Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:16 AM GMT

PDB ID	:	2GBW
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)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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.
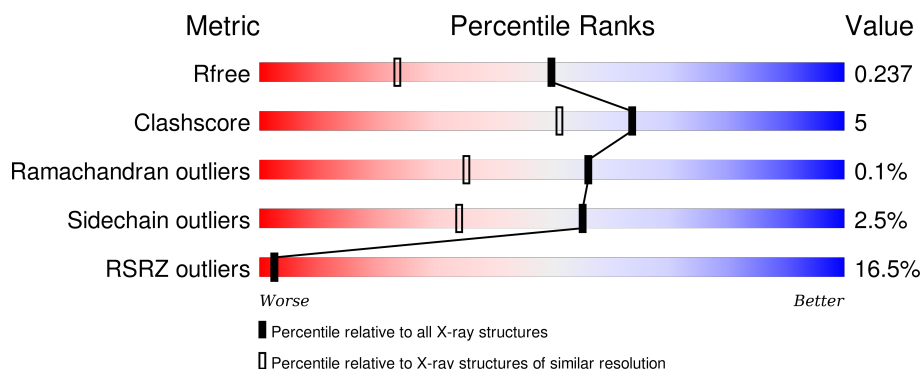
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	14% / 92% / 6% ••
1	C	454	15% / 90% / 7% •
1	E	454	21% / 89% / 9% ••
2	B	174	15% / 79% / 17% • •
2	D	174	14% / 83% / 13% •••

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Mol	Chain	Length	Quality of chain
2	F	174	16% ━━━━━━ 83% 11% ··

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	OXY	E	457	-	-	-	X

2 Entry composition (i)

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 (three-letter code: 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 (three-letter code: FES) (formula: Fe_2S_2).

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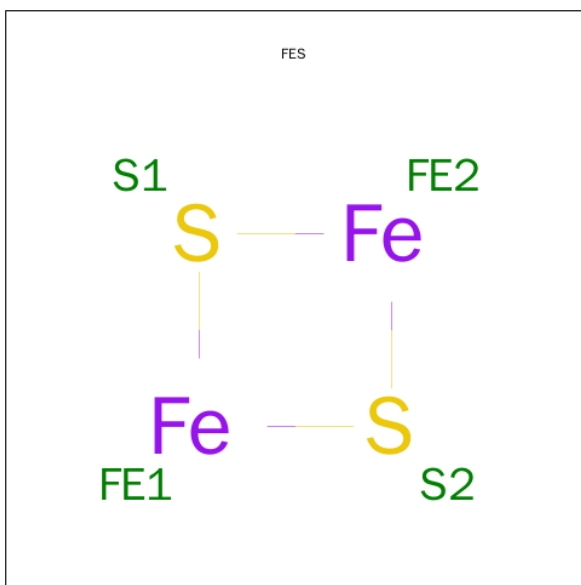
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	C	1	Total	Fe	S	0	0
			4	2	2		
4	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).

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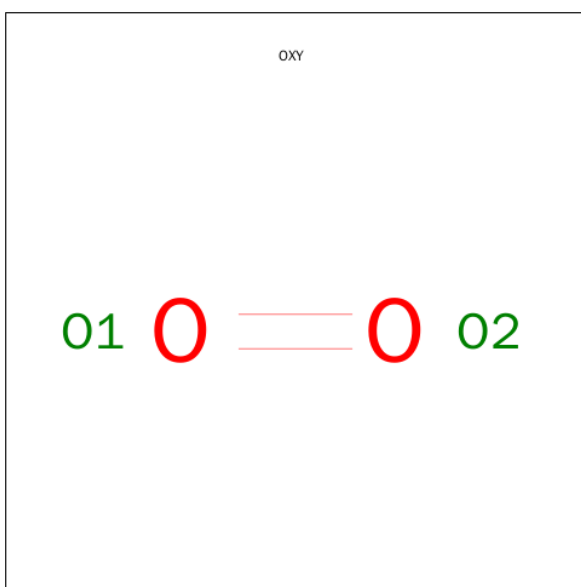
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			2	2		

