



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:48 PM UTC

PDB ID : 2GBX / pdb_00002gbx
Title : Crystal Structure of Biphenyl 2,3-Dioxygenase from *Sphingomonas yanoikuyae* B1 Bound to Biphenyl
Authors : Ferraro, D.J.; Brown, E.N.; Yu, C.; Parales, R.E.; Gibson, D.T.; Ramaswamy, S.
Deposited on : 2006-03-12
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

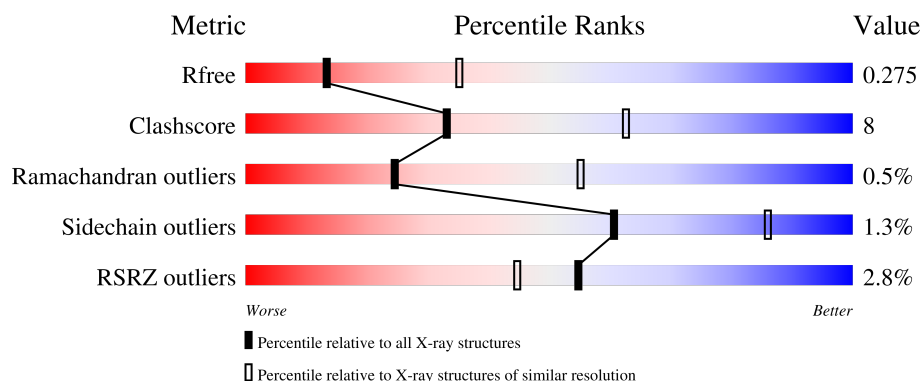
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	454	3% 84% 15% .
1	C	454	2% 80% 18% ..
1	E	454	3% 83% 15% ..
2	B	174	5% 79% 16% ..
2	D	174	3% 75% 21% ..

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Mol	Chain	Length	Quality of chain
2	F	174	3% 82% 13% ...

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15278 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 2,3-Dioxygenase Alpha Subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	1	0
			3569	2265	622	665	17			
1	C	446	Total	C	N	O	S	0	1	0
			3553	2257	620	659	17			
1	E	449	Total	C	N	O	S	0	3	0
			3578	2271	622	668	17			

- Molecule 2 is a protein called Biphenyl 2,3-Dioxygenase Beta Subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	2	0
			1446	914	260	265	7			
2	D	170	Total	C	N	O	S	0	3	0
			1449	916	260	266	7			
2	F	170	Total	C	N	O	S	0	0	0
			1436	906	260	265	5			

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

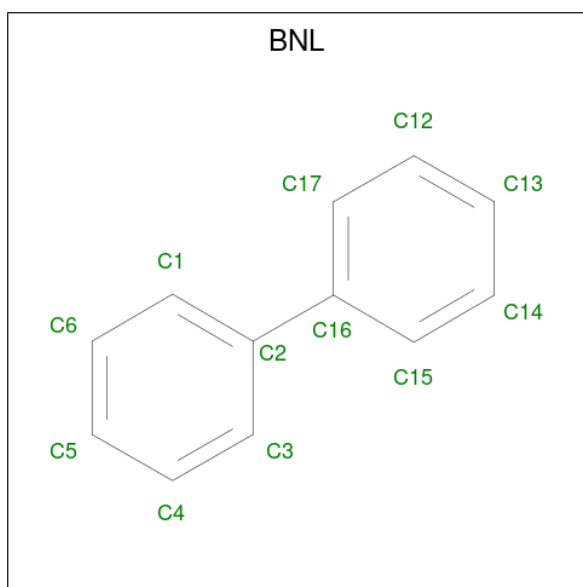
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	E	1	Total	Fe	0	0
			1	1		

- 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 ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	3	Total Zn 3 3	0	0
6	D	3	Total Zn 3 3	0	0
6	F	3	Total Zn 3 3	0	0

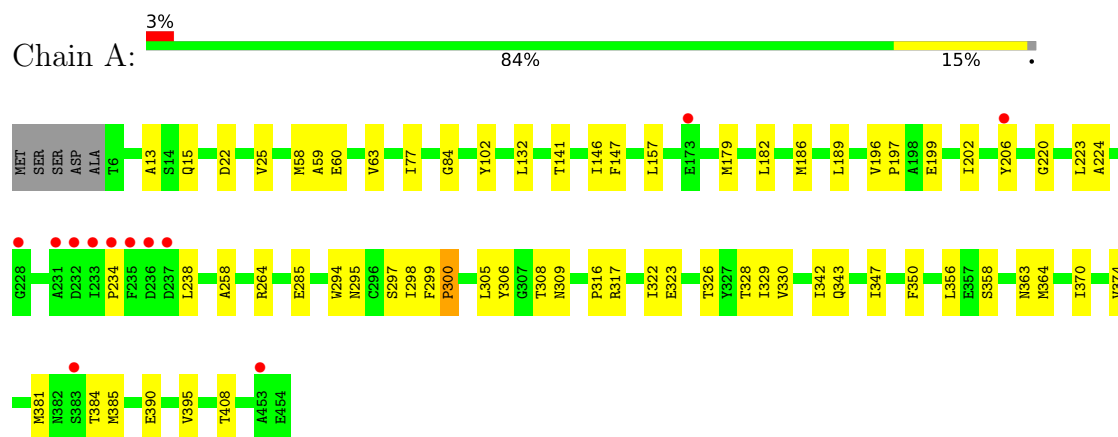
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	45	Total O 45 45	0	0
7	B	29	Total O 29 29	0	0
7	C	29	Total O 29 29	0	0
7	D	25	Total O 25 25	0	0
7	E	45	Total O 45 45	0	0
7	F	14	Total O 14 14	0	0

