



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:06 AM UTC

PDB ID : 1ULJ / pdb_00001ulj
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

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:

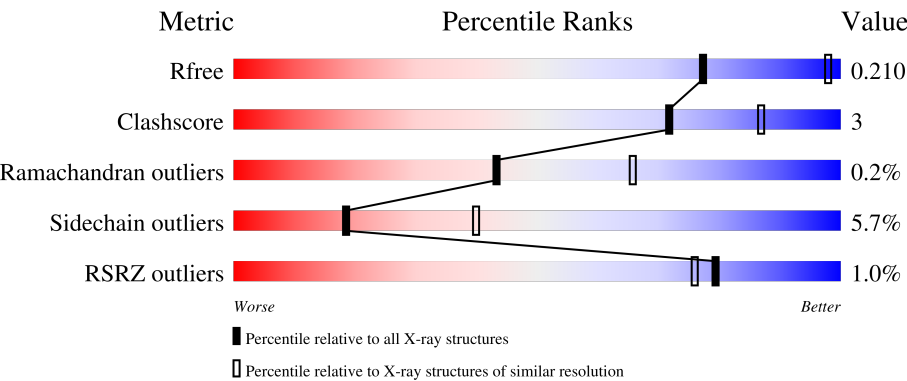
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	% 83% 8% 8%
1	C	460	2% 83% 9% 8%
1	E	460	% 82% 10% 8%
2	B	187	77% 16% 5%
2	D	187	% 83% 10% 5%

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Mol	Chain	Length	Quality of chain
2	F	187	% 82% 12% • 5%

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			

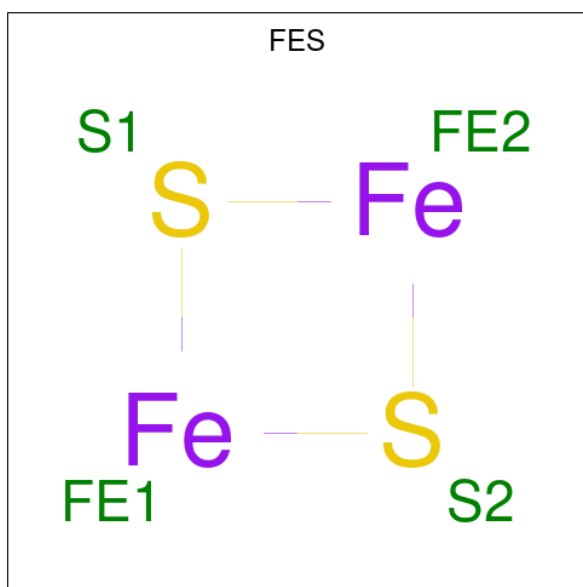
- Molecule 2 is a protein called biphenyl dioxygenase small subunit.

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 (CCD ID: FE2) (formula: Fe).

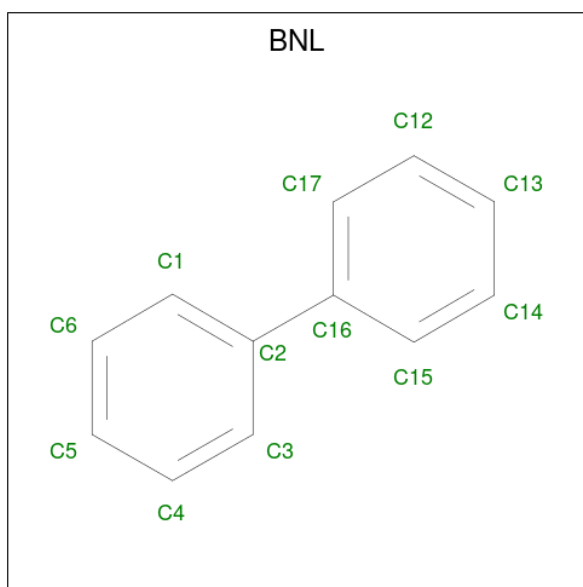
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	E	1	Total	Fe	0	0
			1	1		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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 (CCD ID: BNL) (formula: C₁₂H₁₀).



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

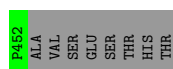
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C 12 12	0	0
5	E	1	Total C 12 12	0	0

- 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



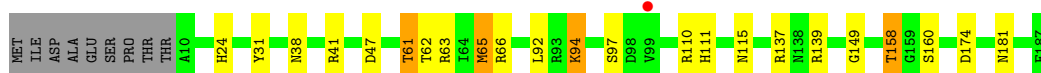
- Molecule 2: biphenyl dioxygenase small subunit

Chain B: 77% 16% 5%



- Molecule 2: biphenyl dioxygenase small subunit

Chain D: 83% 10% 5%



- Molecule 2: biphenyl dioxygenase small subunit

Chain F: 82% 12% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.83Å 137.83Å 237.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.76 – 2.60 36.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (36.76-2.60) 98.3 (36.76-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.184 , 0.234 (Not available) , 0.210	Depositor DCC
R_{free} test set	3522 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 24.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