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

- Molecule 6 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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
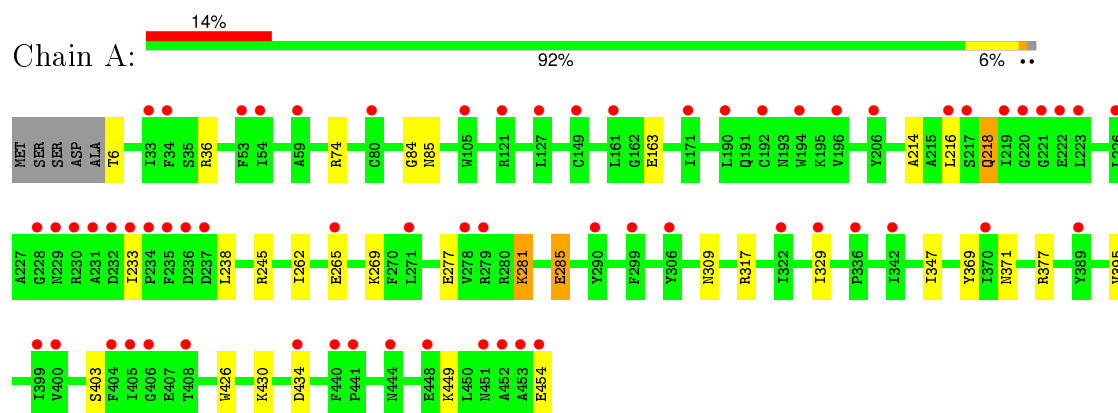
• Molecule 1: Biphenyl 2,3-Dioxygenase Alpha Subunit
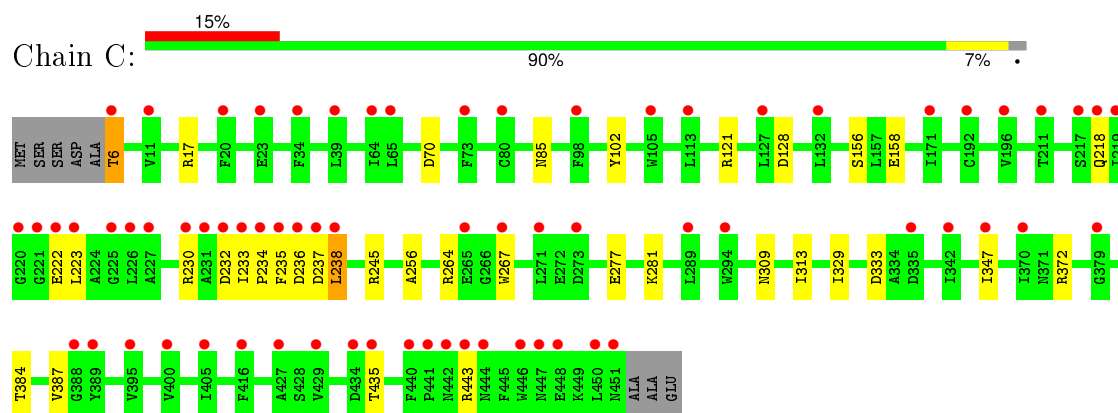
• Molecule 1: Biphenyl 2,3-Dioxygenase Alpha Subunit

