



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:33 pm BST

PDB ID : 1ULJ  
Title : Biphenyl dioxygenase (BphA1A2) in complex with the substrate  
Authors : Furusawa, Y.; Nagarajan, V.; Masai, E.; Tanokura, M.; Fukuda, M.; Senda, T.  
Deposited on : 2003-09-12  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

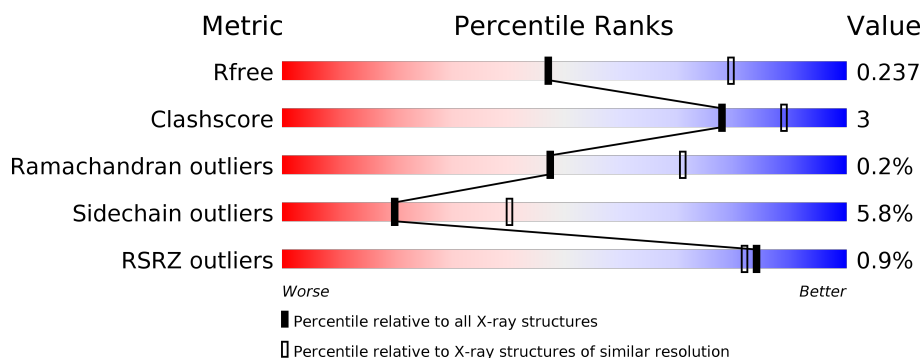
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	460	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>• 8%</div> </div> </div>
1	C	460	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>• 8%</div> </div> </div>
1	E	460	<div> <div></div> <div> <div></div> <div>81%</div> <div>10%</div> <div>• 8%</div> </div> </div>
2	B	187	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>• 5%</div> </div> </div>
2	D	187	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• 5%</div> </div> </div>
2	F	187	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14936 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 large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3377	2129	585	642	21			
1	C	425	Total	C	N	O	S	0	0	0
			3375	2127	585	642	21			
1	E	425	Total	C	N	O	S	0	0	0
			3377	2129	585	642	21			

- Molecule 2 is a protein called biphenyl dioxygenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1484	939	267	273	5			
2	D	178	Total	C	N	O	S	0	0	0
			1489	942	268	274	5			
2	F	177	Total	C	N	O	S	0	0	0
			1484	939	267	273	5			

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

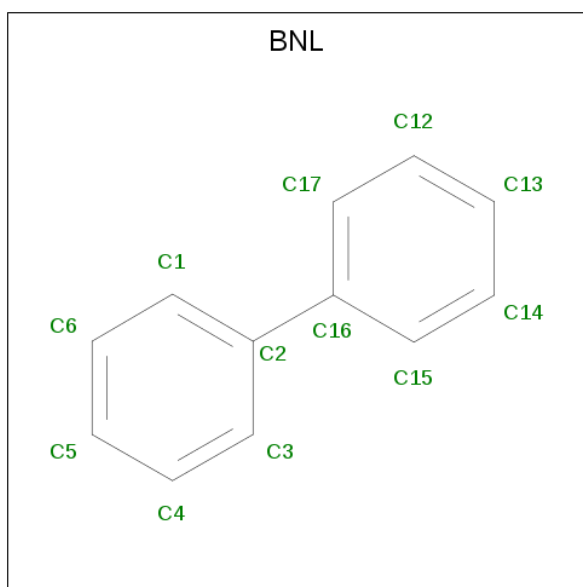
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	E	1	Total	Fe	0	0
			1	1		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

- Molecule 5 is BIPHENYL (three-letter code: BNL) (formula: C<sub>12</sub>H<sub>10</sub>).



