



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:29 AM EDT

PDB ID : 2GBW / pdb_00002gbw
Title : Crystal Structure of Biphenyl 2,3-Dioxygenase from *Sphingomonas yanoikuyae* B1
Authors : Ferraro, D.J.; Brown, E.N.; Yu, C.; Parales, R.E.; Gibson, D.T.; Ramaswamy, S.
Deposited on : 2006-03-12
Resolution : 1.70 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:

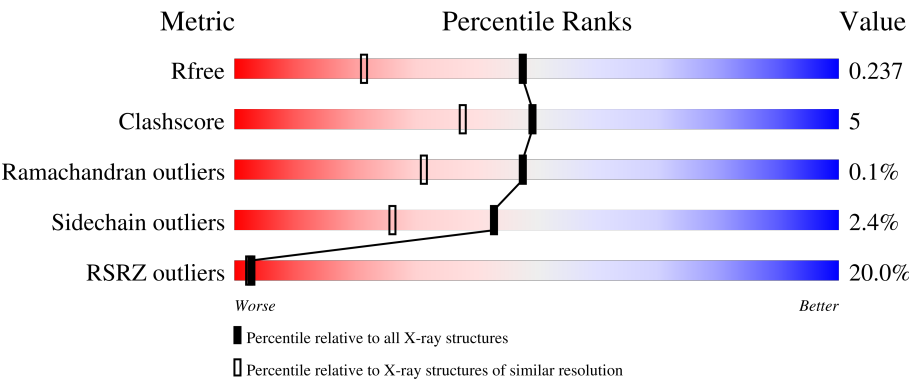
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	20% 92% 7% ..
1	C	454	9% 91% 6% ..
1	E	454	28% 89% 9% ..
2	B	174	32% 78% 18% ..
2	D	174	11% 84% 13% ...

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Mol	Chain	Length	Quality of chain
2	F	174	20% 82% 13% • •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17030 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			

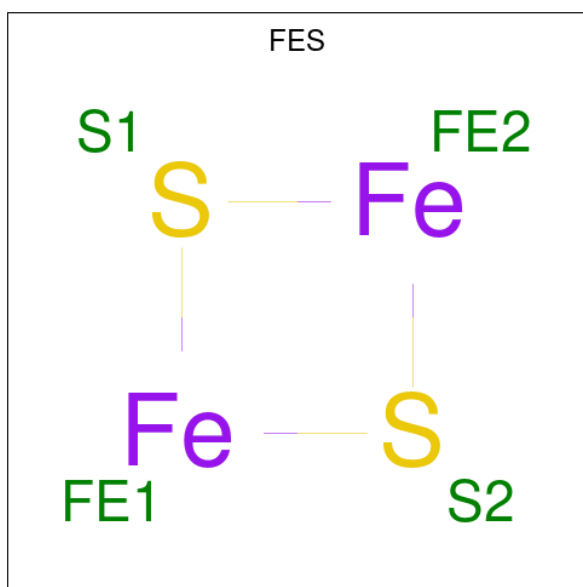
- Molecule 2 is a protein called Biphenyl 2,3-Dioxygenase Beta Subunit.

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).

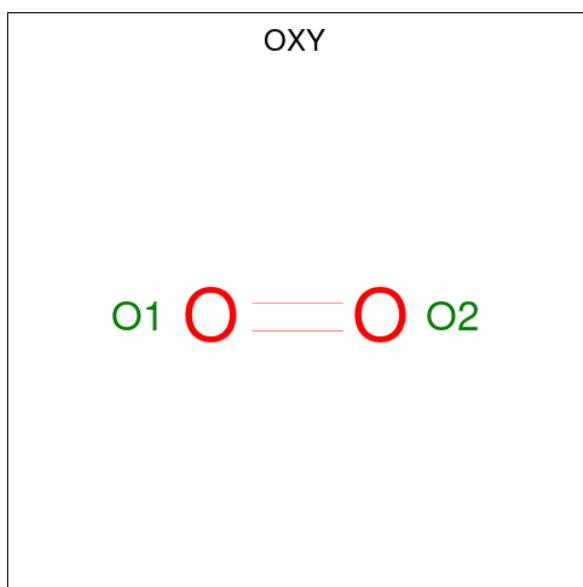
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	E	1	Total	Fe	0	0
			1	1		

- 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 OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	O	0	0
			2	2		
5	E	1	Total	O	0	0
			2	2		

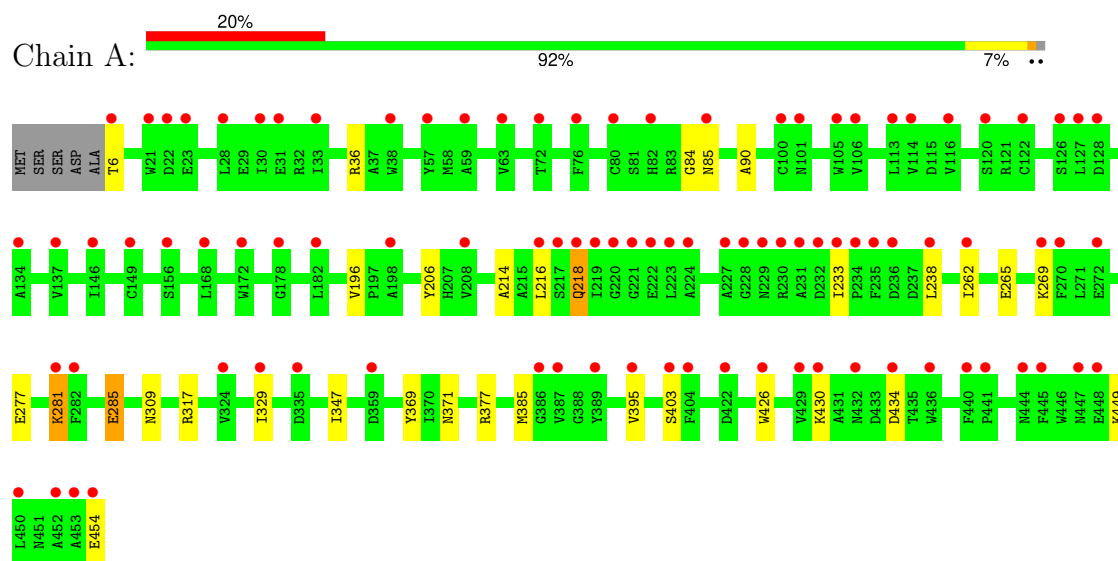
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	502	Total	O	0	0
			502	502		
6	B	250	Total	O	0	0
			250	250		
6	C	441	Total	O	0	0
			441	441		
6	D	232	Total	O	0	0
			232	232		
6	E	354	Total	O	0	0
			354	354		
6	F	199	Total	O	0	0
			199	199		