• Molecule 2: Biphenyl 2,3-Dioxygenase Beta Subunit
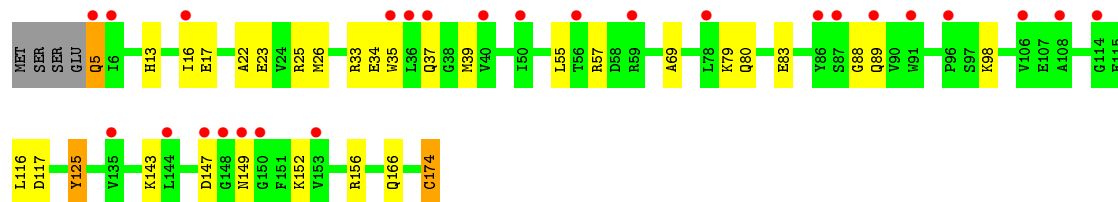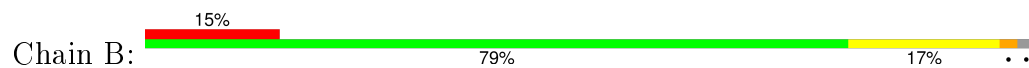
• Molecule 2: Biphenyl 2,3-Dioxygenase Beta Subunit
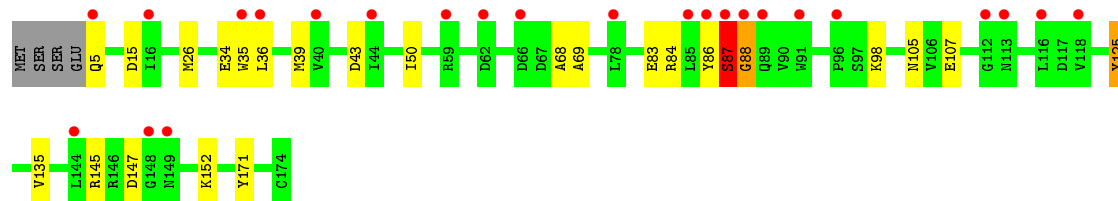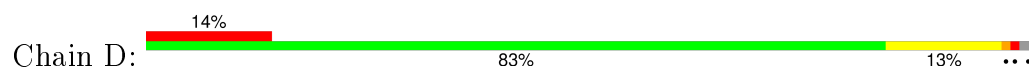
• Molecule 2: Biphenyl 2,3-Dioxygenase Beta Subunit
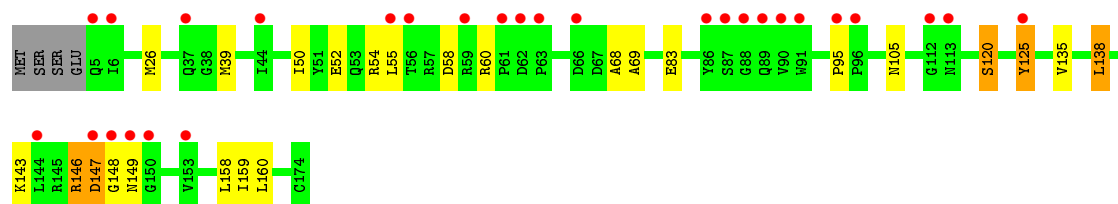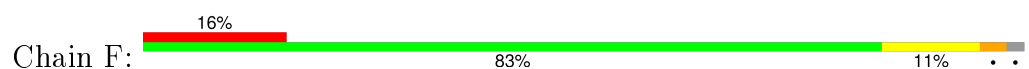
4 Data and refinement statistics (i)

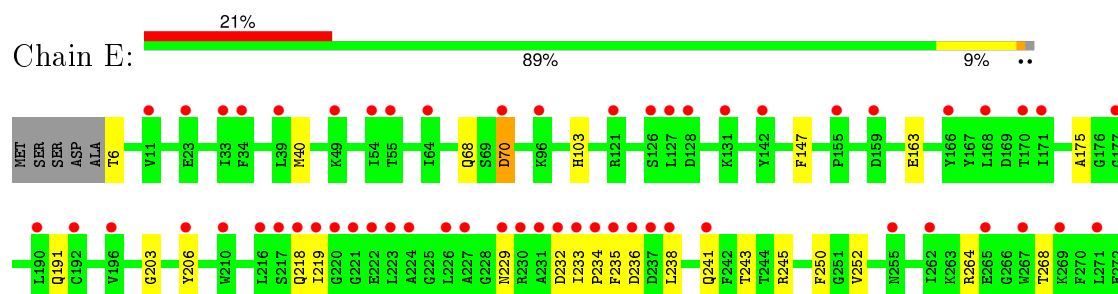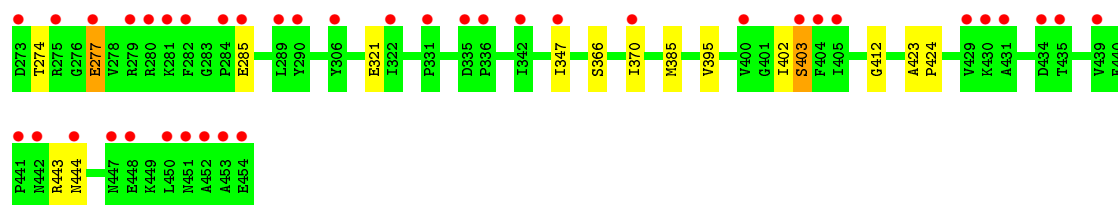| Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	134.96Å 134.96Å 219.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.80 – 1.70 19.79 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (19.80-1.70) 95.2 (19.79-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.228 0.199 , 0.237	Depositor DCC
R_{free} test set	12177 reflections (5.31%)	DCC
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 , 50.2	EDS
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
L-test for twinning [2]	$< |L| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Outliers	1 of 241427 reflections (0.000%)	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, OXY