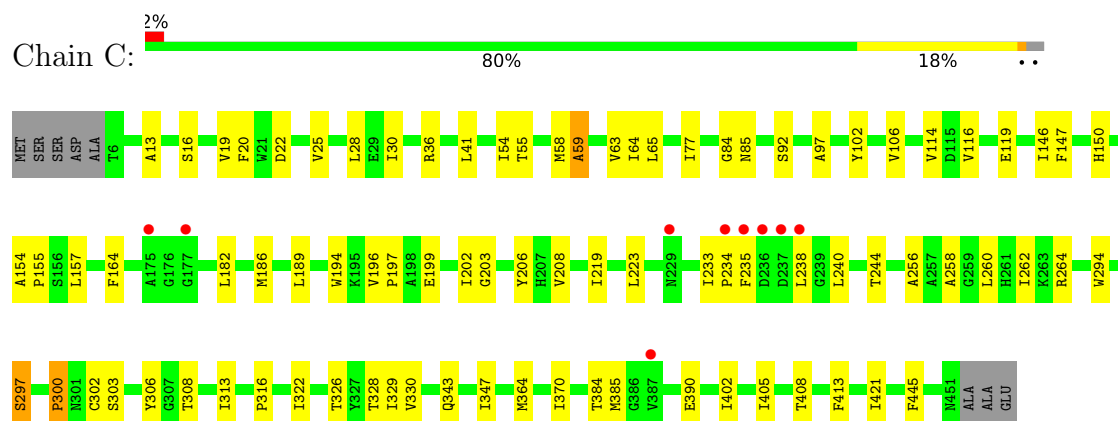
3 Residue-property plots [i](#)

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.

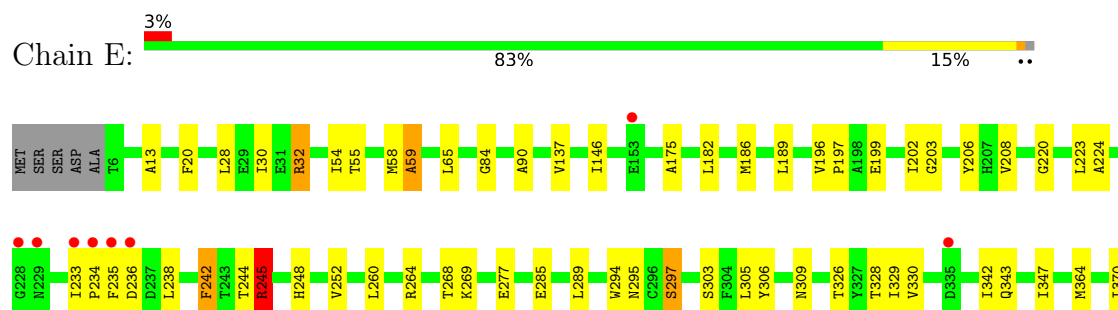
- Molecule 1: Biphenyl 2,3-Dioxygenase Alpha Subunit



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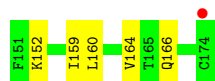
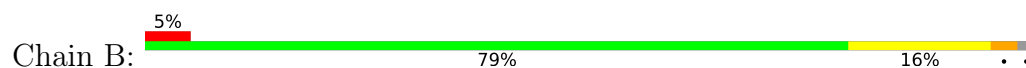


- Molecule 1: Biphenyl 2,3-Dioxygenase Alpha Subunit

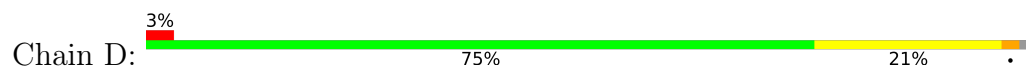




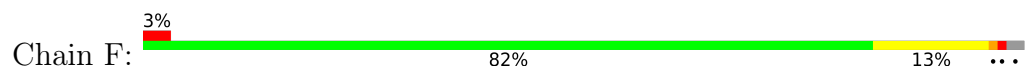
• Molecule 2: Biphenyl 2,3-Dioxygenase Beta Subunit