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

*Continued on next page...*

*Continued from previous page...*

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

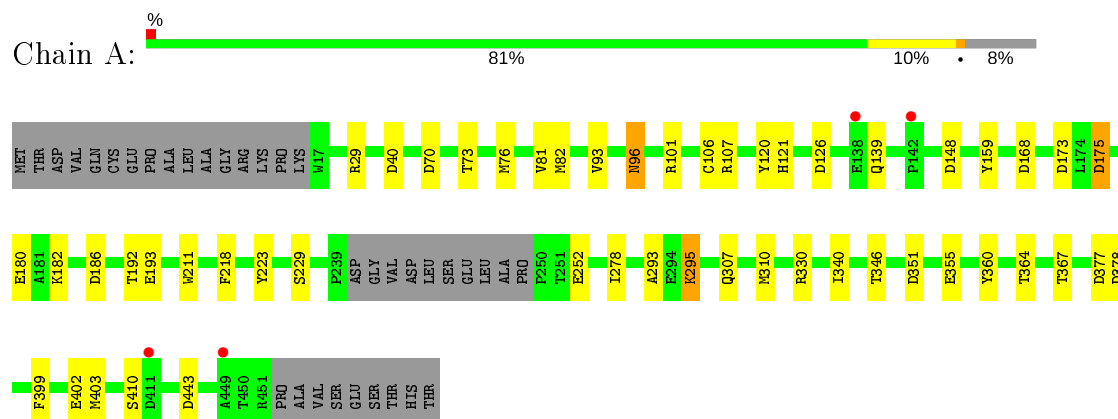
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	71	Total O 71 71	0	0
6	B	32	Total O 32 32	0	0
6	C	45	Total O 45 45	0	0
6	D	42	Total O 42 42	0	0
6	E	73	Total O 73 73	0	0
6	F	36	Total O 36 36	0	0

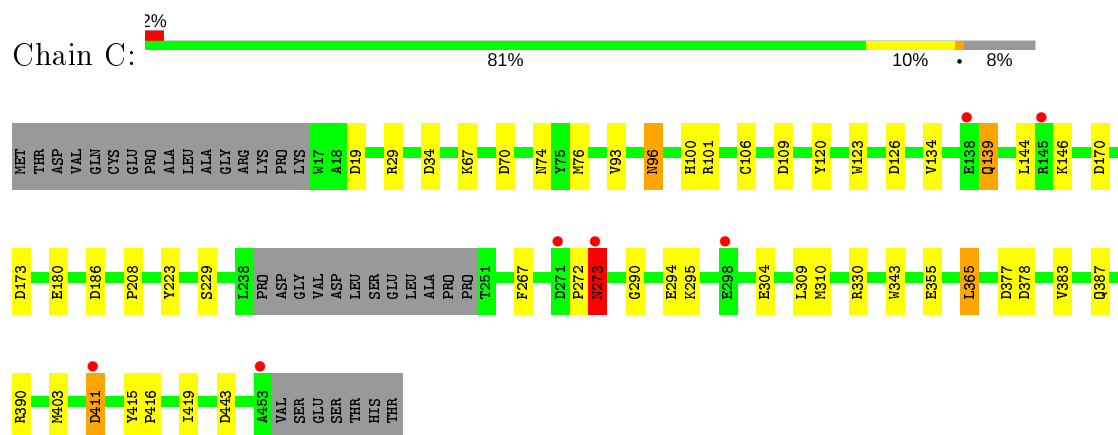
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

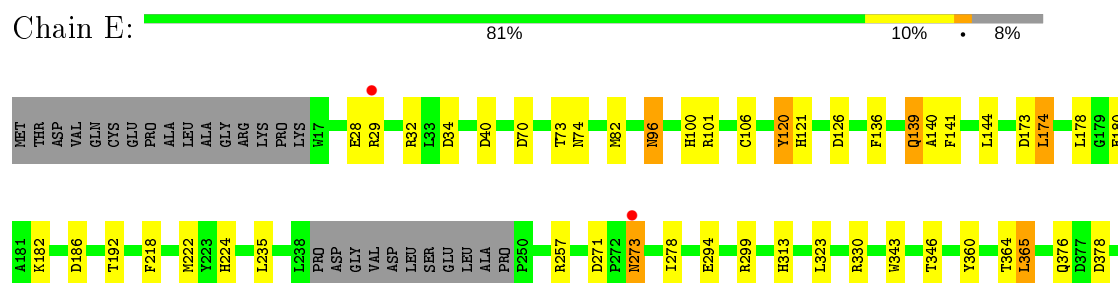
- Molecule 1: biphenyl dioxygenase large subunit