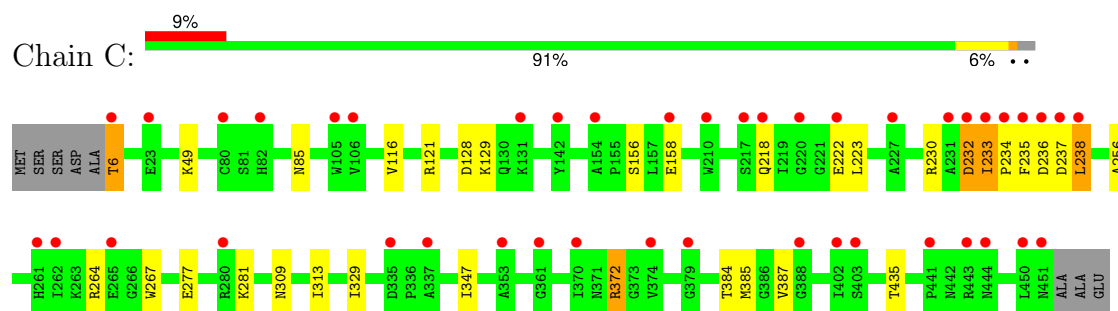
3 Residue-property plots [i](#)

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.

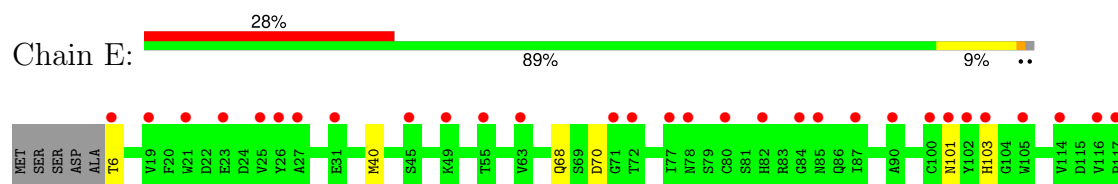
• Molecule 1: Biphenyl 2,3-Dioxygenase Alpha Subunit

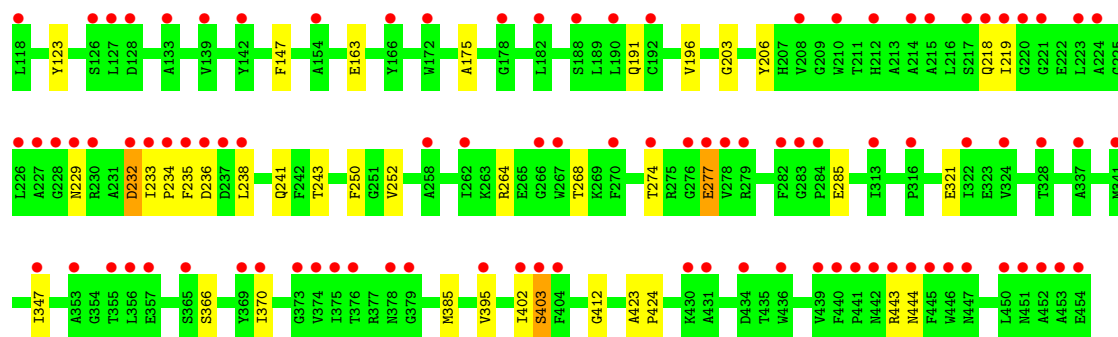


• Molecule 1: Biphenyl 2,3-Dioxygenase Alpha Subunit

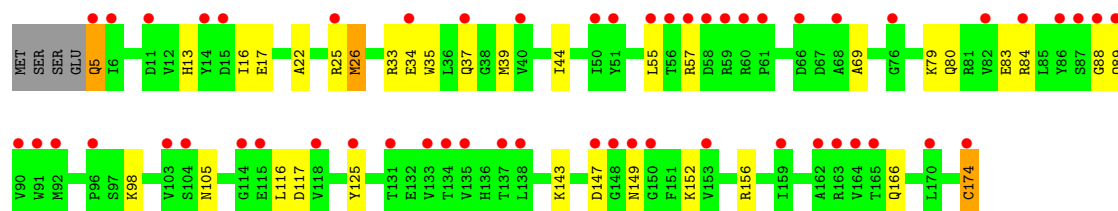
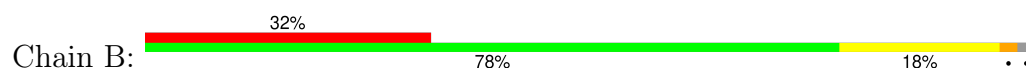