• Molecule 2: Biphenyl 2,3-Dioxygenase Beta Subunit



• Molecule 2: Biphenyl 2,3-Dioxygenase Beta Subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.94Å 133.94Å 219.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.48 – 2.80 19.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.48-2.80) 99.6 (19.48-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.15 (at 2.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.237 , 0.268 0.251 , 0.275	Depositor DCC
R_{free} test set	1132 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.056 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15278	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: FE, FES, BNL, ZN

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	0.43	0/3677	0.62	0/4990
1	C	0.44	0/3661	0.63	0/4967
1	E	0.47	0/3692	0.64	1/5010 (0.0%)
2	B	0.64	2/1487 (0.1%)	0.76	4/2009 (0.2%)
2	D	0.46	0/1493	0.78	4/2017 (0.2%)
2	F	0.42	0/1471	0.61	0/1989
All	All	0.47	2/15481 (0.0%)	0.66	9/20982 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	F	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	39[A]	MET	N-CA	-12.76	1.29	1.46
2	B	39[B]	MET	N-CA	-12.76	1.29	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	39[A]	MET	N-CA-C	-11.24	98.09	114.39
2	D	39[B]	MET	N-CA-C	-11.24	98.09	114.39
2	B	38	GLY	CA-C-N	-10.20	105.01	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	38	GLY	C-N-CA	-10.20	105.01	122.56
2	D	38	GLY	CA-C-N	-9.61	107.28	121.98
2	D	38	GLY	C-N-CA	-9.61	107.28	121.98
2	B	39[A]	MET	N-CA-CB	-8.82	97.68	110.47
2	B	39[B]	MET	N-CA-CB	-8.82	97.68	110.47
1	E	245	ARG	N-CA-C	5.19	117.34	111.11

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	300	PRO	Peptide
2	F	148	GLY	Peptide
2	F	149	ASN	Peptide

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	3569	0	3368	42	0
1	C	3553	0	3360	62	0
1	E	3578	0	3379	62	0
2	B	1446	0	1400	24	0
2	D	1449	0	1405	38	0
2	F	1436	0	1382	28	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	0	0
4	C	4	0	0	0	0
4	E	4	0	0	0	0
5	A	12	0	10	1	0
5	C	12	0	10	2	0
5	E	12	0	10	3	0
6	B	3	0	0	0	0
6	D	3	0	0	0	0
6	F	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	45	0	0	0	0
7	B	29	0	0	0	0
7	C	29	0	0	0	0
7	D	25	0	0	0	0
7	E	45	0	0	1	0
7	F	14	0	0	0	0
All	All	15278	0	14324	230	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 8.

