277	TYR	3.7
2	D	179	LEU	3.7
1	A	283	SER	3.7
1	I	253	LEU	3.6
1	G	333	LEU	3.6
1	A	43	GLN	3.6
1	A	339	ILE	3.6
1	C	320	VAL	3.6
1	K	316	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	58	MET	3.6
1	G	366	ILE	3.6
1	E	297	THR	3.6
2	L	125	PRO	3.6
1	I	429	VAL	3.5
1	K	265	PHE	3.5
1	I	291	LYS	3.5
1	G	253	LEU	3.5
1	G	310	GLY	3.5
1	G	142	ALA	3.5
1	I	302	ALA	3.5
1	K	309	LEU	3.5
1	E	109	ARG	3.5
1	K	291	LYS	3.5
2	D	130	VAL	3.5
1	G	309	LEU	3.4
1	A	421	GLY	3.4
1	C	283	SER	3.4
1	I	130	ALA	3.4
1	K	204	GLY	3.4
1	K	305	ALA	3.4
2	L	100	VAL	3.4
1	E	262	GLY	3.4
1	G	195	ASP	3.4
1	E	253	LEU	3.4
2	B	12	PHE	3.4
1	G	312	THR	3.4
1	A	341	VAL	3.4
1	I	94	LYS	3.4
2	D	165	PHE	3.4
1	I	105	MET	3.3
1	C	420	THR	3.3
1	K	297	THR	3.3
1	I	195	ASP	3.3
1	G	204	GLY	3.3
2	J	9	PHE	3.3
1	G	276	TRP	3.3
1	K	251	MET	3.3
1	C	28	VAL	3.3
1	K	168	TYR	3.3
1	G	339	ILE	3.3
1	I	190	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	305	ALA	3.3
1	K	302	ALA	3.3
1	C	253	LEU	3.3
1	K	457	LEU	3.3
2	D	162	ASN	3.3
1	C	105	MET	3.3
2	F	58	MET	3.3
1	K	310	GLY	3.3
1	K	422	HIS	3.3
1	A	298	GLU	3.3
1	E	348	ASN	3.3
1	K	201	THR	3.2
1	K	311	HIS	3.2
2	J	100	VAL	3.2
2	J	27	ILE	3.2
1	I	425	PHE	3.2
1	I	283	SER	3.2
2	H	75	GLY	3.2
1	G	109	ARG	3.2
1	K	431	TYR	3.2
1	G	198	LEU	3.2
1	G	457	LEU	3.2
2	D	21	LEU	3.2
2	D	180	LEU	3.2
1	K	283	SER	3.2
1	I	109	ARG	3.2
1	I	192	PRO	3.2
2	D	121	GLU	3.2
2	L	169	LYS	3.2
1	K	292	VAL	3.2
1	C	285	LEU	3.2
1	G	431	TYR	3.2
2	H	71	LEU	3.2
1	C	303	GLU	3.2
1	K	315	PRO	3.2
1	K	319	MET	3.2
1	E	434	ALA	3.1
1	G	302	ALA	3.1
2	B	179	LEU	3.1
1	G	201	THR	3.1
1	E	287	VAL	3.1
1	K	52	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	126	ASP	3.1
2	F	184	LEU	3.1
2	F	13	GLU	3.1
1	K	313	GLY	3.1
1	K	361	ASP	3.1
2	D	76	ASP	3.1
1	E	305	ALA	3.1
2	F	17	LYS	3.1
1	A	307	GLN	3.1
1	E	142	ALA	3.1
1	G	335	ALA	3.1
1	C	296	TRP	3.0
1	K	236	THR	3.0
1	A	400	ARG	3.0
2	F	188	PHE	3.0
2	H	9	PHE	3.0
1	A	22	GLU	3.0
1	C	457	LEU	3.0
1	K	320	VAL	3.0
1	I	243	ILE	3.0
1	I	418	SER	3.0
1	I	282	GLY	3.0
1	G	158	TRP	3.0
1	G	249	PRO	3.0
1	C	227	PHE	3.0
2	L	160	ASP	3.0
1	G	105	MET	3.0
1	A	142	ALA	3.0
1	G	268	ALA	3.0
1	I	278	VAL	3.0
1	K	196	VAL	3.0
1	K	416	GLY	3.0