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, 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	0.71	5/3470 (0.1%)	0.86	1/4710 (0.0%)
1	C	0.67	1/3467 (0.0%)	0.87	1/4706 (0.0%)
1	E	0.68	2/3470 (0.1%)	0.86	0/4710
2	B	0.70	0/1519	0.82	0/2047
2	D	0.73	0/1524	0.86	1/2054 (0.0%)
2	F	0.73	0/1519	0.84	0/2047
All	All	0.70	8/14969 (0.1%)	0.86	3/20274 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	MET	SD-CE	-10.04	1.54	1.79
1	C	76	MET	SD-CE	-9.09	1.56	1.79
1	A	82	MET	SD-CE	-6.95	1.62	1.79
1	A	403	MET	SD-CE	-6.64	1.62	1.79
1	E	82	MET	SD-CE	-6.61	1.63	1.79
1	A	222	MET	SD-CE	-6.29	1.63	1.79
1	E	222	MET	SD-CE	-5.57	1.65	1.79
1	A	103	MET	SD-CE	-5.25	1.66	1.79

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	383	VAL	N-CA-C	5.51	116.14	110.36
2	D	139	ARG	N-CA-C	5.42	117.08	108.79
1	A	144	LEU	N-CA-C	5.07	117.90	110.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3377	0	3180	25	0
1	C	3375	0	3177	19	0
1	E	3377	0	3180	21	0
2	B	1484	0	1441	18	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	2	0
5	C	12	0	10	0	0
5	E	12	0	10	2	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	93	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 (93) 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:73:THR:HG22	1:A:82:MET:HE3	1.64	0.80
1:C:76:MET:HE3	1:C:81:VAL:HG11	1.70	0.74
1:A:121:HIS:HB2	4:A:500:FES:S1	2.31	0.71
1:A:223:TYR:CD1	1:A:403:MET:HE1	2.29	0.68
1:A:76:MET:HE3	1:A:81:VAL:HG11	1.75	0.68
1:A:223:TYR:CG	1:A:403:MET:HE1	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:181:ASN:H	2:F:181:ASN:HD22	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
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
1:C:223:TYR:CD2	1:C:403:MET:HE1	2.37	0.60
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: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:C:272:PRO:O	1:C:273:ASN:C	2.52	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:E:271:ASP:CG	1:E:273:ASN:HB2	2.38	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:73:THR:HG22	1:A:82:MET:CE	2.40	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:H	1:C:139:GLN:HE21	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:187:HIS:HE2	1:E:305:ARG:HE	1.63	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
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
1:A:222:MET:HE3	1:A:225:ALA:HB3	1.99	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:222:MET:HE1	5:A:601:BNL:C3	2.46	0.45
1:C:76:MET:HE2	1:C:93:VAL:HG11	1.98	0.44
1:A:175:ASP:OD2	1:A:182:LYS:NZ	2.45	0.44
1:C:56:TRP:CD1	1:C:166:ASN:HD22	2.35	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
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:272:PRO:O	1:E:273:ASN:C	2.62	0.42
1:C:267:PHE:CD2	1:C:309:LEU:HG	2.56	0.41
2:B:57:MET:HE3	2:B:173:ILE:HB	2.03	0.41
1:A:82:MET:HA	1:A:82:MET:HE2	2.01	0.41
1:A:76:MET:HE2	1:A:93:VAL:HG11	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	421/460 (92%)	399 (95%)	22 (5%)	0	100	100
1	C	421/460 (92%)	391 (93%)	29 (7%)	1 (0%)	43	66
1	E	421/460 (92%)	400 (95%)	19 (4%)	2 (0%)	24	46
2	B	175/187 (94%)	167 (95%)	8 (5%)	0	100	100
2	D	176/187 (94%)	168 (96%)	7 (4%)	1 (1%)	21	42
2	F	175/187 (94%)	167 (95%)	8 (5%)	0	100	100
All	All	1789/1941 (92%)	1692 (95%)	93 (5%)	4 (0%)	43	66

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%)	331 (96%)	15 (4%)	26	51
1	C	345/375 (92%)	327 (95%)	18 (5%)	21	44
1	E	346/375 (92%)	327 (94%)	19 (6%)	19	41
2	B	159/167 (95%)	149 (94%)	10 (6%)	16	36
2	D	159/167 (95%)	148 (93%)	11 (7%)	14	32
2	F	159/167 (95%)	145 (91%)	14 (9%)	9	21
All	All	1514/1626 (93%)	1427 (94%)	87 (6%)	18	40

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	82	MET
1	A	101	ARG
1	A	107	ARG
1	A	139	GLN
1	A	175	ASP
1	A	180	GLU
1	A	192	THR
1	A	229	SER
1	A	295	LYS
1	A	310	MET
1	A	355	GLU
1	A	402	GLU
1	A	410	SER
1	A	433	THR
2	B	12	ARG
2	B	41	ARG
2	B	66	ARG
2	B	67	GLU
2	B	68	THR
2	B	76	ARG
2	B	93	ARG