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	0.80	1/3677 (0.0%)	0.76	2/4990 (0.0%)
1	C	0.81	0/3661	0.80	3/4967 (0.1%)
1	E	0.70	0/3692	0.72	0/5010
2	B	0.86	1/1487 (0.1%)	0.85	0/2009
2	D	0.82	0/1493	0.84	0/2017
2	F	0.80	1/1471 (0.1%)	0.86	0/1989
All	All	0.79	3/15481 (0.0%)	0.79	5/20982 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	GLU	CD-OE2	-5.51	1.19	1.25
2	F	125	TYR	CE1-CZ	-5.46	1.31	1.38
2	B	174	CYS	C-OXT	-5.44	1.13	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	70	ASP	CB-CG-OD1	7.42	124.98	118.30
1	A	74	ARG	NE-CZ-NH1	6.23	123.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	17	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	C	333	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	74	ARG	NE-CZ-NH2	-5.15	117.73	120.30

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 (i)

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	26	0
1	C	3553	0	3360	29	0
1	E	3578	0	3379	37	0
2	B	1446	0	1400	35	0
2	D	1449	0	1405	27	0
2	F	1436	0	1382	19	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	4	0
6	D	232	0	0	5	0
6	E	354	0	0	8	0
6	F	199	0	0	3	0
All	All	17030	0	14294	152	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 (152) 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:B:26[A]:MET:HG3	2:B:39[A]:MET:HE1	1.10	1.04
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
1:C:233:ILE:HD12	1:C:233:ILE:N	1.80	0.96
2:D:26[B]:MET:SD	2:D:39[B]:MET:HE1	2.05	0.96
1:E:241:GLN:CG	1:E:403:SER:O	2.15	0.95
2:D:26[B]:MET:SD	2:D:39[B]:MET:HE3	2.10	0.91
1:C:232:ASP:OD1	1:C:233:ILE:CD1	2.27	0.83
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:E:241:GLN:HG3	1:E:403:SER:O	1.82	0.77
1:A:214:ALA:HB1	2:B:88:GLY:HA3	1.64	0.77
1:C:156:SER:OG	1:C:158:GLU:HG2	1.85	0.76
1:E:241:GLN:CD	1:E:403:SER:O	2.25	0.75
1:C:233:ILE:CD1	1:C:233:ILE:N	2.50	0.73
1:A:285:GLU:HG2	1:A:395:VAL:HG11	1.70	0.73
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:NH1	2:F:146:ARG:HG2	2.00	0.69
2:F:159:ILE:HD12	2:F:159:ILE:N	2.07	0.69
2:B:26[A]:MET:HE3	6:B:274:HOH:O	1.91	0.69
1:C:234:PRO:O	1:C:238:LEU:HD13	1.94	0.68
6:A:801:HOH:O	2:B:55:LEU:HD12	1.92	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
2:D:86:TYR:C	2:D:87:SER:OG	2.31	0.67
2:B:26[B]:MET:HE2	2:B:35:TRP:N	2.08	0.67
2:B:26[B]:MET:CE	2:B:35:TRP:N	2.59	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:C:232:ASP:C	1:C:233:ILE:HD12	2.16	0.64
2:B:98:LYS:NZ	6:B:353:HOH:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26[B]:MET:HE2	2:D:35:TRP:N	2.13	0.64
1:E:443:ARG:HD3	6:E:682:HOH:O	1.97	0.64
1:E:241:GLN:HE21	1:E:403:SER:H	1.45	0.63
1:C:223:LEU:HD11	1:C:256:ALA:HB1	1.80	0.63
2:F:26:MET:SD	2:F:39:MET:SD	2.99	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:35:TRP:HA	2:B:39[A]:MET:HE2	1.84	0.60
1:E:206:TYR:CG	1:E:385:MET:HE1	2.37	0.59
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
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:6:THR:HG22	6:E:687:HOH:O	2.02	0.57
1:C:236:ASP:N	1:C:236:ASP:OD1	2.33	0.57