• Molecule 1: Biphenyl 2,3-Dioxygenase Alpha Subunit

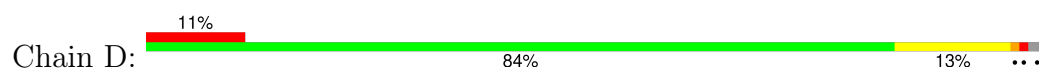




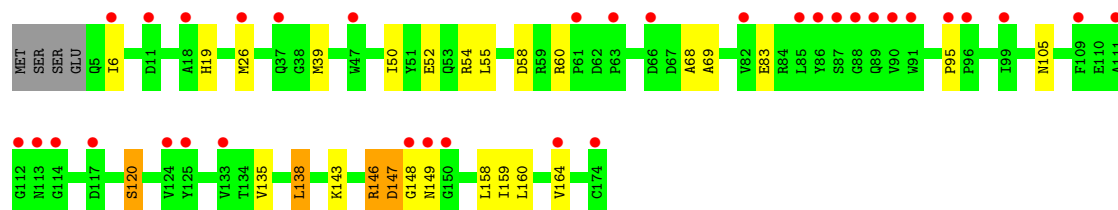
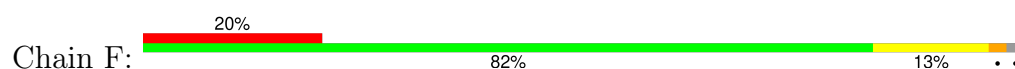
● Molecule 2: Biphenyl 2,3-Dioxygenase Beta Subunit



● 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	134.96Å 134.96Å 219.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.80 – 1.70 19.80 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (19.80-1.70) 95.2 (19.80-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188 , 0.228 0.199 , 0.237	Depositor DCC
R_{free} test set	12180 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17030	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OXY, FES, FE

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	0.96	1/3677 (0.0%)	0.91	0/4990
1	C	0.95	0/3661	0.94	1/4967 (0.0%)
1	E	0.84	0/3692	0.88	2/5010 (0.0%)
2	B	1.01	4/1487 (0.3%)	0.93	0/2009
2	D	0.94	0/1493	0.90	0/2017
2	F	0.93	1/1471 (0.1%)	0.90	1/1989 (0.1%)
All	All	0.93	6/15481 (0.0%)	0.91	4/20982 (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
2	D	0	1
2	F	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	164	VAL	CA-CB	-6.20	1.47	1.54
2	B	26[A]	MET	N-CA	-5.79	1.39	1.46
2	B	26[B]	MET	N-CA	-5.79	1.39	1.46
1	A	90	ALA	CA-CB	-5.41	1.44	1.53
2	B	174	CYS	C-OXT	-5.27	1.13	1.23
2	B	44	ILE	CA-CB	5.20	1.59	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	6	ILE	N-CA-C	6.90	114.38	107.55
1	E	101	ASN	N-CA-C	5.57	119.70	113.02
1	C	232	ASP	N-CA-C	5.45	119.67	113.19
1	E	232	ASP	N-CA-C	5.31	119.24	112.34

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	87	SER	Peptide
2	F	147	ASP	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	28	0
1	C	3553	0	3360	31	0
1	E	3578	0	3379	37	0
2	B	1446	0	1400	36	0
2	D	1449	0	1405	28	0
2	F	1436	0	1382	20	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	1	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
5	E	2	0	0	0	0
6	A	502	0	0	7	0
6	B	250	0	0	7	0
6	C	441	0	0	5	0
6	D	232	0	0	4	0
6	E	354	0	0	8	0
6	F	199	0	0	3	0
All	All	17030	0	14294	158	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 5.