1	K	281	PRO	3.0
1	I	153	PHE	3.0
1	A	179	GLN	3.0
1	A	44	SER	3.0
1	K	287	VAL	3.0
2	D	113	LEU	3.0
2	F	179	LEU	3.0
1	E	250	GLU	3.0
2	F	162	ASN	3.0
1	C	346	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	275	GLY	3.0
1	E	138	PHE	3.0
1	G	43	GLN	2.9
1	G	153	PHE	3.0
1	G	269	TRP	3.0
1	C	109	ARG	2.9
1	C	305	ALA	2.9
1	I	115	ALA	2.9
2	J	168	ALA	2.9
2	B	162	ASN	2.9
2	F	113	LEU	2.9
1	E	215	VAL	2.9
1	I	215	VAL	2.9
1	I	416	GLY	2.9
1	C	43	GLN	2.9
1	A	138	PHE	2.9
1	E	143	PHE	2.9
1	C	214	TRP	2.9
1	E	298	GLU	2.9
1	G	453	SER	2.9
2	F	18	ALA	2.9
1	E	457	LEU	2.9
1	G	284	LEU	2.9
2	F	180	LEU	2.9
1	C	282	GLY	2.9
1	K	262	GLY	2.9
1	C	215	VAL	2.9
1	E	196	VAL	2.9
1	I	297	THR	2.9
1	I	138	PHE	2.9
2	L	188	PHE	2.9
2	L	102	TRP	2.9
1	A	364	ALA	2.9
1	G	203	ALA	2.9
1	G	301	ALA	2.9
1	C	275	GLY	2.9
1	E	43	GLN	2.9
1	G	400	ARG	2.9
2	D	9	PHE	2.9
2	F	128	PHE	2.9
1	C	391	ASN	2.9
1	G	190	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	416	GLY	2.9
1	I	276	TRP	2.9
1	A	48	LEU	2.8
1	C	424	ASP	2.8
1	A	83	VAL	2.8
2	D	155	VAL	2.8
2	H	27	ILE	2.8
1	I	290	PRO	2.8
2	D	70	GLU	2.8
1	A	453	SER	2.8
2	L	90	TYR	2.8
1	E	400	ARG	2.8
1	I	52	ARG	2.8
1	I	314	MET	2.8
2	L	75	GLY	2.8
1	E	285	LEU	2.8
1	A	365	GLU	2.8
1	K	178	VAL	2.8
1	A	334	PRO	2.8
1	E	334	PRO	2.8
1	I	129	ILE	2.8
1	K	248	PRO	2.8
1	C	419	GLN	2.8
2	D	12	PHE	2.8
1	I	431	TYR	2.8
1	I	335	ALA	2.8
1	I	438	ALA	2.8
1	K	268	ALA	2.8
1	K	335	ALA	2.8
2	D	123	ALA	2.8
2	J	70	GLU	2.8
2	L	123	ALA	2.8
1	C	48	LEU	2.8
1	C	50	LEU	2.8
2	D	11	THR	2.8
1	K	39	ILE	2.8
1	A	246	GLY	2.8
1	C	327	PHE	2.8
1	E	210	GLY	2.8
1	K	321	GLY	2.8
1	A	224	ALA	2.8
1	E	335	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	193	TYR	2.8
2	B	123	ALA	2.8
2	D	103	ALA	2.8
2	B	174	LEU	2.8
2	H	113	LEU	2.8
1	K	290	PRO	2.8
1	G	316	VAL	2.8
1	A	19	TRP	2.8
1	C	353	TRP	2.8
1	C	400	ARG	2.7
2	H	162	ASN	2.7
1	A	430	GLY	2.7
2	L	9	PHE	2.7
1	K	301	ALA	2.7
2	F	159	ALA	2.7
1	K	198	LEU	2.7
1	E	76	THR	2.7
1	G	334	PRO	2.7
1	K	318	ARG	2.7
2	D	67	ARG	2.7
1	A	215	VAL	2.7
1	C	341	VAL	2.7
1	G	178	VAL	2.7
1	G	294	GLN	2.7
1	I	178	VAL	2.7
1	I	196	VAL	2.7
1	G	311	HIS	2.7
1	K	314	MET	2.7
2	L	58	MET	2.7
2	L	44	GLU	2.7
1	E	246	GLY	2.7