1:A:277:GLU:OE2	1:A:281:LYS:HD2	2.06	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:317:ARG:NH2	6:A:738:HOH:O	2.38	0.55
1:E:347:ILE:HG21	2:F:69:ALA:O	2.08	0.54
2:F:146:ARG:NH1	2:F:146:ARG:CG	2.62	0.54
1:E:175:ALA:HB1	1:E:277[A]:GLU:HG3	1.89	0.54
2:B:26[B]:MET:HE1	2:B:34:GLU:C	2.28	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
2:B:5:GLN:N	6:B:377:HOH:O	2.43	0.52
2:F:138:LEU:N	2:F:138:LEU:HD23	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
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:347:ILE:HG21	2:B:69:ALA:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:26[B]:MET:HE1	2:B:35:TRP:N	2.27	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
2:D:86:TYR:O	2:D:87:SER:OG	2.30	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: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
2:D:26[B]:MET:HE2	2:D:35:TRP:CA	2.44	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:B:35:TRP:HD1	2:B:39[A]:MET:CE	2.26	0.47
2:F:146:ARG:NH1	6:F:306:HOH:O	2.46	0.47
2:D:125:TYR:OH	2:F:135:VAL:HG11	2.14	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:E:40:MET:HE2	1:E:147:PHE:CZ	2.50	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:A:214:ALA:HB2	2:B:88:GLY:CA	2.45	0.46
1:A:369:TYR:OH	6:A:624:HOH:O	2.15	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
2:D:98:LYS:NZ	6:D:392:HOH:O	2.48	0.45
1:C:128:ASP:HB3	6:C:671:HOH:O	2.16	0.45
1:E:243:THR:OG1	1:E:412:GLY:HA3	2.16	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:147:ASP:O	2:F:148:GLY:C	2.56	0.43
2:F:52:GLU:HG3	2:F:54:ARG:HG3	2.00	0.43
1:E:443:ARG:CD	6:E:682:HOH:O	2.63	0.43
1:E:250:PHE:HE2	1:E:252:VAL:CG2	2.30	0.43
1:E:219:ILE:HD11	6:E:745:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:HIS:HE1	2:B:17:GLU:OE2	2.02	0.43
2:D:26[B]:MET:HE1	2:D:34:GLU:C	2.39	0.43
2:D:50:ILE:HD12	2:D:68:ALA:HB1	2.01	0.42
2:B:22:ALA:O	2:B:26[A]:MET:HG2	2.18	0.42
2:B:26[B]:MET:HE2	2:B:35:TRP:CA	2.48	0.42
1:A:262:ILE:HD12	2:B:80:GLN:NE2	2.34	0.42
2:B:156:ARG:NH1	2:B:174:CYS:O	2.52	0.42
1:A:371:ASN:HB3	1:A:377:ARG:HB3	2.02	0.42
1:C:230:ARG:HG3	1:C:233:ILE:HD13	2.01	0.42
1:E:40:MET:CE	1:E:147:PHE:CZ	3.02	0.42
1:A:84:GLY:O	1:E:370:ILE:HG21	2.19	0.42
1:A:36:ARG:HG2	1:A:426:TRP:NE1	2.34	0.42
2:B:23:GLU:HA	2:B:39[A]:MET:HE3	2.01	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:232:ASP:CG	1:E:233:ILE:HG13	2.41	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:E:206:TYR:CD2	1:E:385:MET:HE1	2.56	0.40
1:A:265:GLU:O	1:A:269:LYS:HG3	2.21	0.40
1:A:6:THR:HG22	6:A:822:HOH:O	2.20	0.40
2:F:158:LEU:C	2:F:159:ILE:HD12	2.41	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
1:C:237:ASP:C	1:C:238:LEU:HD12	2.42	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	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%)	52	32
2	B	170/174 (98%)	166 (98%)	4 (2%)	0	100	100
2	D	171/174 (98%)	166 (97%)	4 (2%)	1 (1%)	30	12
2	F	168/174 (97%)	164 (98%)	4 (2%)	0	100	100
All	All	1852/1884 (98%)	1790 (97%)	60 (3%)	2 (0%)	56	35