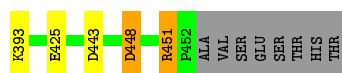


- Molecule 1: biphenyl dioxygenase large subunit

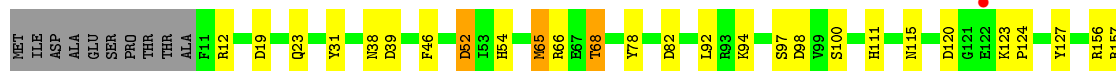
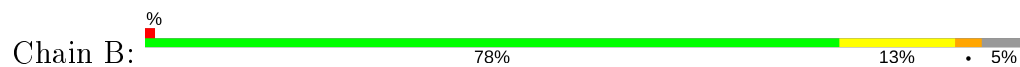


- Molecule 1: biphenyl dioxygenase large subunit

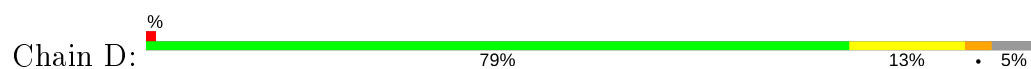




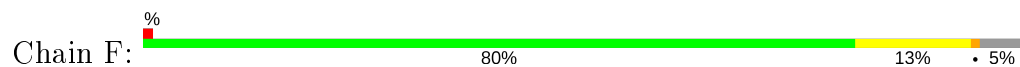
- Molecule 2: biphenyl dioxygenase small subunit



- Molecule 2: biphenyl dioxygenase small subunit



- Molecule 2: biphenyl dioxygenase small subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.83Å 137.83Å 237.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.76 – 2.60 36.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (36.76-2.60) 98.3 (36.74-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.64 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.184 , 0.234 0.190 , 0.237	Depositor DCC
$R_{free}$ test set	3522 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 27.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14936	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, BNL

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	0.52	0/3470	0.79	11/4710 (0.2%)
1	C	0.50	0/3467	0.80	12/4706 (0.3%)
1	E	0.52	0/3470	0.81	11/4710 (0.2%)
2	B	0.55	0/1519	0.81	6/2047 (0.3%)
2	D	0.56	0/1524	0.85	7/2054 (0.3%)
2	F	0.57	0/1519	0.86	9/2047 (0.4%)
All	All	0.53	0/14969	0.81	56/20274 (0.3%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	70	ASP	CB-CG-OD2	8.78	126.20	118.30
1	C	173	ASP	CB-CG-OD2	8.30	125.77	118.30
1	E	173	ASP	CB-CG-OD2	8.18	125.66	118.30
1	A	186	ASP	CB-CG-OD2	8.03	125.52	118.30
1	A	173	ASP	CB-CG-OD2	7.95	125.46	118.30
1	C	378	ASP	CB-CG-OD2	7.61	125.15	118.30
2	D	137	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	C	443	ASP	CB-CG-OD2	7.44	125.00	118.30
1	C	109	ASP	CB-CG-OD2	7.30	124.87	118.30
2	F	39	ASP	CB-CG-OD2	7.25	124.83	118.30
1	A	70	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	40	ASP	CB-CG-OD2	7.07	124.66	118.30
1	A	443	ASP	CB-CG-OD2	6.97	124.57	118.30
1	E	186	ASP	CB-CG-OD2	6.95	124.55	118.30
1	E	126	ASP	CB-CG-OD2	6.87	124.48	118.30
1	E	443	ASP	CB-CG-OD2	6.79	124.41	118.30
1	E	365	LEU	CA-CB-CG	6.67	130.65	115.30
2	D	83	ASP	CB-CG-OD2	6.52	124.17	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	120	ASP	CB-CG-OD2	6.46	124.11	118.30
1	C	365	LEU	CA-CB-CG	6.43	130.09	115.30
1	A	126	ASP	CB-CG-OD2	6.40	124.06	118.30
1	C	70	ASP	CB-CG-OD2	6.38	124.04	118.30
1	E	448	ASP	CB-CG-OD2	6.31	123.98	118.30
1	C	170	ASP	CB-CG-OD2	6.14	123.83	118.30
2	F	137	ARG	NE-CZ-NH2	-6.09	117.25	120.30
2	F	145	ASP	CB-CG-OD2	6.09	123.78	118.30
2	F	82	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	378	ASP	CB-CG-OD2	5.92	123.62	118.30
2	F	156	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	34	ASP	CB-CG-OD2	5.86	123.57	118.30
2	D	137	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	E	378	ASP	CB-CG-OD2	5.78	123.50	118.30
1	E	40	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	351	ASP	CB-CG-OD2	5.77	123.49	118.30
1	C	186	ASP	CB-CG-OD2	5.64	123.38	118.30
2	B	98	ASP	CB-CG-OD2	5.63	123.36	118.30
2	F	83	ASP	CB-CG-OD2	5.60	123.34	118.30
2	D	156	ARG	NE-CZ-NH1	5.59	123.09	120.30
2	F	47	ASP	CB-CG-OD2	5.55	123.30	118.30
2	B	39	ASP	CB-CG-OD2	5.55	123.29	118.30
2	B	174	ASP	CB-CG-OD2	5.55	123.29	118.30
2	D	145	ASP	CB-CG-OD2	5.51	123.26	118.30
2	F	156	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	377	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	168	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	148	ASP	CB-CG-OD2	5.31	123.08	118.30
2	F	120	ASP	CB-CG-OD2	5.28	123.05	118.30
2	D	82	ASP	CB-CG-OD2	5.25	123.03	118.30
1	C	19	ASP	CB-CG-OD2	5.23	123.01	118.30
1	E	34	ASP	CB-CG-OD2	5.21	122.99	118.30
2	B	52	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	411	ASP	CB-CG-OD2	5.10	122.89	118.30
2	B	19	ASP	CB-CG-OD2	5.10	122.89	118.30
2	B	120	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	126	ASP	CB-CG-OD2	5.04	122.83	118.30
1	E	365	LEU	CB-CG-CD2	5.01	119.51	111.00