1	E	384	PHE	2.7
2	B	159	ALA	2.7
2	B	188	PHE	2.7
1	I	48	LEU	2.7
2	F	67	ARG	2.7
2	F	141	LEU	2.7
2	L	122	THR	2.7
1	I	315	PRO	2.7
1	C	348	ASN	2.7
1	A	448	MET	2.7
1	I	95	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	303	GLU	2.7
1	G	94	LYS	2.7
1	K	235	GLY	2.7
1	A	163	ALA	2.7
1	E	245	ALA	2.7
1	G	74	LEU	2.7
1	K	312	THR	2.7
1	E	365	GLU	2.7
1	G	181	PRO	2.7
1	I	348	ASN	2.7
2	B	13	GLU	2.7
1	C	254	SER	2.7
1	A	350	ILE	2.7
1	C	24	ILE	2.7
1	C	292	VAL	2.7
1	C	310	GLY	2.7
1	K	299	GLY	2.7
2	B	14	TRP	2.7
2	D	143	ARG	2.7
1	A	455	ALA	2.6
1	E	455	ALA	2.6
1	A	293	THR	2.6
1	E	425	PHE	2.6
1	G	194	MET	2.6
2	H	58	MET	2.6
1	A	348	ASN	2.6
1	C	316	VAL	2.6
1	E	216	ILE	2.6
1	G	393	VAL	2.6
1	C	417	ARG	2.6
1	C	273	GLY	2.6
1	G	282	GLY	2.6
1	G	289	GLY	2.6
1	C	19	TRP	2.6
1	I	303	GLU	2.6
1	K	296	TRP	2.6
1	A	245	ALA	2.6
1	K	130	ALA	2.6
1	C	222	PHE	2.6
1	G	423	PRO	2.6
1	K	459	PRO	2.6
1	C	140	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	341	VAL	2.6
1	I	330	CYS	2.6
1	K	124	GLY	2.6
1	K	324	MET	2.6
1	G	348	ASN	2.6
1	C	302	ALA	2.6
2	H	149	ALA	2.6
1	A	415	LEU	2.6
1	C	82	PRO	2.6
1	C	89	LYS	2.6
1	C	459	PRO	2.6
1	A	153	PHE	2.6
1	C	29	ASP	2.6
1	G	415	LEU	2.6
1	I	61	LEU	2.6
2	J	136	LEU	2.6
1	I	96	PHE	2.6
1	I	199	ASP	2.6
1	I	457	LEU	2.6
1	K	332	PHE	2.6
2	D	115	SER	2.6
1	A	243	ILE	2.6
1	E	243	ILE	2.6
1	E	247	ILE	2.6
1	K	186	TYR	2.6
1	K	432	VAL	2.6
2	F	145	VAL	2.6
1	A	303	GLU	2.6
1	C	365	GLU	2.6
1	C	262	GLY	2.6
1	C	389	GLY	2.6
1	C	440	GLY	2.6
1	I	131	GLY	2.6
1	I	311	HIS	2.6
1	C	334	PRO	2.6
1	C	331	SER	2.6
1	C	392	TRP	2.6
1	E	19	TRP	2.6
2	L	163	LEU	2.6
2	L	180	LEU	2.6
1	C	425	PHE	2.5
2	B	26	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	136	VAL	2.5
1	I	287	VAL	2.5
1	A	122	TYR	2.5
1	K	402	TYR	2.5
1	C	335	ALA	2.5
1	K	223	ALA	2.5
2	B	16	SER	2.5
1	G	35	LEU	2.5
1	A	392	TRP	2.5
1	C	384	PHE	2.5
1	G	384	PHE	2.5
1	I	173	PHE	2.5
1	I	85	MET	2.5
1	E	93	ILE	2.5
2	D	66	ILE	2.5
1	E	291	LYS	2.5
1	I	442	TYR	2.5
1	C	330	CYS	2.5
1	A	294	GLN	2.5
1	K	238	THR	2.5
1	K	192	PRO	2.5
1	E	309	LEU	2.5
1	K	187	LEU	2.5
1	A	381	GLY	2.5
2	F	169	LYS	2.5
1	E	252	ASP	2.5
1	G	307	GLN	2.5
2	D	68	GLU	2.5
2	B	122	THR	2.5
1	G	245	ALA	2.5
1	I	181	PRO	2.5