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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%)	57	36
1	C	371/375 (99%)	362 (98%)	9 (2%)	57	36
1	E	374/375 (100%)	369 (99%)	5 (1%)	76	62
2	B	155/157 (99%)	150 (97%)	5 (3%)	46	24
2	D	156/157 (99%)	151 (97%)	5 (3%)	46	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	153/157 (98%)	145 (95%)	8 (5%)	29	10
All	All	1581/1596 (99%)	1540 (97%)	41 (3%)	55	32

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LEU
1	A	218	GLN
1	A	238	LEU
1	A	245	ARG
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	125	TYR
2	B	149	ASN
1	C	6	THR
1	C	85	ASN
1	C	102	TYR
1	C	222	GLU
1	C	238	LEU
1	C	245	ARG
1	C	264	ARG
1	C	267	TRP
1	C	443	ARG
2	D	5	GLN
2	D	36	LEU
2	D	87	SER
2	D	105	ASN
2	D	125	TYR
1	E	70	ASP
1	E	245	ARG
1	E	277[A]	GLU
1	E	277[B]	GLU
1	E	403	SER
2	F	105	ASN
2	F	120	SER
2	F	125	TYR

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Mol	Chain	Res	Type
2	F	138	LEU
2	F	143	LYS
2	F	146	ARG
2	F	149	ASN
2	F	160	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	125	ASN
1	A	218	GLN
2	B	5	GLN
2	B	13	HIS
2	B	80	GLN
2	B	89	GLN
1	C	125	ASN
1	C	218	GLN
2	D	13	HIS
2	D	31	GLN
1	E	200	ASN
1	E	241	GLN
1	E	246	HIS
1	E	378	ASN

5.3.3　RNA (i)

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 carbohydrates 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	$\#|Z| > 2$
4	FES	A	455	1	0,4,4	0.00	-	0,4,4	0.00	-
5	OXY	A	457	3	1,1,1	0.29	0	0,0,0	0.00	-
4	FES	C	455	1	0,4,4	0.00	-	0,4,4	0.00	-
5	OXY	C	457	3	1,1,1	0.31	0	0,0,0	0.00	-
4	FES	E	455	1	0,4,4	0.00	-	0,4,4	0.00	-
5	OXY	E	457	3	1,1,1	0.37	0	0,0,0	0.00	-

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	A	455	1	-	0/0/4/4	0/1/1/1
5	OXY	A	457	3	-	0/0/0/0	0/0/0/0
4	FES	C	455	1	-	0/0/4/4	0/1/1/1
5	OXY	C	457	3	-	0/0/0/0	0/0/0/0
4	FES	E	455	1	-	0/0/4/4	0/1/1/1
5	OXY	E	457	3	-	0/0/0/0	0/0/0/0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	1.10	63 (14%)	4	4	30, 41, 56, 77	0
1	C	446/454 (98%)	1.07	69 (15%)	3	3	23, 29, 45, 54	0
1	E	449/454 (98%)	1.31	96 (21%)	1	1	26, 33, 56, 68	0
2	B	170/174 (97%)	1.07	26 (15%)	3	3	36, 42, 55, 67	0
2	D	170/174 (97%)	1.01	24 (14%)	4	4	24, 29, 41, 52	0
2	F	170/174 (97%)	1.19	28 (16%)	2	2	26, 32, 47, 57	0
All	All	1854/1884 (98%)	1.14	306 (16%)	2	2	23, 35, 51, 77	0

All (306) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	87	SER	11.1
1	E	453	ALA	10.9
2	D	87	SER	10.2
2	F	149	ASN	10.1
1	C	450	LEU	9.0
1	E	237	ASP	8.8
1	A	453	ALA	8.6
1	A	454	GLU	8.5
1	C	238	LEU	8.5
1	E	233	ILE	8.4
1	C	232	ASP	8.2
1	C	234	PRO	8.1
1	C	235	PHE	8.0
1	C	233	ILE	7.9
2	B	149	ASN	7.9
1	A	452	ALA	7.8
1	A	233	ILE	7.5
2	D	59	ARG	7.4
2	F	88	GLY	7.4