All (158) 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)
2:D:26[B]:MET:SD	2:D:39[B]:MET:CE	2.31	1.19
2:F:146:ARG:HH11	2:F:146:ARG:HG2	1.19	1.03
2:B:26[A]:MET:HG3	2:B:39[A]:MET:CE	1.91	1.00
2:D:26[B]:MET:SD	2:D:39[B]:MET:HE3	2.02	0.99
2:B:26[A]:MET:HG3	2:B:39[A]:MET:HE1	1.46	0.97
1:C:233:ILE:N	1:C:233:ILE:HD12	1.80	0.96
1:E:241:GLN:CG	1:E:403:SER:O	2.15	0.95
2:B:35:TRP:HD1	2:B:39[A]:MET:HE3	1.34	0.93
2:B:26[B]:MET:HE1	2:B:35:TRP:N	1.85	0.92
2:D:26[B]:MET:SD	2:D:39[B]:MET:HE1	2.13	0.88
1:C:232:ASP:OD1	1:C:233:ILE:CD1	2.27	0.83
1:E:241:GLN:CD	1:E:403:SER:O	2.25	0.80
2:B:35:TRP:CD1	2:B:39[A]:MET:HE3	2.17	0.79
2:D:26[B]:MET:SD	2:D:39[B]:MET:SD	2.81	0.79
2:F:146:ARG:HH11	2:F:146:ARG:CG	1.95	0.79
1:A:214:ALA:CB	2:B:88:GLY:HA3	2.12	0.78
1:A:214:ALA:HB1	2:B:88:GLY:HA3	1.64	0.77
1:E:241:GLN:HG3	1:E:403:SER:O	1.82	0.77
1:C:156:SER:OG	1:C:158:GLU:HG2	1.85	0.76
2:B:26[A]:MET:HG3	2:B:39[A]:MET:HE2	1.68	0.76
2:B:26[B]:MET:HE1	2:B:34:GLU:C	2.10	0.76
1:A:285:GLU:HG2	1:A:395:VAL:HG11	1.70	0.73
1:C:233:ILE:N	1:C:233:ILE:CD1	2.50	0.73
2:D:86:TYR:C	2:D:87:SER:OG	2.31	0.72
6:E:667:HOH:O	2:F:55:LEU:HD12	1.89	0.71
1:C:232:ASP:OD1	1:C:233:ILE:HD11	1.89	0.71
1:C:232:ASP:OD1	1:C:233:ILE:HD12	1.91	0.71
1:A:85:ASN:HB2	6:A:790:HOH:O	1.89	0.70
2:F:146:ARG:HG2	2:F:146:ARG:NH1	2.00	0.69
2:F:159:ILE:N	2:F:159:ILE:HD12	2.07	0.69
1:C:232:ASP:C	1:C:233:ILE:HD12	2.16	0.69
2:B:26[A]:MET:HE3	6:B:274:HOH:O	1.92	0.69
6:A:801:HOH:O	2:B:55:LEU:HD12	1.92	0.68
1:C:234:PRO:O	1:C:238:LEU:HD13	1.94	0.68
1:C:372:ARG:NH2	6:C:492:HOH:O	2.26	0.68
1:C:6:THR:N	6:C:773:HOH:O	2.26	0.68
1:A:403:SER:O	6:A:678:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26[B]:MET:CE	2:B:35:TRP:N	2.59	0.66
2:B:26[A]:MET:CG	2:B:39[A]:MET:HE1	2.22	0.66
1:E:241:GLN:NE2	1:E:403:SER:O	2.29	0.66
2:F:120:SER:HB2	6:F:188:HOH:O	1.97	0.65
1:E:443:ARG:HD3	6:E:682:HOH:O	1.97	0.64
2:D:26[B]:MET:HE1	2:D:35:TRP:N	2.13	0.63
1:C:223:LEU:HD11	1:C:256:ALA:HB1	1.80	0.63
1:E:241:GLN:HE21	1:E:403:SER:H	1.45	0.63
2:F:26:MET:SD	2:F:39:MET:SD	2.99	0.61
2:B:98:LYS:NZ	6:B:353:HOH:O	2.30	0.61
1:E:229:ASN:ND2	6:E:519:HOH:O	2.25	0.61
2:D:145:ARG:HD2	6:D:316:HOH:O	2.00	0.60
2:D:43:ASP:OD1	2:D:145:ARG:NH2	2.34	0.60
2:B:33:ARG:O	2:B:37:GLN:HG3	2.02	0.59
1:C:277:GLU:OE2	1:C:281[A]:LYS:HE2	2.01	0.59
2:D:88:GLY:HA2	6:D:344:HOH:O	2.01	0.59
1:E:234:PRO:O	1:E:238:LEU:HD13	2.02	0.59
2:D:26[B]:MET:HE1	2:D:35:TRP:HA	1.85	0.58
1:C:218:GLN:HE22	2:D:83:GLU:HB2	1.68	0.58
2:D:26[B]:MET:CE	2:D:35:TRP:N	2.67	0.57
1:E:206:TYR:CG	1:E:385:MET:HE1	2.39	0.57
1:C:236:ASP:N	1:C:236:ASP:OD1	2.33	0.57
1:E:6:THR:HG22	6:E:687:HOH:O	2.02	0.57
2:D:86:TYR:C	2:D:87:SER:HG	2.10	0.57
2:D:26[B]:MET:HE1	2:D:34:GLU:C	2.29	0.56
1:A:277:GLU:OE2	1:A:281:LYS:HD2	2.06	0.56
2:F:19:HIS:CE1	2:F:39:MET:HE2	2.41	0.56
1:A:214:ALA:HB2	2:B:88:GLY:HA3	1.86	0.56
1:E:444:ASN:ND2	6:E:710:HOH:O	2.38	0.56
2:D:145:ARG:CD	6:D:316:HOH:O	2.54	0.56
1:E:285:GLU:HG2	1:E:395:VAL:HG11	1.88	0.55
2:F:50:ILE:HD12	2:F:68:ALA:HB1	1.88	0.55
1:A:369:TYR:OH	6:A:624:HOH:O	2.15	0.55
1:A:317:ARG:NH2	6:A:738:HOH:O	2.38	0.55
2:D:26[B]:MET:HE1	2:D:35:TRP:CA	2.37	0.54
1:E:347:ILE:HG21	2:F:69:ALA:O	2.08	0.54
1:E:175:ALA:HB1	1:E:277[A]:GLU:HG3	1.89	0.54
2:F:146:ARG:CG	2:F:146:ARG:NH1	2.62	0.54
1:E:175:ALA:CB	1:E:277[A]:GLU:HG3	2.37	0.54
1:C:230:ARG:HG3	1:C:233:ILE:CD1	2.38	0.53
1:A:233:ILE:O	1:C:121:ARG:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:GLN:N	6:B:377:HOH:O	2.43	0.52
1:C:49:LYS:NZ	6:C:745:HOH:O	2.43	0.52
2:F:138:LEU:HD23	2:F:138:LEU:N	2.25	0.52
1:C:235:PHE:HA	1:C:238:LEU:HD22	1.91	0.52
1:E:250:PHE:CE2	1:E:252:VAL:CG2	2.93	0.51