2	B	125	PRO	2.5
1	A	187	LEU	2.5
1	C	45	LEU	2.5
1	I	183	LEU	2.5
2	L	179	LEU	2.5
1	A	52	ARG	2.5
1	G	332	PHE	2.5
1	E	214	TRP	2.5
1	I	263	ASN	2.5
1	G	196	VAL	2.4
1	G	358	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	86	VAL	2.4
1	K	24	ILE	2.5
2	H	145	VAL	2.4
2	L	54	ILE	2.5
1	A	250	GLU	2.4
1	A	252	ASP	2.4
1	I	189	ASP	2.4
1	C	297	THR	2.4
1	G	283	SER	2.4
1	K	300	PRO	2.4
1	C	438	ALA	2.4
1	C	448	MET	2.4
1	K	41	ALA	2.4
2	D	176	ALA	2.4
2	L	19	ALA	2.4
1	A	399	LEU	2.4
1	E	61	LEU	2.4
1	I	285	LEU	2.4
1	C	311	HIS	2.4
1	A	222	PHE	2.4
1	K	270	GLY	2.4
1	K	425	PHE	2.4
1	A	296	TRP	2.4
1	A	393	VAL	2.4
1	C	352	VAL	2.4
1	C	366	ILE	2.4
1	I	339	ILE	2.4
1	K	339	ILE	2.4
2	D	44	GLU	2.4
1	E	316	VAL	2.4
2	D	119	VAL	2.4
2	H	100	VAL	2.4
1	G	291	LYS	2.4
1	I	268	ALA	2.4
2	D	133	ALA	2.4
2	H	42	ALA	2.4
1	K	48	LEU	2.4
2	B	180	LEU	2.4
2	F	23	LEU	2.4
1	E	421	GLY	2.4
1	G	275	GLY	2.4
1	K	43	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	L	78	ASP	2.4
1	C	393	VAL	2.4
1	E	24	ILE	2.4
1	E	165	VAL	2.4
1	C	276	TRP	2.4
1	E	276	TRP	2.4
1	G	454	TRP	2.4
1	I	229	SER	2.4
1	I	254	SER	2.4
1	A	431	TYR	2.4
1	G	186	TYR	2.4
2	B	73	TYR	2.4
2	D	178	THR	2.4
2	D	125	PRO	2.4
2	F	56	TYR	2.4
2	F	137	TYR	2.4
1	A	335	ALA	2.4
1	G	438	ALA	2.4
1	K	234	ALA	2.4
1	I	171	LEU	2.4
2	J	179	LEU	2.4
2	D	126	ASP	2.4
2	F	76	ASP	2.4
1	I	332	PHE	2.4
2	L	47	PHE	2.4
1	A	395	ILE	2.4
1	C	287	VAL	2.4
1	E	52	ARG	2.4
1	E	53	VAL	2.4
1	G	165	VAL	2.4
1	I	320	VAL	2.4
1	K	194	MET	2.4
1	K	450	SER	2.4
1	G	185	THR	2.4
1	G	205	THR	2.4
1	G	202	PRO	2.4
1	G	296	TRP	2.4
1	A	232	TYR	2.3
1	E	295	TYR	2.3
1	I	168	TYR	2.3
1	G	267	ALA	2.3
1	I	23	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	284	LEU	2.3
1	I	161	LEU	2.3
2	L	174	LEU	2.3
2	B	160	ASP	2.3
1	G	85	MET	2.3
2	B	134	PHE	2.3
2	B	186	MET	2.3
2	J	128	PHE	2.3
1	C	93	ILE	2.3
1	G	243	ILE	2.3
1	G	247	ILE	2.3
1	G	326	ILE	2.3
1	A	86	VAL	2.3
1	A	292	VAL	2.3
1	C	165	VAL	2.3
1	C	172	VAL	2.3
1	K	331	SER	2.3
1	G	290	PRO	2.3
1	K	31	GLU	2.3
2	H	70	GLU	2.3
1	C	224	ALA	2.3
1	E	166	ALA	2.3
1	E	370	TYR	2.3
1	K	286	ALA	2.3
1	G	304	LEU	2.3
1	I	313	GLY	2.3
2	J	184	LEU	2.3
1	E	361	ASP	2.3
1	G	424	ASP	2.3
1	G	319	MET	2.3