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	3377	0	3180	20	0
1	C	3375	0	3177	17	0
1	E	3377	0	3180	20	0
2	B	1484	0	1441	17	0
2	D	1489	0	1446	13	0
2	F	1484	0	1441	11	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	4	0	0	1	0
4	C	4	0	0	0	0
4	E	4	0	0	1	0
5	A	12	0	10	1	0
5	C	12	0	10	0	0
5	E	12	0	10	3	0
6	A	71	0	0	0	0
6	B	32	0	0	0	0
6	C	45	0	0	1	0
6	D	42	0	0	0	0
6	E	73	0	0	0	0
6	F	36	0	0	0	0
All	All	14936	0	13895	84	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 (84) 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:121:HIS:HB2	4:A:500:FES:S1	2.31	0.71
2:F:181:ASN:HD22	2:F:181:ASN:H	1.42	0.66
1:C:96:ASN:HD21	1:C:106:CYS:H	1.42	0.65
1:E:448:ASP:O	1:E:451:ARG:HG2	1.98	0.63
1:A:96:ASN:HD21	1:A:106:CYS:H	1.46	0.63
2:B:38:ASN:HD21	2:B:111:HIS:H	1.47	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:GLU:HG3	6:C:1020:HOH:O	2.00	0.61
2:D:61:THR:CG2	2:D:63:ARG:HE	2.14	0.61
2:B:181:ASN:H	2:B:181:ASN:HD22	1.51	0.59
1:E:346:THR:OG1	1:E:364:THR:HG21	2.03	0.59
1:C:290:GLY:O	1:C:294:GLU:HG2	2.05	0.57
2:F:181:ASN:HD22	2:F:181:ASN:N	2.02	0.57
2:D:38:ASN:HD21	2:D:111:HIS:H	1.51	0.56
2:B:31:TYR:CD1	2:F:115:ASN:HA	2.41	0.56
1:E:271:ASP:OD1	1:E:273:ASN:HB2	2.06	0.55
1:A:73:THR:HG22	1:A:82:MET:HE3	1.89	0.55
1:E:96:ASN:HD21	1:E:106:CYS:H	1.55	0.54
2:D:115:ASN:HA	2:F:31:TYR:CG	2.43	0.53
1:E:73:THR:HG22	1:E:82:MET:CE	2.39	0.52
2:B:31:TYR:CG	2:F:115:ASN:HA	2.45	0.52
1:E:360:TYR:O	1:E:364:THR:HB	2.10	0.52
1:C:208:PRO:HD2	1:C:383:VAL:HG22	1.90	0.52
2:B:174:ASP:OD2	2:D:110:ARG:HB2	2.09	0.52
1:A:73:THR:HG22	1:A:82:MET:CE	2.40	0.52
1:A:293:ALA:HB1	1:A:307:GLN:HG2	1.91	0.51
1:A:360:TYR:O	1:A:364:THR:HB	2.10	0.51
2:F:38:ASN:HD21	2:F:111:HIS:H	1.60	0.49
1:C:100:HIS:NE2	1:E:425:GLU:OE2	2.34	0.48
2:D:62:THR:OG1	2:F:108:ARG:NH2	2.46	0.48
1:A:364:THR:HG23	2:B:78:TYR:HE1	1.79	0.48
1:A:193:GLU:OE2	1:A:295:LYS:NZ	2.41	0.48
2:B:127:TYR:OH	2:B:157:ARG:NH2	2.47	0.48
1:E:313:HIS:HA	1:E:323:LEU:HD23	1.96	0.48
2:F:30:TYR:HE1	2:F:129:VAL:HG11	1.78	0.48
1:C:377:ASP:OD2	2:D:94:LYS:NZ	2.47	0.48
1:A:403:MET:HG3	1:E:140:ALA:HB1	1.94	0.48
1:C:123:TRP:NE1	1:C:134:VAL:HG13	2.29	0.48
2:B:54:HIS:NE2	2:B:82:ASP:OD2	2.42	0.48
2:B:115:ASN:HA	2:D:31:TYR:CD1	2.49	0.47
1:C:139:GLN:HE21	1:C:139:GLN:H	1.62	0.47
1:C:272:PRO:O	1:C:273:ASN:C	2.52	0.47