2:F:58:ASP:OD1	2:F:60:ARG:HD3	2.11	0.51
1:C:313:ILE:N	1:C:313:ILE:HD12	2.26	0.51
2:B:26[B]:MET:HE1	2:B:35:TRP:CA	2.41	0.50
1:E:218:GLN:NE2	2:F:83:GLU:HB2	2.27	0.50
2:B:25:ARG:HD3	2:D:107:GLU:OE1	2.11	0.50
1:A:206:TYR:CG	1:A:385:MET:HE1	2.47	0.50
1:A:347:ILE:HG21	2:B:69:ALA:O	2.12	0.50
1:A:206:TYR:CD2	1:A:385:MET:HE1	2.47	0.50
2:B:166:GLN:NE2	6:B:359:HOH:O	2.45	0.50
1:E:235:PHE:O	1:E:238:LEU:HB2	2.12	0.49
1:E:191:GLN:OE1	1:E:321:GLU:OE2	2.31	0.49
1:A:218:GLN:O	1:A:218:GLN:HG3	2.11	0.49
1:C:347:ILE:HG21	2:D:69:ALA:O	2.13	0.49
1:E:206:TYR:CD1	1:E:385:MET:HE1	2.48	0.49
1:E:175:ALA:HB2	1:E:274:THR:HB	1.94	0.49
2:B:79:LYS:HE3	6:B:417:HOH:O	2.13	0.48
2:F:147:ASP:O	2:F:148:GLY:C	2.56	0.48
2:B:25:ARG:CZ	6:B:274:HOH:O	2.61	0.48
2:D:147:ASP:OD2	2:D:152:LYS:NZ	2.31	0.48
1:A:430:LYS:CD	6:A:803:HOH:O	2.61	0.48
2:D:84:ARG:HD3	2:D:171:TYR:CZ	2.49	0.47
2:D:125:TYR:OH	2:F:135:VAL:HG11	2.14	0.47
2:F:146:ARG:NH1	6:F:306:HOH:O	2.46	0.47
1:C:230:ARG:HG3	1:C:233:ILE:HD11	1.95	0.47
1:E:264:ARG:HD2	1:E:268:THR:HG21	1.95	0.47
1:A:85:ASN:HD22	1:E:366:SER:HB3	1.80	0.47
1:A:214:ALA:CB	2:B:88:GLY:CA	2.89	0.47
1:C:218:GLN:NE2	2:D:83:GLU:HB2	2.30	0.47
2:D:15:ASP:OD2	6:D:342:HOH:O	2.21	0.47
1:C:385:MET:HE2	1:E:123:TYR:CE2	2.50	0.46
1:A:214:ALA:HB2	2:B:88:GLY:CA	2.45	0.46
1:A:85:ASN:ND2	1:E:366:SER:HB3	2.30	0.46
1:A:233:ILE:O	1:C:121:ARG:CD	2.64	0.46
1:E:232:ASP:CG	1:E:233:ILE:HG13	2.41	0.46
1:C:128:ASP:HB3	6:C:671:HOH:O	2.16	0.45
2:F:158:LEU:C	2:F:159:ILE:HD12	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:THR:OG1	1:E:412:GLY:HA3	2.16	0.45
1:C:237:ASP:C	1:C:238:LEU:HD12	2.42	0.45
1:A:309:ASN:HB3	1:A:329:ILE:O	2.18	0.44
1:E:103:HIS:HB2	4:E:455:FES:S1	2.58	0.44
2:D:26[B]:MET:CE	2:D:35:TRP:CA	2.96	0.44
1:A:218:GLN:HE22	2:B:83:GLU:HB2	1.83	0.43
2:B:16:ILE:HD11	2:B:116:LEU:HD13	1.99	0.43
2:F:52:GLU:HG3	2:F:54:ARG:HG3	2.00	0.43
1:E:250:PHE:HE2	1:E:252:VAL:CG2	2.30	0.43
1:E:443:ARG:CD	6:E:682:HOH:O	2.63	0.43
1:E:219:ILE:HD11	6:E:745:HOH:O	2.19	0.43
2:B:13:HIS:HE1	2:B:17:GLU:OE2	2.02	0.43
2:D:43:ASP:CG	2:D:145:ARG:HH22	2.23	0.43
2:D:50:ILE:HD12	2:D:68:ALA:HB1	2.01	0.42
1:A:262:ILE:HD12	2:B:80:GLN:NE2	2.34	0.42
1:A:371:ASN:HB3	1:A:377:ARG:HB3	2.02	0.42
2:B:22:ALA:O	2:B:26[A]:MET:HG2	2.18	0.42
2:B:156:ARG:NH1	2:B:174:CYS:O	2.52	0.42
1:C:230:ARG:HG3	1:C:233:ILE:HD13	2.01	0.42
1:A:36:ARG:HG2	1:A:426:TRP:NE1	2.34	0.42
1:A:84:GLY:O	1:E:370:ILE:HG21	2.19	0.42
1:E:40:MET:CE	1:E:147:PHE:CZ	3.02	0.42
1:C:309:ASN:HB3	1:C:329:ILE:O	2.20	0.42
1:C:435:THR:O	1:C:435:THR:OG1	2.32	0.42
2:B:117:ASP:OD1	2:B:143:LYS:HE3	2.19	0.41
2:D:26[B]:MET:CE	2:D:35:TRP:HA	2.50	0.41
1:C:384:THR:O	1:C:387:VAL:HG22	2.21	0.41
1:E:68:GLN:HB2	1:E:70:ASP:OD1	2.21	0.41
2:B:125:TYR:OH	2:D:135:VAL:HG11	2.20	0.41
1:E:423:ALA:HA	1:E:424:PRO:HD3	1.94	0.41
2:B:37:GLN:NE2	6:B:366:HOH:O	2.53	0.41
2:B:147:ASP:OD2	2:B:152:LYS:HE3	2.21	0.41
1:E:236:ASP:HB3	1:E:402:ILE:CD1	2.51	0.41
1:A:6:THR:HG22	6:A:822:HOH:O	2.20	0.40
1:A:265:GLU:O	1:A:269:LYS:HG3	2.21	0.40
2:B:83:GLU:O	2:B:84:ARG:C	2.61	0.40
1:E:163:GLU:OE1	6:E:527:HOH:O	2.21	0.40
1:C:435:THR:HG23	6:C:775:HOH:O	2.20	0.40
2:F:95:PRO:HD3	6:F:326:HOH:O	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%)	434 (97%)	14 (3%)	0	100	100
1	C	445/454 (98%)	427 (96%)	18 (4%)	0	100	100
1	E	450/454 (99%)	433 (96%)	16 (4%)	1 (0%)	43	28
2	B	170/174 (98%)	166 (98%)	4 (2%)	0	100	100
2	D	171/174 (98%)	166 (97%)	4 (2%)	1 (1%)	21	9
2	F	168/174 (97%)	164 (98%)	4 (2%)	0	100	100
All	All	1852/1884 (98%)	1790 (97%)	60 (3%)	2 (0%)	48	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	88	GLY
1	E	203	GLY