1	I	89	LYS	2.3
1	K	138	PHE	2.3
2	D	188	PHE	2.3
1	A	216	ILE	2.3
1	C	395	ILE	2.3
1	K	326	ILE	2.3
1	I	82	PRO	2.3
1	I	293	THR	2.3
1	I	334	PRO	2.3
1	K	322	GLN	2.3
1	K	334	PRO	2.3
1	G	263	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	437	ALA	2.3
1	A	45	LEU	2.3
1	A	270	GLY	2.3
1	G	122	TYR	2.3
1	G	442	TYR	2.3
1	I	269	TRP	2.3
1	I	273	GLY	2.3
1	I	277	TYR	2.3
1	K	71	GLY	2.3
1	K	284	LEU	2.3
2	B	113	LEU	2.3
2	D	141	LEU	2.3
2	H	174	LEU	2.3
1	I	448	MET	2.3
1	K	448	MET	2.3
1	A	54	PHE	2.3
1	C	306	GLU	2.3
1	K	22	GLU	2.3
1	K	323	HIS	2.3
2	D	185	SER	2.3
2	J	98	SER	2.3
1	A	129	ILE	2.3
1	G	322	GLN	2.3
1	K	216	ILE	2.3
1	K	243	ILE	2.3
1	K	28	VAL	2.3
1	G	300	PRO	2.3
1	G	420	THR	2.3
1	I	21	PRO	2.3
1	K	400	ARG	2.3
1	E	364	ALA	2.3
1	G	182	ASP	2.3
1	I	163	ALA	2.3
1	I	174	ALA	2.3
1	I	204	GLY	2.3
1	A	35	LEU	2.3
2	B	163	LEU	2.3
1	A	442	TYR	2.3
1	C	46	TYR	2.3
1	K	454	TRP	2.3
1	A	435	GLU	2.2
1	G	157	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	74	SER	2.2
1	E	378	PHE	2.2
1	G	96	PHE	2.2
1	G	265	PHE	2.2
1	E	395	ILE	2.2
1	I	312	THR	2.2
1	I	363	PRO	2.2
1	K	67	VAL	2.2
1	K	165	VAL	2.2
2	F	94	ARG	2.2
1	A	207	ALA	2.2
1	A	437	ALA	2.2
1	E	313	GLY	2.2
1	G	321	GLY	2.2
1	I	413	MET	2.2
1	I	304	LEU	2.2
1	I	415	LEU	2.2
1	K	133	LEU	2.2
1	K	253	LEU	2.2
1	I	193	TYR	2.2
2	D	87	GLU	2.2
2	F	26	GLU	2.2
2	F	87	GLU	2.2
1	A	254	SER	2.2
1	A	326	ILE	2.2
1	C	76	THR	2.2
1	C	347	PRO	2.2
1	G	93	ILE	2.2
1	G	107	ILE	2.2
1	I	217	PRO	2.2
1	I	423	PRO	2.2
2	B	124	THR	2.2
2	B	147	ILE	2.2
2	D	135	ILE	2.2
2	B	96	VAL	2.2
1	C	413	MET	2.2
1	G	413	MET	2.2
1	I	252	ASP	2.2
1	K	288	MET	2.2
1	K	246	GLY	2.2
1	C	180	ALA	2.2
1	E	156	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	234	ALA	2.2
1	I	157	GLU	2.2
1	K	203	ALA	2.2
1	K	354	ALA	2.2
1	E	59	LEU	2.2
1	K	161	LEU	2.2
1	K	304	LEU	2.2
2	D	16	SER	2.2
1	C	342	TRP	2.2
1	I	19	TRP	2.2
1	C	94	LYS	2.2
1	C	153	PHE	2.2
1	C	216	ILE	2.2
1	E	459	PRO	2.2
1	K	327	PHE	2.2
1	A	275	GLY	2.2
1	A	203	ALA	2.2
1	E	311	HIS	2.2
1	E	407	GLN	2.2
1	E	419	GLN	2.2
1	G	354	ALA	2.2
1	K	190	ALA	2.2
1	K	411	ALA	2.2
2	F	149	ALA	2.2
1	A	50	LEU	2.2
1	K	333	LEU	2.2
2	D	184	LEU	2.2
1	E	229	SER	2.2
1	I	370	TYR	2.2