1:C:96:ASN:HD21	1:C:106:CYS:N	2.12	0.46
2:D:115:ASN:HA	2:F:31:TYR:CD1	2.50	0.46
1:E:120:TYR:CG	1:E:121:HIS:CE1	3.03	0.46
1:A:211:TRP:HA	1:A:340:ILE:HG21	1.97	0.46
1:E:218:PHE:HA	5:E:2001:BNL:H13	1.97	0.46
1:A:159:TYR:CE1	1:A:182:LYS:HG2	2.51	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:PHE:HB3	1:E:144:LEU:HB2	1.99	0.45
1:C:76:MET:CE	1:C:93:VAL:HG11	2.46	0.45
2:B:115:ASN:HA	2:D:31:TYR:CG	2.51	0.45
1:A:82:MET:O	1:A:93:VAL:HA	2.17	0.45
1:C:304:GLU:O	1:C:309:LEU:HD13	2.15	0.45
2:D:158:THR:HG23	2:D:160:SER:H	1.81	0.45
1:A:223:TYR:CD1	1:A:403:MET:HE1	2.52	0.44
1:A:175:ASP:OD2	1:A:182:LYS:NZ	2.45	0.44
1:E:271:ASP:CG	1:E:273:ASN:HB2	2.38	0.44
1:A:346:THR:OG1	1:A:364:THR:HG21	2.18	0.43
2:B:23:GLN:HG3	2:D:24:HIS:ND1	2.32	0.43
2:D:149:GLY:HA2	2:D:174:ASP:OD2	2.18	0.43
1:A:218:PHE:HA	5:A:601:BNL:H13	2.00	0.43
1:C:223:TYR:CD2	1:C:403:MET:HE1	2.53	0.43
2:B:52:ASP:OD2	2:B:156:ARG:NH2	2.51	0.43
2:B:46:PHE:CD1	2:B:92:LEU:HD13	2.54	0.43
2:B:123:LYS:CG	2:B:124:PRO:HD2	2.49	0.43
1:E:174:LEU:HD22	1:E:178:LEU:HG	2.01	0.43
1:E:74:ASN:HA	1:E:343:TRP:CZ3	2.54	0.42
2:B:97:SER:HB3	2:B:100:SER:HB2	2.01	0.42
2:B:65:MET:O	2:B:68:THR:HG23	2.19	0.42
1:E:121:HIS:HB2	4:E:500:FES:S1	2.59	0.42
1:A:278:ILE:O	1:A:367:THR:HG21	2.20	0.42
1:E:222:MET:HE3	5:E:2001:BNL:H15	2.01	0.42
1:C:76:MET:HE1	1:C:93:VAL:HG11	2.01	0.41
1:C:267:PHE:CD2	1:C:309:LEU:HG	2.56	0.41
1:A:76:MET:CE	1:A:81:VAL:HG11	2.50	0.41
1:C:74:ASN:HA	1:C:343:TRP:CZ3	2.56	0.41
1:E:278:ILE:HD11	5:E:2001:BNL:H5	2.03	0.41
1:A:159:TYR:CZ	1:A:182:LYS:HG2	2.55	0.41
1:A:399:PHE:HB3	1:E:100:HIS:O	2.20	0.41
1:C:415:TYR:HA	1:C:416:PRO:HD3	1.95	0.41
2:D:61:THR:HG21	2:D:63:ARG:HH21	1.86	0.41
2:F:42:PHE:O	2:F:46:PHE:HD1	2.05	0.40
2:F:181:ASN:H	2:F:181:ASN:ND2	2.16	0.40
2:B:158:THR:HG22	2:B:160:SER:H	1.86	0.40
1:E:136:PHE:HA	1:E:139:GLN:HE21	1.85	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	421/460 (92%)	399 (95%)	22 (5%)	0	100	100
1	C	421/460 (92%)	391 (93%)	29 (7%)	1 (0%)	47	71
1	E	421/460 (92%)	400 (95%)	19 (4%)	2 (0%)	29	52
2	B	175/187 (94%)	167 (95%)	8 (5%)	0	100	100
2	D	176/187 (94%)	168 (96%)	7 (4%)	1 (1%)	25	47
2	F	175/187 (94%)	167 (95%)	8 (5%)	0	100	100
All	All	1789/1941 (92%)	1692 (95%)	93 (5%)	4 (0%)	47	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	273	ASN
1	C	273	ASN
1	E	376	GLN
2	D	65	MET