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%)	363 (98%)	9 (2%)	43	26
1	C	371/375 (99%)	361 (97%)	10 (3%)	39	23
1	E	374/375 (100%)	370 (99%)	4 (1%)	65	54
2	B	155/157 (99%)	150 (97%)	5 (3%)	34	17
2	D	156/157 (99%)	152 (97%)	4 (3%)	40	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	153/157 (98%)	146 (95%)	7 (5%)	24 9
All	All	1581/1596 (99%)	1542 (98%)	39 (2%)	43 24

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	VAL
1	A	216	LEU
1	A	218	GLN
1	A	238	LEU
1	A	281	LYS
1	A	285	GLU
1	A	434	ASP
1	A	449	LYS
1	A	454	GLU
2	B	5	GLN
2	B	57	ARG
2	B	89	GLN
2	B	105	ASN
2	B	149	ASN
1	C	6	THR
1	C	85	ASN
1	C	116	VAL
1	C	129	LYS
1	C	222	GLU
1	C	233	ILE
1	C	238	LEU
1	C	264	ARG
1	C	267	TRP
1	C	372	ARG
2	D	5	GLN
2	D	36	LEU
2	D	87	SER
2	D	105	ASN
1	E	196	VAL
1	E	277[A]	GLU
1	E	277[B]	GLU
1	E	403	SER
2	F	105	ASN
2	F	120	SER
2	F	138	LEU
2	F	143	LYS

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Mol	Chain	Res	Type
2	F	146	ARG
2	F	149	ASN
2	F	160	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	109	GLN
1	A	124	HIS
1	A	125	ASN
1	A	218	GLN
2	B	5	GLN
2	B	13	HIS
2	B	31	GLN
2	B	80	GLN
2	B	89	GLN
2	B	127	ASN
2	B	166	GLN
1	C	101	ASN
1	C	200	ASN
1	C	218	GLN
2	D	5	GLN
2	D	13	HIS
2	D	166	GLN
1	E	12	ASN
1	E	200	ASN
1	E	241	GLN
1	E	246	HIS
1	E	444	ASN
2	F	13	HIS
2	F	89	GLN
2	F	166	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	OXY	E	457	3	1,1,1	0.22	0	-		
4	FES	A	455	1	0,4,4	-	-	-		
5	OXY	A	457	3	1,1,1	0.15	0	-		
4	FES	E	455	1	0,4,4	-	-	-		
5	OXY	C	457	3	1,1,1	0.17	0	-		
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
4	FES	C	455	1	-	-	0/1/1/1
4	FES	A	455	1	-	-	0/1/1/1
4	FES	E	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	455	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	449/454 (98%)	1.52	93 (20%) 2 2	26, 41, 56, 77	1 (0%)
1	C	446/454 (98%)	1.08	43 (9%) 13 14	21, 29, 45, 54	1 (0%)
1	E	449/454 (98%)	1.62	125 (27%) 1 1	19, 33, 56, 68	3 (0%)
2	B	170/174 (97%)	1.79	55 (32%) 1 1	25, 42, 55, 67	2 (1%)
2	D	170/174 (97%)	1.02	20 (11%) 9 9	17, 29, 41, 52	3 (1%)
2	F	170/174 (97%)	1.36	34 (20%) 3 2	26, 32, 47, 57	0
All	All	1854/1884 (98%)	1.40	370 (19%) 3 2	17, 35, 51, 77	10 (0%)