1	E	89	LYS	2.2
1	K	263	ASN	2.2
1	A	214	TRP	2.2
1	A	413	MET	2.2
1	G	58	TRP	2.2
1	C	237	THR	2.2
1	G	21	PRO	2.1
1	G	426	PRO	2.1
1	G	456	THR	2.2
1	I	128	ASP	2.2
1	I	167	THR	2.2
1	K	195	ASP	2.2
1	K	420	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	126	ASP	2.2
1	A	425	PHE	2.1
1	C	208	ILE	2.1
1	K	153	PHE	2.1
1	K	306	GLU	2.1
2	D	82	PHE	2.1
2	L	172	ILE	2.1
1	I	165	VAL	2.1
1	G	416	GLY	2.1
1	K	88	GLN	2.1
1	K	414	GLY	2.1
1	I	422	HIS	2.1
1	I	443	HIS	2.1
1	A	41	ALA	2.1
1	I	245	ALA	2.1
1	A	417	ARG	2.1
1	C	161	LEU	2.1
1	G	133	LEU	2.1
2	F	174	LEU	2.1
2	L	113	LEU	2.1
2	L	141	LEU	2.1
2	J	52	LYS	2.1
1	A	40	TYR	2.1
1	G	251	MET	2.1
1	G	448	MET	2.1
1	I	433	TYR	2.1
1	A	361	ASP	2.1
1	C	361	ASP	2.1
1	E	22	GLU	2.1
1	G	128	ASP	2.1
2	H	76	ASP	2.1
2	H	160	ASP	2.1
1	G	315	PRO	2.1
2	F	122	THR	2.1
2	H	125	PRO	2.1
1	I	220	TRP	2.1
1	C	350	ILE	2.1
1	C	375	ILE	2.1
1	E	208	ILE	2.1
1	G	378	PHE	2.1
2	B	9	PHE	2.1
1	E	282	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	209	GLY	2.1
1	I	262	GLY	2.1
1	K	275	GLY	2.1
2	F	150	GLY	2.1
1	C	75	ALA	2.1
1	I	166	ALA	2.1
1	I	360	ALA	2.1
1	I	362	ALA	2.1
1	I	434	ALA	2.1
1	K	180	ALA	2.1
1	K	364	ALA	2.1
2	H	176	ALA	2.1
1	A	60	LEU	2.1
1	A	94	LYS	2.1
1	A	285	LEU	2.1
1	C	291	LYS	2.1
1	I	92	SER	2.1
1	I	240	LEU	2.1
2	H	180	LEU	2.1
2	L	16	SER	2.1
1	G	314	MET	2.1
1	C	22	GLU	2.1
1	K	18	ASN	2.1
1	I	361	ASP	2.1
1	K	177	ASP	2.1
1	C	402	TYR	2.1
1	I	186	TYR	2.1
2	B	31	TYR	2.1
1	C	452	PRO	2.1
1	C	456	THR	2.1
1	E	217	PRO	2.1
1	E	356	THR	2.1
1	G	137	PRO	2.1
1	G	281	PRO	2.1
1	I	201	THR	2.1
1	I	300	PRO	2.1
2	B	15	PRO	2.1
2	H	124	THR	2.1
1	A	39	ILE	2.1
1	G	242	GLY	2.1
1	G	246	GLY	2.1
1	I	67	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	341	VAL	2.1
1	E	91	LYS	2.1
1	C	166	ALA	2.1
1	G	117	ALA	2.1
1	G	180	ALA	2.1
2	F	48	ALA	2.1
1	E	183	LEU	2.1
1	I	27	LEU	2.1
2	H	16	SER	2.1
2	H	49	LEU	2.1
2	H	166	SER	2.1
1	A	288	MET	2.1
1	A	306	GLU	2.1
1	G	228	CYS	2.1
1	I	228	CYS	2.1
1	I	324	MET	2.1
2	B	121	GLU	2.1
2	L	121	GLU	2.1
2	F	175	ASP	2.1
1	K	264	GLN	2.1
1	A	217	PRO	2.1
1	E	372	ARG	2.1
1	G	192	PRO	2.1
1	G	323	HIS	2.1
1	G	433	TYR	2.1
1	I	400	ARG	2.1
1	I	459	PRO	2.1
2	B	178	THR	2.1