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Mol	Chain	Res	Type	RSRZ
1	C	237	ASP	7.3
1	E	454	GLU	7.3
2	F	6	ILE	7.2
2	F	148	GLY	7.0
1	E	450	LEU	6.9
2	B	5	GLN	6.7
1	E	452	ALA	6.6
2	F	59	ARG	6.6
2	F	86	TYR	6.5
1	E	234	PRO	6.4
1	E	230	ARG	6.4
1	E	431	ALA	6.3
1	E	232	ASP	6.3
1	E	235	PHE	6.2
1	E	220	GLY	6.2
1	A	234	PRO	6.1
1	C	231	ALA	6.1
1	A	232	ASP	5.8
1	E	236	ASP	5.7
1	E	218	GLN	5.6
1	A	219	ILE	5.6
1	E	434	ASP	5.4
2	B	59	ARG	5.3
1	C	230	ARG	5.3
1	E	219	ILE	5.2
1	E	171	ILE	5.1
1	E	238	LEU	5.0
2	F	91	TRP	5.0
1	A	223	LEU	4.8
2	D	5	GLN	4.8
1	C	444	ASN	4.7
2	D	112	GLY	4.7
2	B	6	ILE	4.7
2	B	86	TYR	4.7
1	E	451	ASN	4.7
1	A	235	PHE	4.7
2	D	88	GLY	4.7
2	B	148	GLY	4.6
1	A	230	ARG	4.6
1	A	451	ASN	4.6
1	C	451	ASN	4.5
1	E	231	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	226	LEU	4.4
1	C	236	ASP	4.4
1	A	221	GLY	4.4
1	A	231	ALA	4.3
1	C	6	THR	4.3
1	A	228	GLY	4.3
1	A	400	VAL	4.3
1	C	448	GLU	4.2
2	D	86	TYR	4.2
1	A	405	ILE	4.1
2	F	5	GLN	4.0
2	F	112	GLY	4.0
1	E	405	ILE	4.0
1	C	217	SER	4.0
1	C	222	GLU	4.0
1	C	221	GLY	3.9
1	A	448	GLU	3.9
1	E	222	GLU	3.9
1	E	279	ARG	3.9
2	F	113	ASN	3.9
2	B	89	GLN	3.8
1	E	221	GLY	3.8
1	C	443	ARG	3.8
1	E	282	PHE	3.8
1	E	444	ASN	3.8
1	E	430	LYS	3.7
1	A	226	LEU	3.7
2	B	147	ASP	3.6
1	C	289	LEU	3.6
2	B	56	THR	3.6
1	E	447	ASN	3.6
1	E	223	LEU	3.6
1	C	267	TRP	3.6
1	A	290	TYR	3.6
1	A	399	ILE	3.6
2	F	87	SER	3.5
1	A	434	ASP	3.5
2	D	149	ASN	3.5
2	B	40	VAL	3.5
2	B	150	GLY	3.4
1	E	441	PRO	3.4
1	E	335	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	434	ASP	3.4
2	F	150	GLY	3.4
2	D	113	ASN	3.4
1	A	194	TRP	3.4
1	E	127	LEU	3.3
1	A	236	ASP	3.3
1	E	229	ASN	3.3
1	E	336	PRO	3.3
1	A	222	GLU	3.3
2	D	148	GLY	3.3
1	E	284	PRO	3.2
2	F	62	ASP	3.2
2	D	144	LEU	3.2
2	F	37	GLN	3.2
1	A	53	PHE	3.2
1	A	237	ASP	3.2
2	D	40	VAL	3.2
1	A	322	ILE	3.2
1	E	128	ASP	3.2
1	C	447	ASN	3.2
1	C	219	ILE	3.2
1	E	442	ASN	3.1
1	E	206	TYR	3.1
2	D	16	ILE	3.1
2	D	91	TRP	3.1
1	E	280	ARG	3.1
1	A	370	ILE	3.0
1	A	127	LEU	3.0
2	B	144	LEU	3.0
1	C	441	PRO	3.0
2	D	96	PRO	3.0
1	E	217	SER	3.0
2	F	96	PRO	2.9
1	E	11	VAL	2.9
1	A	444	ASN	2.9