### 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	346/375 (92%)	329 (95%)	17 (5%)	25	48
1	C	345/375 (92%)	326 (94%)	19 (6%)	21	43
1	E	346/375 (92%)	326 (94%)	20 (6%)	20	40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	159/167 (95%)	152 (96%)	7 (4%)	28	53
2	D	159/167 (95%)	145 (91%)	14 (9%)	10	19
2	F	159/167 (95%)	148 (93%)	11 (7%)	15	31
All	All	1514/1626 (93%)	1426 (94%)	88 (6%)	20	40

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	96	ASN
1	A	101	ARG
1	A	107	ARG
1	A	120	TYR
1	A	139	GLN
1	A	175	ASP
1	A	180	GLU
1	A	192	THR
1	A	229	SER
1	A	252	GLU
1	A	295	LYS
1	A	310	MET
1	A	330	ARG
1	A	355	GLU
1	A	402	GLU
1	A	410	SER
2	B	12	ARG
2	B	65	MET
2	B	66	ARG
2	B	68	THR
2	B	94	LYS
2	B	158	THR
2	B	181	ASN
1	C	29	ARG
1	C	67	LYS
1	C	96	ASN
1	C	101	ARG
1	C	120	TYR
1	C	139	GLN
1	C	144	LEU
1	C	146	LYS
1	C	180	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	229	SER
1	C	273	ASN
1	C	295	LYS
1	C	310	MET
1	C	330	ARG
1	C	365	LEU
1	C	387	GLN
1	C	390	ARG
1	C	411	ASP
1	C	419	ILE
2	D	41	ARG
2	D	47	ASP
2	D	61	THR
2	D	65	MET
2	D	66	ARG
2	D	83	ASP
2	D	89	ARG
2	D	92	LEU
2	D	97	SER
2	D	98	ASP
2	D	137	ARG
2	D	157	ARG
2	D	158	THR
2	D	181	ASN
1	E	28	GLU
1	E	29	ARG
1	E	32	ARG
1	E	96	ASN
1	E	101	ARG
1	E	120	TYR
1	E	139	GLN
1	E	174	LEU
1	E	180	GLU
1	E	182	LYS
1	E	192	THR
1	E	224	HIS
1	E	235	LEU
1	E	257	ARG
1	E	294	GLU
1	E	299	ARG
1	E	330	ARG
1	E	365	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	393	LYS
1	E	451	ARG
2	F	51	GLU
2	F	66	ARG
2	F	76	ARG
2	F	92	LEU
2	F	93	ARG
2	F	94	LYS
2	F	97	SER
2	F	98	ASP
2	F	137	ARG
2	F	158	THR
2	F	181	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	217	GLN
1	A	381	ASN
1	A	434	GLN
2	B	38	ASN
2	B	43	GLN
2	B	181	ASN
1	C	96	ASN
1	C	139	GLN
1	C	153	GLN
1	C	333	HIS
1	C	362	GLN
1	C	381	ASN
1	C	434	GLN
2	D	38	ASN
2	D	143	GLN
2	D	181	ASN
1	E	96	ASN
1	E	139	GLN
1	E	153	GLN
1	E	308	GLN
1	E	381	ASN
1	E	434	GLN
2	F	38	ASN
2	F	86	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	F	143	GLN
2	F	181	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 3 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	$\# Z  > 2$
5	BNL	A	601	-	13,13,13	1.16	1 (7%)	16,16,16	0.78	0
4	FES	A	500	1	0,4,4	0.00	-	-		
4	FES	C	500	1	0,4,4	0.00	-	-		
4	FES	E	500	1	0,4,4	0.00	-	-		
5	BNL	E	2001	-	13,13,13	1.15	1 (7%)	16,16,16	0.59	0
5	BNL	C	1001	-	13,13,13	1.21	1 (7%)	16,16,16	0.90	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BNL	A	601	-	-	4/4/4/4	0/2/2/2
4	FES	A	500	1	-	-	0/1/1/1
4	FES	C	500	1	-	-	0/1/1/1
4	FES	E	500	1	-	-	0/1/1/1
5	BNL	E	2001	-	-	3/4/4/4	0/2/2/2
5	BNL	C	1001	-	-	4/4/4/4	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1001	BNL	C16-C2	-3.98	1.39	1.49
5	A	601	BNL	C16-C2	-3.89	1.39	1.49
5	E	2001	BNL	C16-C2	-3.61	1.40	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	BNL	C17-C16-C2-C1
5	A	601	BNL	C17-C16-C2-C3
5	A	601	BNL	C15-C16-C2-C1
5	A	601	BNL	C15-C16-C2-C3
5	C	1001	BNL	C17-C16-C2-C1
5	E	2001	BNL	C15-C16-C2-C3
5	C	1001	BNL	C15-C16-C2-C1
5	E	2001	BNL	C15-C16-C2-C1
5	C	1001	BNL	C17-C16-C2-C3
5	E	2001	BNL	C17-C16-C2-C3
5	C	1001	BNL	C15-C16-C2-C3