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Mol	Chain	Res	Type
2	B	94	LYS
2	B	158	THR
2	B	181	ASN
1	C	29	ARG
1	C	67	LYS
1	C	101	ARG
1	C	139	GLN
1	C	144	LEU
1	C	146	LYS
1	C	180	GLU
1	C	229	SER
1	C	235	LEU
1	C	273	ASN
1	C	274	LEU
1	C	295	LYS
1	C	310	MET
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	92	LEU
2	D	94	LYS
2	D	97	SER
2	D	137	ARG
2	D	158	THR
2	D	181	ASN
1	E	29	ARG
1	E	32	ARG
1	E	101	ARG
1	E	138	GLU
1	E	139	GLN
1	E	174	LEU
1	E	180	GLU
1	E	182	LYS
1	E	192	THR
1	E	224	HIS

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Mol	Chain	Res	Type
1	E	235	LEU
1	E	257	ARG
1	E	294	GLU
1	E	299	ARG
1	E	365	LEU
1	E	383	VAL
1	E	393	LYS
1	E	402	GLU
1	E	451	ARG
2	F	41	ARG
2	F	51	GLU
2	F	66	ARG
2	F	76	ARG
2	F	89	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	173	ILE
2	F	181	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	130	ASN
1	A	307	GLN
1	A	381	ASN
1	A	407	GLN
1	A	434	GLN
2	B	24	HIS
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

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Mol	Chain	Res	Type
1	C	381	ASN
1	C	407	GLN
2	D	24	HIS
2	D	38	ASN
2	D	143	GLN
2	D	181	ASN
1	E	96	ASN
1	E	97	GLN
1	E	139	GLN
1	E	289	GLN
1	E	363	GLN
1	E	381	ASN
1	E	392	HIS
1	E	407	GLN
1	E	434	GLN
2	F	38	ASN
2	F	43	GLN
2	F	86	GLN
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 oligosaccharides 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	C	1001	-	13,13,13	1.27	1 (7%)	16,16,16	0.94	0
4	FES	E	500	1	0,4,4	-	-	-		
5	BNL	A	601	-	13,13,13	1.22	1 (7%)	16,16,16	0.81	0
4	FES	C	500	1	0,4,4	-	-	-		
5	BNL	E	2001	-	13,13,13	1.23	1 (7%)	16,16,16	0.62	0
4	FES	A	500	1	0,4,4	-	-	-		

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1001	BNL	C16-C2	-4.18	1.39	1.49
5	A	601	BNL	C16-C2	-4.08	1.39	1.49
5	E	2001	BNL	C16-C2	-3.79	1.40	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
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

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	500	FES	1	0
5	A	601	BNL	2	0
5	E	2001	BNL	2	0
4	A	500	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	425/460 (92%)	-0.35	3 (0%) 84 82	17, 28, 47, 61	0
1	C	425/460 (92%)	-0.22	9 (2%) 63 58	17, 30, 51, 63	0
1	E	425/460 (92%)	-0.30	4 (0%) 81 78	17, 29, 46, 57	0
2	B	177/187 (94%)	-0.38	0 100 100	17, 28, 41, 51	0
2	D	178/187 (95%)	-0.31	1 (0%) 85 83	16, 27, 47, 51	0
2	F	177/187 (94%)	-0.31	1 (0%) 85 83	17, 28, 46, 52	0
All	All	1807/1941 (93%)	-0.30	18 (0%) 79 76	16, 29, 47, 63	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	250	PRO	4.0
1	C	238	LEU	3.3
1	C	453	ALA	3.1
1	A	250	PRO	3.0
2	D	99	VAL	2.6
1	E	273	ASN	2.5
1	C	251	THR	2.4
1	C	273	ASN	2.4
2	F	100	SER	2.3
1	E	238	LEU	2.2
1	A	143	GLY	2.2
1	C	272	PRO	2.2
1	C	143	GLY	2.1
1	C	270	GLY	2.1
1	E	235	LEU	2.1
1	C	138	GLU	2.1
1	A	274	LEU	2.1
1	C	311	ALA	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($\text{\AA}^2$)	Q<0.9
5	BNL	E	2001	12/12	0.87	0.17	40,44,47,47	0
5	BNL	C	1001	12/12	0.90	0.19	63,64,66,66	0
5	BNL	A	601	12/12	0.91	0.14	49,49,51,51	0
4	FES	C	500	4/4	0.99	0.04	28,31,31,32	0
4	FES	E	500	4/4	0.99	0.03	21,23,24,26	0
3	FE2	C	600	1/1	0.99	0.02	50,50,50,50	0
3	FE2	E	600	1/1	0.99	0.03	33,33,33,33	0
4	FES	A	500	4/4	0.99	0.04	31,33,34,35	0
3	FE2	A	600	1/1	1.00	0.03	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.