All (230) 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:E:245:ARG:HG3	1:E:245:ARG:HH11	1.09	1.17
1:C:58:MET:HE2	1:C:150:HIS:NE2	1.72	1.02
2:D:95:PRO:HB2	2:D:96:PRO:HD2	1.45	0.99
1:E:245:ARG:HD2	1:E:245:ARG:C	1.87	0.99
2:F:95:PRO:HB2	2:F:96:PRO:CD	1.96	0.96
1:E:245:ARG:HD2	1:E:245:ARG:O	1.69	0.91
2:F:148:GLY:C	2:F:149:ASN:HD22	1.78	0.90
2:D:16:ILE:HD11	2:D:116:LEU:HD13	1.59	0.85
1:E:245:ARG:C	1:E:245:ARG:CD	2.49	0.84
1:C:223:LEU:HD11	1:C:256:ALA:HB1	1.59	0.84
1:C:297:SER:HG	1:C:303:SER:HG	1.15	0.83
2:F:95:PRO:CB	2:F:96:PRO:HD3	2.07	0.83
1:E:245:ARG:HG3	1:E:245:ARG:NH1	1.89	0.82
1:E:245:ARG:O	1:E:245:ARG:CD	2.30	0.80
1:E:245:ARG:HH11	1:E:245:ARG:CG	1.89	0.78
2:F:95:PRO:CB	2:F:96:PRO:CD	2.57	0.77
2:B:16:ILE:HD11	2:B:116:LEU:HD13	1.65	0.76
1:A:370:ILE:HG21	1:C:84:GLY:O	1.86	0.76
2:F:149:ASN:N	2:F:149:ASN:ND2	2.34	0.76
2:F:93:GLU:C	2:F:95:PRO:O	2.30	0.75
2:F:149:ASN:HD22	2:F:149:ASN:N	1.86	0.72
1:A:132:LEU:HD21	1:E:382:ASN:HD22	1.53	0.72
2:D:94:ASP:OD1	2:F:56:THR:OG1	2.04	0.71
1:A:84:GLY:O	1:E:370:ILE:HG21	1.90	0.71
1:C:58:MET:HE2	1:C:150:HIS:HE2	1.55	0.71
1:C:58:MET:CE	1:C:150:HIS:NE2	2.51	0.70
2:F:16:ILE:HD11	2:F:116:LEU:HD13	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:MET:HE2	1:C:150:HIS:CE1	2.28	0.69
2:D:95:PRO:HB2	2:D:96:PRO:CD	2.22	0.69
1:C:58:MET:O	1:C:59:ALA:HB3	1.93	0.67
1:E:245:ARG:NH1	1:E:245:ARG:CG	2.53	0.67
1:C:233:ILE:HD11	1:C:238:LEU:HD21	1.78	0.66
2:D:26[B]:MET:SD	2:D:39[B]:MET:HE3	2.36	0.66
2:D:93:GLU:O	2:D:96:PRO:N	2.30	0.65
2:B:34:GLU:OE1	2:B:34:GLU:N	2.30	0.64
1:A:309:ASN:HD22	1:A:342:ILE:HG21	1.63	0.63
2:B:26[A]:MET:HG3	2:B:39[A]:MET:HE1	1.80	0.63
2:D:24:VAL:HB	2:F:105:ASN:HD21	1.64	0.63
1:C:370:ILE:HG21	1:E:84:GLY:O	1.99	0.63
2:F:95:PRO:HB2	2:F:96:PRO:HD2	1.82	0.62
1:A:13:ALA:HB3	1:A:384:THR:HG22	1.82	0.61
2:D:64:THR:C	2:D:66:ASP:H	2.08	0.60
2:F:147:ASP:O	2:F:148:GLY:C	2.43	0.59
2:D:95:PRO:CB	2:D:96:PRO:CD	2.79	0.59
1:C:182:LEU:HD11	1:C:330:VAL:HG21	1.84	0.58
1:E:58:MET:O	1:E:59:ALA:HB3	2.02	0.58
1:C:58:MET:CE	1:C:150:HIS:CE1	2.86	0.58
2:D:64:THR:O	2:D:66:ASP:N	2.36	0.58
1:E:285:GLU:HG2	1:E:395:VAL:HG11	1.85	0.58
1:A:60:GLU:HG2	1:E:372:ARG:NH1	2.18	0.58
1:C:208:VAL:HG21	5:C:458:BNL:C3	2.34	0.58
2:D:92:MET:HG2	2:D:128:ARG:NH2	2.19	0.57
1:A:358:SER:O	2:B:92:MET:SD	2.63	0.57
1:A:285:GLU:HG2	1:A:395:VAL:HG11	1.87	0.56
1:C:402:ILE:HD11	1:C:445:PHE:HZ	1.69	0.56
1:E:175:ALA:HB1	1:E:277[A]:GLU:CD	2.30	0.56
1:E:295:ASN:HA	1:E:305:LEU:HD23	1.87	0.56
1:C:54:ILE:HG22	1:C:92:SER:HB3	1.88	0.55
1:C:63:VAL:HG12	1:C:77:ILE:HD13	1.89	0.55
1:A:328:THR:HG21	1:A:343:GLN:HA	1.87	0.55
1:C:13:ALA:HB3	1:C:384:THR:HG22	1.87	0.55
2:F:148:GLY:O	2:F:149:ASN:ND2	2.30	0.55
2:B:33:ARG:HB2	2:B:34:GLU:OE1	2.07	0.55
1:A:60:GLU:HG2	1:E:372:ARG:HH11	1.72	0.55
1:C:219:ILE:HG23	1:C:262:ILE:CD1	2.37	0.55
1:E:13:ALA:HB3	1:E:384:THR:HG22	1.89	0.55
1:A:206:TYR:CD2	1:A:385:MET:HE1	2.42	0.54
2:D:123:LEU:HD13	2:D:137:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:ARG:HD2	1:E:268:THR:HG21	1.90	0.54
2:F:94:ASP:N	2:F:95:PRO:O	2.40	0.54
1:C:58:MET:O	1:C:59:ALA:CB	2.55	0.53
1:E:328:THR:HG21	1:E:343:GLN:HA	1.89	0.53
1:C:65:LEU:HD21	1:C:146:ILE:HD12	1.89	0.53
1:E:55:THR:HG23	1:E:90:ALA:O	2.07	0.53
1:E:55:THR:CG2	1:E:90:ALA:O	2.57	0.53
2:D:50:ILE:HD12	2:D:68:ALA:HB1	1.91	0.53
1:E:234:PRO:O	1:E:238:LEU:HD13	2.09	0.53
2:B:123:LEU:HD13	2:B:137:THR:HG22	1.90	0.53
1:C:328:THR:HG21	1:C:343:GLN:HA	1.90	0.52
1:E:55:THR:OG1	7:E:481:HOH:O	2.13	0.52