1	G	235	GLY	2.1
1	I	310	GLY	2.1
1	A	24	ILE	2.1
1	A	247	ILE	2.1
1	G	132	LYS	2.1
2	H	66	ILE	2.1
1	I	84	VAL	2.1
1	I	358	VAL	2.1
1	K	378	PHE	2.1
2	F	119	VAL	2.1
1	C	454	TRP	2.1
1	G	392	TRP	2.1
1	A	280	GLU	2.0
1	C	41	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	441	MET	2.0
2	F	121	GLU	2.0
2	F	168	ALA	2.1
1	E	251	MET	2.0
1	E	314	MET	2.0
1	E	413	MET	2.0
1	A	198	LEU	2.0
1	C	27	LEU	2.0
1	C	415	LEU	2.0
1	E	161	LEU	2.0
2	D	173	LEU	2.0
2	F	173	LEU	2.0
1	C	428	ASN	2.0
2	B	182	ASN	2.0
1	C	199	ASP	2.0
1	E	386	GLN	2.0
1	I	88	GLN	2.0
1	K	199	ASP	2.0
1	K	317	ARG	2.0
2	D	94	ARG	2.0
1	C	328	PRO	2.0
1	I	420	THR	2.0
2	D	107	PRO	2.0
1	C	232	TYR	2.0
1	E	79	GLY	2.0
1	G	168	TYR	2.0
2	B	17	LYS	2.0
1	G	313	GLY	2.0
1	K	271	GLY	2.0
1	K	395	ILE	2.0
2	D	27	ILE	2.0
2	F	66	ILE	2.0
2	F	135	ILE	2.0
1	A	53	VAL	2.0
1	A	287	VAL	2.0
1	A	383	VAL	2.0
1	C	53	VAL	2.0
1	E	153	PHE	2.0
1	G	138	PHE	2.0
1	G	352	VAL	2.0
2	F	44	GLU	2.0
2	L	187	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	110	SER	2.0
1	E	220	TRP	2.0
1	E	445	TRP	2.0
1	G	214	TRP	2.0
1	I	180	ALA	2.0
2	J	102	TRP	2.0
1	A	391	ASN	2.0
1	I	410	ASN	2.0
1	G	187	LEU	2.0
1	G	244	LEU	2.0
1	I	50	LEU	2.0
1	I	60	LEU	2.0
1	I	198	LEU	2.0
1	I	309	LEU	2.0
1	I	399	LEU	2.0
1	K	240	LEU	2.0
2	H	50	LEU	2.0
1	A	36	ASP	2.0
1	A	372	ARG	2.0
1	C	52	ARG	2.0
1	G	52	ARG	2.0
2	F	143	ARG	2.0
1	C	218	CYS	2.0
1	G	155	LYS	2.0
1	E	167	THR	2.0
1	G	248	PRO	2.0
1	K	131	GLY	2.0
2	D	73	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
5	1IT	C	1451	13/13	0.86	0.17	61,61,61,61	0
5	1IT	A	1460	13/13	0.87	0.16	61,61,61,61	0
5	1IT	E	1451	13/13	0.91	0.28	29,29,29,29	13
4	FE2	I	901	1/1	0.94	0.10	55,55,55,55	0
3	FES	G	900	4/4	0.94	0.10	54,54,55,55	0
3	FES	I	900	4/4	0.95	0.10	58,58,58,58	0
3	FES	A	900	4/4	0.96	0.07	29,30,31,31	0
4	FE2	G	901	1/1	0.97	0.08	57,57,57,57	0
3	FES	K	900	4/4	0.97	0.08	57,57,57,58	0
4	FE2	K	901	1/1	0.97	0.07	57,57,57,57	0
3	FES	E	900	4/4	0.98	0.06	31,32,32,32	0
4	FE2	C	901	1/1	0.99	0.05	33,33,33,33	0
4	FE2	E	901	1/1	0.99	0.04	41,41,41,41	0
3	FES	C	900	4/4	0.99	0.05	31,32,33,33	0
4	FE2	A	901	1/1	0.99	0.06	33,33,33,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.