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	BNL	1	0
4	A	500	FES	1	0
4	E	500	FES	1	0
5	E	2001	BNL	3	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	425/460 (92%)	-0.49	4 (0%) 84 82	17, 28, 47, 61	0
1	C	425/460 (92%)	-0.38	7 (1%) 72 68	17, 30, 51, 63	0
1	E	425/460 (92%)	-0.45	2 (0%) 91 89	17, 29, 46, 57	0
2	B	177/187 (94%)	-0.61	1 (0%) 89 88	17, 28, 41, 51	0
2	D	178/187 (95%)	-0.47	1 (0%) 89 88	16, 27, 47, 51	0
2	F	177/187 (94%)	-0.54	1 (0%) 89 88	17, 28, 46, 52	0
All	All	1807/1941 (93%)	-0.47	16 (0%) 84 82	16, 29, 47, 63	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	122	GLU	3.0
1	C	138	GLU	2.9
2	B	122	GLU	2.8
1	C	273	ASN	2.7
1	C	453	ALA	2.3
1	C	298	GLU	2.3
1	A	449	ALA	2.3
1	A	142	PRO	2.1
1	E	273	ASN	2.1
1	A	138	GLU	2.1
1	A	411	ASP	2.1
1	E	29	ARG	2.1
1	C	271	ASP	2.0
1	C	411	ASP	2.0
2	D	12	ARG	2.0
1	C	145	ARG	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 carbohydrates 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	BNL	C	1001	12/12	0.80	0.37	63,64,66,66	0
5	BNL	E	2001	12/12	0.89	0.27	40,44,47,47	0
5	BNL	A	601	12/12	0.91	0.29	49,49,51,51	0
3	FE2	C	600	1/1	0.98	0.11	50,50,50,50	0
4	FES	E	500	4/4	0.99	0.07	21,23,24,26	0
3	FE2	A	600	1/1	0.99	0.07	32,32,32,32	0
4	FES	A	500	4/4	0.99	0.05	31,33,34,35	0
4	FES	C	500	4/4	0.99	0.04	28,31,31,32	0
3	FE2	E	600	1/1	0.99	0.08	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.