1:C:106:VAL:HG13	1:C:114:VAL:HG23	1.92	0.52
1:E:30:ILE:HG22	1:E:30:ILE:O	2.10	0.51
2:F:147:ASP:O	2:F:149:ASN:N	2.43	0.51
1:C:199:GLU:O	1:C:202:ILE:HG22	2.10	0.51
1:E:175:ALA:HB1	1:E:277[A]:GLU:OE2	2.10	0.51
1:A:316:PRO:HA	1:A:322:ILE:HG22	1.91	0.51
2:B:26[A]:MET:HG3	2:B:39[A]:MET:CE	2.41	0.51
1:A:223:LEU:HD13	5:A:457:BNL:H13	1.93	0.51
1:C:294:TRP:HB2	1:C:306:TYR:HB3	1.93	0.51
1:E:182:LEU:HD11	1:E:330:VAL:HG21	1.93	0.51
1:E:186:MET:HE3	1:E:326:THR:HB	1.92	0.51
1:C:219:ILE:HG23	1:C:262:ILE:HD11	1.93	0.51
2:D:118:VAL:HG21	2:D:144:LEU:HD12	1.93	0.51
1:E:245:ARG:O	1:E:245:ARG:HD3	2.11	0.50
2:D:32:TYR:CE2	2:D:85:LEU:HD13	2.47	0.50
1:E:242:PHE:N	1:E:242:PHE:CD2	2.79	0.49
2:B:164:VAL:HB	2:F:131:THR:HG22	1.93	0.49
1:C:234:PRO:O	1:C:238:LEU:HD13	2.13	0.49
1:A:199:GLU:O	1:A:202:ILE:HG22	2.12	0.49
1:C:347:ILE:HG21	2:D:69:ALA:O	2.13	0.48
1:A:182:LEU:HD11	1:A:330:VAL:HG21	1.95	0.48
1:C:258:ALA:HB1	1:C:264:ARG:HD3	1.95	0.48
2:B:26[A]:MET:HE2	2:B:26[A]:MET:HA	1.95	0.48
2:D:93:GLU:O	2:D:95:PRO:C	2.56	0.48
1:A:220:GLY:HA2	1:A:224:ALA:HB2	1.95	0.48
1:C:240:LEU:HD23	1:C:402:ILE:O	2.13	0.48
1:E:65:LEU:HD21	1:E:146:ILE:HD12	1.95	0.48
2:B:8:VAL:CG2	2:B:108:ALA:HB3	2.44	0.48
1:A:179:MET:HE2	1:A:329:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:VAL:HG21	2:D:108:ALA:HB3	1.96	0.48
2:B:32:TYR:CE2	2:B:85:LEU:HD13	2.49	0.47
2:D:26[A]:MET:HE2	2:D:26[A]:MET:HA	1.97	0.47
1:E:58:MET:SD	1:E:137:VAL:HG11	2.54	0.47
1:E:370:ILE:HG13	1:E:376:THR:HG21	1.97	0.47
2:B:93:GLU:OE2	2:B:97:SER:OG	2.30	0.47
1:A:347:ILE:HG21	2:B:69:ALA:O	2.14	0.47
2:B:125:TYR:CG	2:D:137:THR:HG21	2.50	0.47
1:E:206:TYR:CD2	1:E:385:MET:HE1	2.49	0.47
2:F:160:LEU:HD21	2:F:170:LEU:HD13	1.95	0.47
1:A:22:ASP:OD2	1:A:25:VAL:HG23	2.14	0.47
2:B:8:VAL:HG21	2:B:108:ALA:HB3	1.97	0.47
2:F:46:TYR:HB2	2:F:78:LEU:HD11	1.96	0.47
2:D:44:ILE:HG21	2:D:78:LEU:HD12	1.96	0.47
1:C:223:LEU:HD11	1:C:256:ALA:CB	2.39	0.47
2:D:64:THR:C	2:D:66:ASP:N	2.72	0.47
1:E:294:TRP:HB2	1:E:306:TYR:HB3	1.97	0.47
1:C:147:PHE:CD2	1:C:157:LEU:HD21	2.51	0.46
1:C:164:PHE:HB2	1:C:244:THR:HG21	1.97	0.46
1:C:196:VAL:HB	1:C:197:PRO:HD3	1.98	0.46
1:E:260:LEU:HD11	5:E:459:BNL:C14	2.46	0.46
1:E:347:ILE:HG21	2:F:69:ALA:O	2.15	0.46
2:D:165:THR:HG21	2:D:170:LEU:HG	1.97	0.46
1:C:186:MET:HE3	1:C:326:THR:HB	1.98	0.46
2:F:138:LEU:HD21	2:F:158:LEU:HD22	1.97	0.46
1:C:189:LEU:HD12	2:D:166:GLN:HG2	1.97	0.46
1:C:154:ALA:HB1	1:C:155:PRO:HD2	1.97	0.46
1:A:234:PRO:O	1:A:238:LEU:HD13	2.15	0.46
1:E:32:ARG:O	1:E:420:MET:HE3	2.15	0.46
2:F:159:ILE:N	2:F:159:ILE:HD12	2.31	0.46
1:E:30:ILE:O	1:E:30:ILE:CG2	2.63	0.46
1:A:63:VAL:HG12	1:A:77:ILE:HD13	1.99	0.46
1:C:106:VAL:HG13	1:C:114:VAL:CG2	2.46	0.45
1:E:196:VAL:HB	1:E:197:PRO:HD3	1.99	0.45
1:A:141:THR:HG22	1:A:146:ILE:HG12	1.99	0.45
1:A:189:LEU:HD12	2:B:166:GLN:HG2	1.98	0.45
2:D:26[B]:MET:SD	2:D:39[B]:MET:CE	3.03	0.45
1:E:20:PHE:CZ	1:E:196:VAL:HG22	2.52	0.45
1:E:28:LEU:O	1:E:32:ARG:HB2	2.15	0.45
1:A:364:MET:HE2	1:A:364:MET:HA	1.98	0.45
2:B:94:ASP:HA	2:B:95:PRO:HA	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:TYR:CG	2:F:137:THR:HG21	2.52	0.45
1:C:313:ILE:N	1:C:313:ILE:HD12	2.31	0.45
1:E:199:GLU:O	1:E:202:ILE:HG22	2.16	0.45
2:D:125:TYR:CB	2:F:137:THR:HG21	2.47	0.45
1:C:116:VAL:HG23	1:C:119:GLU:HB2	1.99	0.45
1:E:244:THR:OG1	1:E:248:HIS:O	2.30	0.44
1:A:350:PHE:CE2	1:A:356:LEU:HD22	2.51	0.44
2:D:32:TYR:HB2	2:D:82:VAL:HG13	2.00	0.44
1:C:22:ASP:OD2	1:C:25:VAL:HG23	2.17	0.44