All (370) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	453	ALA	7.5
1	C	231	ALA	7.1
1	A	453	ALA	6.9
2	F	86	TYR	6.2
1	C	235	PHE	6.2
1	C	450	LEU	5.8
1	C	237	ASP	5.0
2	B	149	ASN	5.0
1	C	234	PRO	4.9
1	A	228	GLY	4.7
1	E	232	ASP	4.6
1	E	237	ASP	4.6
2	B	87	SER	4.6
1	C	238	LEU	4.6
1	E	233	ILE	4.6
2	D	86	TYR	4.6
1	A	404	PHE	4.5
1	A	235	PHE	4.4
1	A	452	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	232	ASP	4.4
2	F	149	ASN	4.4
1	A	233	ILE	4.4
2	B	133	VAL	4.3
2	F	88	GLY	4.1
1	E	235	PHE	4.1
2	B	6	ILE	4.1
2	B	125	TYR	4.0
1	E	431	ALA	4.0
1	E	450	LEU	3.9
2	B	91	TRP	3.9
1	E	236	ASP	3.9
1	E	224	ALA	3.9
1	E	85	ASN	3.9
2	B	174	CYS	3.9
1	E	403	SER	3.8
1	E	220	GLY	3.8
2	B	164	VAL	3.8
1	E	404	PHE	3.8
1	C	233	ILE	3.8
1	A	224	ALA	3.7
2	D	87	SER	3.7
2	F	148	GLY	3.7
1	A	219	ILE	3.7
1	A	236	ASP	3.6
2	B	86	TYR	3.6
2	B	50	ILE	3.6
1	A	220	GLY	3.6
2	D	59	ARG	3.6
2	B	55	LEU	3.6
1	A	234	PRO	3.5
1	E	218	GLN	3.5
1	C	236	ASP	3.4
1	C	217	SER	3.4
2	F	91	TRP	3.4
1	E	118	LEU	3.4
2	B	56	THR	3.4
2	F	125	TYR	3.4
1	E	447	ASN	3.4
1	C	222	GLU	3.3
1	E	282	PHE	3.3
1	A	230	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	279	ARG	3.3
1	E	262	ILE	3.3
1	C	441	PRO	3.3
1	E	452	ALA	3.3
1	C	451	ASN	3.3
2	B	114	GLY	3.3
1	E	190	LEU	3.3
1	A	238	LEU	3.2
1	A	232	ASP	3.2
1	A	422	ASP	3.2
1	E	454	GLU	3.2
2	F	113	ASN	3.2
1	E	238	LEU	3.2
1	E	446	TRP	3.2
2	D	88	GLY	3.2
2	B	58	ASP	3.2
1	E	82	HIS	3.2
1	A	116	VAL	3.2
1	E	370	ILE	3.1
2	B	162	ALA	3.1
1	A	426	TRP	3.1
1	E	172	TRP	3.1
2	F	87	SER	3.1
1	E	373	GLY	3.1
1	E	337	ALA	3.1
2	B	84	ARG	3.0
1	A	216	LEU	3.0
1	E	45	SER	3.0
2	B	135	VAL	3.0
2	F	82	VAL	3.0
1	A	105	TRP	3.0
1	A	335	ASP	3.0
1	E	100	CYS	3.0
1	E	276	GLY	3.0
1	A	454	GLU	3.0
2	B	147	ASP	3.0
1	A	134	ALA	3.0
2	B	5	GLN	3.0
1	A	222	GLU	3.0
1	E	101	ASN	3.0
2	B	82	VAL	2.9
2	F	18	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	80	CYS	2.9
1	E	84	GLY	2.9
1	E	283	GLY	2.9
1	E	374	VAL	2.9
1	E	227	ALA	2.9
1	A	223	LEU	2.9
1	C	262	ILE	2.9
2	D	174	CYS	2.9
1	A	429	VAL	2.9
1	E	439	VAL	2.9
1	E	375	ILE	2.9
2	F	61	PRO	2.9
1	E	105	TRP	2.9
1	E	376	THR	2.8
1	A	231	ALA	2.8
1	E	228	GLY	2.8
2	B	150	GLY	2.8
2	F	174	CYS	2.8
2	D	91	TRP	2.8
1	C	158	GLU	2.8
1	E	215	ALA	2.8
2	F	112	GLY	2.8
1	E	182	LEU	2.8
1	E	223	LEU	2.8
1	A	444	ASN	2.8
2	B	37	GLN	2.8
2	F	150	GLY	2.8
1	E	188	SER	2.8
1	E	214	ALA	2.8
1	A	120	SER	2.8
1	A	403	SER	2.8
2	D	5	GLN	2.7
1	A	441	PRO	2.7
2	F	26	MET	2.7
1	E	369	TYR	2.7
1	A	434	ASP	2.7
1	C	402	ILE	2.7
1	E	208	VAL	2.7
2	F	90	VAL	2.7
1	E	192	CYS	2.7
2	B	57	ARG	2.7
1	C	403	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	262	ILE	2.7
1	E	87	ILE	2.7
1	E	219	ILE	2.7
2	F	6	ILE	2.7
1	A	221	GLY	2.7
2	B	76	GLY	2.7
1	E	442	ASN	2.7
1	C	353	ALA	2.7
2	D	80	GLN	2.7
2	B	170	LEU	2.7
2	B	14	TYR	2.7
1	A	281	LYS	2.7
2	D	96	PRO	2.6
2	B	89	GLN	2.6
1	E	444	ASN	2.6
2	B	90	VAL	2.6
2	F	133	VAL	2.6
2	F	47	TRP	2.6
1	E	434	ASP	2.6
1	E	23	GLU	2.6
2	B	68	ALA	2.6
1	E	430	LYS	2.6
2	B	138	LEU	2.6
1	E	63	VAL	2.6
2	B	40	VAL	2.6
1	A	30	ILE	2.6
1	A	272	GLU	2.6
2	D	56	THR	2.6
2	F	66	ASP	2.6
2	F	117	ASP	2.6
1	A	100	CYS	2.6
1	A	218	GLN	2.6
2	F	164	VAL	2.6
1	E	212	HIS	2.5
2	F	85	LEU	2.5
1	A	229	ASN	2.5
1	E	378	ASN	2.5
1	A	448	GLU	2.5
1	C	23	GLU	2.5
1	E	355	THR	2.5
2	D	85	LEU	2.5
1	A	395	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	37	GLN	2.5
1	A	33	ILE	2.5
1	E	77	ILE	2.5
2	B	59	ARG	2.5
1	A	38	TRP	2.5
1	C	105	TRP	2.5
1	C	218	GLN	2.5
1	A	445	PHE	2.5
1	E	127	LEU	2.5
1	E	270	PHE	2.5