1:C:316:PRO:HA	1:C:322:ILE:HG22	1.99	0.44
1:C:41:LEU:HD21	1:C:58:MET:SD	2.58	0.44
1:E:223:LEU:HD13	5:E:459:BNL:H13	2.00	0.44
1:E:297:SER:OG	1:E:303:SER:OG	2.12	0.44
1:A:196:VAL:HB	1:A:197:PRO:HD3	2.00	0.44
1:C:28:LEU:CD2	1:C:421:ILE:HG23	2.48	0.44
1:C:329:ILE:HG23	1:C:329:ILE:O	2.18	0.44
2:D:32:TYR:CB	2:D:82:VAL:HG13	2.48	0.44
2:B:35:TRP:C	2:B:37:GLN:H	2.26	0.44
1:E:329:ILE:HG23	1:E:329:ILE:O	2.18	0.44
1:E:402:ILE:HD12	1:E:403:SER:N	2.32	0.44
1:C:97:ALA:HB1	1:C:106:VAL:CG2	2.47	0.43
2:B:131:THR:HG22	2:D:164:VAL:HB	2.00	0.43
2:D:123:LEU:HD13	2:D:137:THR:CG2	2.48	0.43
1:E:402:ILE:HD12	1:E:403:SER:HB2	2.00	0.43
2:B:138:LEU:HG	2:B:160:LEU:HD23	2.00	0.43
1:A:258:ALA:HB1	1:A:264:ARG:HD3	2.00	0.43
1:C:302:CYS:SG	1:C:303:SER:N	2.92	0.43
1:E:252:VAL:HG21	1:E:289:LEU:HD22	2.01	0.43
1:E:330:VAL:HG12	1:E:342:ILE:HG21	2.00	0.43
2:F:70:ILE:HD13	2:F:170:LEU:HD12	1.99	0.43
1:C:55:THR:HG22	1:C:64:ILE:HG12	2.00	0.43
1:E:235:PHE:CD1	1:E:405:ILE:HD12	2.53	0.43
1:A:294:TRP:HB2	1:A:306:TYR:HB3	2.00	0.43
1:C:206:TYR:CG	1:C:385:MET:HE1	2.54	0.43
1:C:235:PHE:CD1	1:C:405:ILE:HD12	2.54	0.43
1:A:317:ARG:HD2	1:A:323:GLU:HB2	2.01	0.43
1:A:308:THR:HG21	1:A:350:PHE:CD2	2.54	0.42
1:A:363:ASN:HA	1:C:85:ASN:HD21	1.84	0.42
1:E:233:ILE:HD11	1:E:235:PHE:CE1	2.54	0.42
1:A:59:ALA:HA	1:A:316:PRO:HD2	2.01	0.42
1:C:223:LEU:HD23	5:C:458:BNL:H13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:GLY:HA2	1:E:224:ALA:HB2	2.00	0.42
1:A:58:MET:O	1:A:59:ALA:HB3	2.20	0.42
2:B:38:GLY:O	2:B:152:LYS:HG2	2.18	0.42
1:A:102:TYR:OH	1:E:364:MET:HE1	2.19	0.42
1:C:54:ILE:HG22	1:C:92:SER:CB	2.49	0.42
1:E:58:MET:O	1:E:59:ALA:CB	2.67	0.42
1:A:295:ASN:HA	1:A:305:LEU:HD23	2.02	0.42
1:A:147:PHE:CD2	1:A:157:LEU:HD21	2.55	0.42
2:D:122:ILE:HD11	2:D:140:ARG:CZ	2.49	0.42
1:A:299:PHE:HA	1:A:300:PRO:HA	1.69	0.42
2:B:159:ILE:N	2:B:159:ILE:HD12	2.34	0.42
2:D:125:TYR:CE1	2:D:135:VAL:HG22	2.55	0.42
1:E:402:ILE:HD12	1:E:403:SER:CB	2.50	0.42
1:A:374:VAL:HG11	1:C:30:ILE:CG2	2.49	0.42
1:C:28:LEU:HD23	1:C:421:ILE:HG23	2.00	0.42
2:B:35:TRP:CD1	2:B:39[B]:MET:HB2	2.55	0.42
2:D:138:LEU:HD23	2:D:138:LEU:N	2.34	0.42
1:C:260:LEU:HD12	1:C:308:THR:OG1	2.20	0.41
2:F:55:LEU:HD13	2:F:57:ARG:NH1	2.35	0.41
2:D:8:VAL:CG2	2:D:108:ALA:HB3	2.49	0.41
1:C:16:SER:O	1:C:19:VAL:HG22	2.20	0.41
1:C:364:MET:HE2	1:C:364:MET:HA	2.01	0.41
2:D:125:TYR:HB3	2:F:137:THR:HG21	2.03	0.41
1:E:208:VAL:HG21	5:E:459:BNL:C3	2.51	0.41
1:C:194:TRP:HA	1:C:322:ILE:HG21	2.02	0.41
2:D:70:ILE:HD13	2:D:170:LEU:HD12	2.02	0.41
1:A:186:MET:HE3	1:A:326:THR:HB	2.02	0.41
1:A:15:GLN:HB2	1:A:381:MET:HE3	2.03	0.41
2:B:20:TYR:O	2:B:24:VAL:HG23	2.21	0.41
1:E:309:ASN:HD22	1:E:342:ILE:CG2	2.33	0.41
1:A:390:GLU:OE1	1:A:408:THR:HG23	2.21	0.41
1:C:20:PHE:CE2	1:C:196:VAL:HG22	2.56	0.40
2:D:127:ASN:ND2	2:F:162:ALA:HB2	2.36	0.40
1:C:202:ILE:HD13	1:C:413:PHE:HB2	2.04	0.40
1:C:390:GLU:OE1	1:C:408:THR:HG23	2.21	0.40
1:E:189:LEU:HD12	2:F:166:GLN:HG2	2.04	0.40
1:E:236:ASP:CG	1:E:402:ILE:HD13	2.46	0.40
1:E:244:THR:OG1	1:E:248:HIS:HB2	2.22	0.40
1:A:364:MET:HE1	1:C:102:TYR:OH	2.21	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	448/454 (99%)	422 (94%)	25 (6%)	1 (0%)	43	72
1	C	445/454 (98%)	407 (92%)	35 (8%)	3 (1%)	18	47
1	E	450/454 (99%)	425 (94%)	23 (5%)	2 (0%)	30	60
2	B	170/174 (98%)	163 (96%)	7 (4%)	0	100	100
2	D	171/174 (98%)	159 (93%)	11 (6%)	1 (1%)	21	51
2	F	168/174 (97%)	156 (93%)	10 (6%)	2 (1%)	10	34
All	All	1852/1884 (98%)	1732 (94%)	111 (6%)	9 (0%)	24	55

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	59	ALA
2	F	148	GLY
2	F	96	PRO
1	E	59	ALA
1	C	203	GLY
2	D	150	GLY
1	E	203	GLY
1	A	300	PRO
1	C	300	PRO

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	372/375 (99%)	370 (100%)	2 (0%)	81	93
1	C	371/375 (99%)	369 (100%)	2 (0%)	81	93
1	E	374/375 (100%)	367 (98%)	7 (2%)	50	81
2	B	155/157 (99%)	151 (97%)	4 (3%)	40	75
2	D	156/157 (99%)	154 (99%)	2 (1%)	61	86
2	F	153/157 (98%)	150 (98%)	3 (2%)	48	80
All	All	1581/1596 (99%)	1561 (99%)	20 (1%)	61	86

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	SER
1	A	298	ILE
2	B	37	GLN
2	B	73	ASP
2	B	93	GLU
2	B	97	SER
1	C	36	ARG
1	C	297	SER
2	D	66	ASP
2	D	92	MET
1	E	32	ARG
1	E	54	ILE
1	E	242	PHE
1	E	245	ARG
1	E	269	LYS
1	E	297	SER
1	E	447	ASN
2	F	97	SER
2	F	147	ASP
2	F	149	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	125	ASN
1	A	150	HIS
1	A	309	ASN
2	B	31	GLN