1	A	227	ALA	2.5
2	F	95	PRO	2.5
1	E	278	VAL	2.5
2	B	148	GLY	2.5
1	A	31	GLU	2.5
1	E	128	ASP	2.4
1	A	28	LEU	2.4
1	A	282	PHE	2.4
2	B	60	ARG	2.4
1	E	324	VAL	2.4
1	E	229	ASN	2.4
2	F	11	ASP	2.4
1	A	269	LYS	2.4
2	B	25	ARG	2.4
1	A	82	HIS	2.4
1	E	103	HIS	2.4
1	A	149	CYS	2.4
1	A	21	TRP	2.4
1	A	127	LEU	2.4
1	C	379	GLY	2.4
1	E	234	PRO	2.4
1	A	389	TYR	2.4
2	B	51	TYR	2.4
1	A	387	VAL	2.4
1	E	139	VAL	2.4
2	B	118	VAL	2.4
1	E	217	SER	2.4
1	E	365	SER	2.4
1	A	450	LEU	2.4
2	D	22	ALA	2.4
1	E	210	TRP	2.4
1	C	265	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	395	VAL	2.4
1	E	341	MET	2.4
1	E	71	GLY	2.3
2	B	88	GLY	2.3
1	E	284	PRO	2.3
1	E	133	ALA	2.3
1	A	436	TRP	2.3
1	E	142	TYR	2.3
1	E	267	TRP	2.3
1	A	208	VAL	2.3
1	A	85	ASN	2.3
2	D	149	ASN	2.3
1	A	178	GLY	2.3
2	F	114	GLY	2.3
1	E	441	PRO	2.3
2	B	61	PRO	2.3
2	D	98	LYS	2.3
2	F	96	PRO	2.3
1	E	55	THR	2.3
2	B	134	THR	2.3
1	E	154	ALA	2.3
1	A	113	LEU	2.3
1	E	356	LEU	2.3
2	D	55	LEU	2.3
2	B	159	ILE	2.3
1	E	117	PRO	2.3
1	C	6	THR	2.3
1	C	80	CYS	2.3
2	F	111	ALA	2.3
1	E	440	PHE	2.3
1	E	102	TYR	2.3
1	E	166	TYR	2.3
1	A	22	ASP	2.3
2	D	150	GLY	2.3
1	A	114	VAL	2.3
1	A	137	VAL	2.3
2	F	63	PRO	2.2
1	A	6	THR	2.2
1	E	80	CYS	2.2
1	C	444	ASN	2.2
1	A	182	LEU	2.2
2	D	148	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	261	HIS	2.2
1	C	374	VAL	2.2
1	E	114	VAL	2.2
1	E	116	VAL	2.2
2	B	153	VAL	2.2
1	A	72	THR	2.2
1	C	280	ARG	2.2
1	E	6	THR	2.2
1	E	274	THR	2.2
1	E	328	THR	2.2
2	B	131	THR	2.2
2	B	137	THR	2.2
1	C	210	TRP	2.2
1	E	21	TRP	2.2
1	E	436	TRP	2.2
1	E	451	ASN	2.2
1	C	227	ALA	2.2
2	D	66	ASP	2.2
1	C	220	GLY	2.2
1	E	221	GLY	2.2
1	E	266	GLY	2.2
1	E	357	GLU	2.2
1	A	76	PHE	2.2
1	A	270	PHE	2.2
1	C	82	HIS	2.2
1	E	347	ILE	2.2
1	E	443	ARG	2.2
2	F	99	ILE	2.2
2	B	165	THR	2.2
1	A	430	LYS	2.2
1	A	128	ASP	2.2
1	C	337	ALA	2.2
1	E	27	ALA	2.2
1	E	90	ALA	2.2
1	E	258	ALA	2.2
2	B	15	ASP	2.2
2	B	66	ASP	2.2
2	D	111	ALA	2.2
1	A	172	TRP	2.2
1	E	178	GLY	2.2
2	B	163	ARG	2.2
1	A	432	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	49	LYS	2.2
1	A	146	ILE	2.2
2	B	96	PRO	2.2
1	A	126	SER	2.2
2	B	92	MET	2.1
1	E	353	ALA	2.1
1	C	361	GLY	2.1
1	C	388	GLY	2.1
2	B	104	SER	2.1
1	E	316	PRO	2.1
2	F	109	PHE	2.1
2	F	89	GLN	2.1
1	E	402	ILE	2.1
1	C	443	ARG	2.1
1	A	59	ALA	2.1
1	A	63	VAL	2.1
1	C	154	ALA	2.1
1	E	25	VAL	2.1
1	A	447	ASN	2.1
1	A	217	SER	2.1
1	A	359	ASP	2.1
1	C	335	ASP	2.1
1	E	72	THR	2.1
1	A	57	TYR	2.1
1	E	322	ILE	2.1
1	E	19	VAL	2.1
2	B	34	GLU	2.1
1	E	126	SER	2.1
2	B	11	ASP	2.1
1	A	168	LEU	2.1
1	E	226	LEU	2.1
1	E	230	ARG	2.1
1	A	440	PHE	2.1
1	A	329	ILE	2.1
1	C	142	TYR	2.1
1	C	370	ILE	2.1
1	E	26	TYR	2.1
1	E	445	PHE	2.1
1	E	277[A]	GLU	2.0
1	A	106	VAL	2.0
1	A	324	VAL	2.0
1	C	106	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	103	VAL	2.0
1	C	131	LYS	2.0
1	A	23	GLU	2.0
1	E	31	GLU	2.0
2	B	115	GLU	2.0
1	A	101	ASN	2.0
1	A	386	GLY	2.0
1	E	78	ASN	2.0
1	E	379	GLY	2.0
2	D	37	GLN	2.0
1	E	313	ILE	2.0
1	A	198	ALA	2.0
1	A	156	SER	2.0
1	A	122	CYS	2.0
2	F	124	VAL	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	OXY	C	457	2/2	0.83	0.17	29,29,29,29	2
5	OXY	E	457	2/2	0.83	0.18	24,24,24,26	2
5	OXY	A	457	2/2	0.90	0.14	21,21,21,22	2
4	FES	A	455	4/4	0.99	0.06	37,38,38,39	0
4	FES	C	455	4/4	0.99	0.15	23,24,25,25	0
4	FES	E	455	4/4	0.99	0.18	28,29,29,30	0
3	FE	A	456	1/1	0.99	0.04	37,37,37,37	0
3	FE	C	456	1/1	0.99	0.16	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FE	E	456	1/1	0.99	0.15	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.