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Mol	Chain	Res	Type
2	B	80	GLN
2	B	89	GLN
2	B	130	GLN
2	B	166	GLN
1	C	125	ASN
1	C	193	ASN
1	C	200	ASN
1	C	218	GLN
1	C	295	ASN
1	C	301	ASN
1	C	309	ASN
1	C	382	ASN
1	C	451	ASN
2	D	5	GLN
2	D	127	ASN
2	D	130	GLN
1	E	86	GLN
1	E	109	GLN
1	E	191	GLN
1	E	218	GLN
1	E	241	GLN
1	E	309	ASN
1	E	378	ASN
1	E	382	ASN
1	E	447	ASN
2	F	37	GLN
2	F	105	ASN
2	F	130	GLN
2	F	149	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 18 ligands modelled in this entry, 12 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	E	459	-	13,13,13	0.49	0	16,16,16	0.60	0
5	BNL	A	457	-	13,13,13	0.47	0	16,16,16	0.59	0
5	BNL	C	458	-	13,13,13	0.45	0	16,16,16	0.67	0
4	FES	E	455	1	0,4,4	-	-	-		
4	FES	A	455	1	0,4,4	-	-	-		
4	FES	C	455	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	E	459	-	-	0/4/4/4	0/2/2/2
5	BNL	A	457	-	-	0/4/4/4	0/2/2/2
5	BNL	C	458	-	-	0/4/4/4	0/2/2/2
4	FES	E	455	1	-	-	0/1/1/1
4	FES	A	455	1	-	-	0/1/1/1
4	FES	C	455	1	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	459	BNL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	457	BNL	1	0
5	C	458	BNL	2	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	449/454 (98%)	0.25	12 (2%) 56 46	23, 32, 50, 56	1 (0%)
1	C	446/454 (98%)	0.40	9 (2%) 65 56	28, 41, 54, 58	1 (0%)
1	E	449/454 (98%)	0.13	12 (2%) 56 46	17, 27, 41, 48	3 (0%)
2	B	170/174 (97%)	0.41	8 (4%) 36 29	19, 33, 39, 40	2 (1%)
2	D	170/174 (97%)	0.38	6 (3%) 47 38	21, 36, 45, 45	3 (1%)
2	F	170/174 (97%)	0.39	5 (2%) 53 43	30, 34, 39, 40	0
All	All	1854/1884 (98%)	0.30	52 (2%) 55 45	17, 35, 50, 58	10 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	235	PHE	5.0
2	B	87	SER	4.8
1	A	236	ASP	4.5
2	B	149	ASN	4.0
1	A	235	PHE	3.9
2	B	94	ASP	3.7
1	E	235	PHE	3.4
2	F	174	CYS	3.4
1	E	236	ASP	3.4
1	A	453	ALA	3.4
2	D	174	CYS	3.3
1	E	228	GLY	3.3
2	D	147	ASP	3.2
1	A	234	PRO	3.2
1	A	231	ALA	3.2
1	A	228	GLY	3.1
2	D	148	GLY	3.1
1	A	232	ASP	3.0
2	D	149	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	234	PRO	2.9
1	C	236	ASP	2.9
2	B	174	CYS	2.9
1	E	234	PRO	2.8
2	F	87	SER	2.8
1	C	177	GLY	2.8
1	A	233	ILE	2.8
1	E	335	ASP	2.7
2	D	87	SER	2.7
2	B	88	GLY	2.6
2	B	59	ARG	2.5
1	E	453	ALA	2.5
2	B	147	ASP	2.5
2	F	148	GLY	2.5
1	E	454	GLU	2.4
1	A	237	ASP	2.4
1	C	175	ALA	2.4
2	B	150	GLY	2.3
1	A	173	GLU	2.3
1	E	153	GLU	2.3
1	E	229	ASN	2.2
1	E	448	GLU	2.2
1	A	383	SER	2.2
2	D	5	GLN	2.2
1	C	237	ASP	2.2
1	E	233	ILE	2.1
2	F	147	ASP	2.1
1	E	451	ASN	2.1
2	F	149	ASN	2.1
1	C	387	VAL	2.1
1	C	238	LEU	2.1
1	A	206	TYR	2.0
1	C	229	ASN	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

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	BNL	C	458	12/12	0.83	0.18	60,60,60,60	0
6	ZN	D	469	1/1	0.83	0.13	98,98,98,98	0
6	ZN	F	466	1/1	0.84	0.11	84,84,84,84	0
6	ZN	B	460	1/1	0.86	0.09	60,60,60,60	0
3	FE	A	456	1/1	0.87	0.08	31,31,31,31	0
3	FE	E	456	1/1	0.89	0.09	20,20,20,20	0
6	ZN	B	468	1/1	0.89	0.15	83,83,83,83	0
5	BNL	A	457	12/12	0.91	0.14	58,58,58,58	0
3	FE	C	456	1/1	0.91	0.07	33,33,33,33	0
6	ZN	F	463	1/1	0.92	0.06	54,54,54,54	0
6	ZN	F	467	1/1	0.92	0.13	56,56,56,56	0
5	BNL	E	459	12/12	0.94	0.09	29,29,29,29	0
6	ZN	D	465	1/1	0.94	0.12	54,54,54,54	0
4	FES	E	455	4/4	0.95	0.05	18,18,18,18	0
4	FES	C	455	4/4	0.97	0.05	30,30,30,30	0
6	ZN	B	464	1/1	0.97	0.04	51,51,51,51	0
6	ZN	D	462	1/1	0.98	0.04	54,54,54,54	0
4	FES	A	455	4/4	0.98	0.05	16,16,16,16	0

6.5 Other polymers

There are no such residues in this entry.