1	C	442	ASN	2.9
1	A	220	GLY	2.9
1	E	224	ALA	2.9
2	B	96	PRO	2.9
1	C	127	LEU	2.9
1	E	121	ARG	2.9
1	A	171	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	50	ILE	2.9
1	A	271	LEU	2.8
1	E	177	GLY	2.8
1	A	342	ILE	2.8
1	C	11	VAL	2.8
2	D	85	LEU	2.8
1	A	217	SER	2.8
1	A	440	PHE	2.8
2	B	114	GLY	2.8
1	E	404	PHE	2.8
1	A	441	PRO	2.8
1	C	405	ILE	2.8
2	F	144	LEU	2.8
1	A	265	GLU	2.8
2	F	95	PRO	2.8
1	E	370	ILE	2.7
2	F	44	ILE	2.7
1	C	226	LEU	2.7
1	E	168	LEU	2.7
1	E	70	ASP	2.7
1	E	192	CYS	2.7
1	C	171	ILE	2.7
1	E	170	THR	2.7
2	D	89	GLN	2.7
2	F	125	TYR	2.7
1	A	216	LEU	2.7
2	B	35	TRP	2.7
2	B	91	TRP	2.7
2	D	35	TRP	2.7
1	C	335	ASP	2.7
1	E	23	GLU	2.6
1	A	33	ILE	2.6
1	A	121	ARG	2.6
1	E	49	LYS	2.6
2	F	63	PRO	2.6
1	A	406	GLY	2.6
1	E	126	SER	2.6
2	F	147	ASP	2.6
1	E	255	ASN	2.6
1	C	342	ILE	2.6
2	D	62	ASP	2.6
1	E	448	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	262	ILE	2.6
1	C	388	GLY	2.6
1	E	39	LEU	2.6
1	E	227	ALA	2.5
1	E	429	VAL	2.5
1	E	271	LEU	2.5
1	E	196	VAL	2.5
1	A	279	ARG	2.5
1	E	273	ASP	2.5
1	C	113	LEU	2.5
1	A	306	TYR	2.5
1	E	269	LYS	2.5
1	E	281	LYS	2.5
2	F	61	PRO	2.5
1	C	400	VAL	2.5
1	C	65	LEU	2.5
1	E	347	ILE	2.5
1	E	400	VAL	2.5
1	C	435	THR	2.4
1	E	285	GLU	2.4
1	E	403	SER	2.4
1	C	132	LEU	2.4
2	B	16	ILE	2.4
1	A	389	TYR	2.4
1	C	20	PHE	2.4
1	E	267	TRP	2.4
2	F	90	VAL	2.4
1	E	190	LEU	2.4
1	E	306	TYR	2.4
1	C	105	TRP	2.4
1	C	225	GLY	2.4
2	D	118	VAL	2.4
1	E	216	LEU	2.3
1	C	370	ILE	2.3
1	E	439	VAL	2.3
2	F	153	VAL	2.3
1	C	223	LEU	2.3
2	D	36	LEU	2.3
1	E	342	ILE	2.3
1	C	389	TYR	2.3
2	B	108	ALA	2.3
1	C	220	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	347	ILE	2.3
1	E	265	GLU	2.3
1	A	408	THR	2.3
1	A	80	CYS	2.3
1	C	395	VAL	2.3
1	C	227	ALA	2.3
2	B	36	LEU	2.3
1	E	435	THR	2.3
2	B	106	VAL	2.3
1	E	277[A]	GLU	2.2
1	E	289	LEU	2.2
1	E	275	ARG	2.2
1	A	54	ILE	2.2
1	C	64	ILE	2.2
1	E	210	TRP	2.2
1	E	322	ILE	2.2
1	C	379	GLY	2.2
1	C	23	GLU	2.2
1	A	59	ALA	2.2
1	E	241	GLN	2.2
1	E	142	TYR	2.2
1	E	159	ASP	2.2
2	B	153	VAL	2.2
1	C	218	GLN	2.2
1	E	34	PHE	2.2
2	F	55	LEU	2.2
1	C	294	TRP	2.2
1	A	196	VAL	2.2
1	C	196	VAL	2.2
1	C	265	GLU	2.2
1	C	39	LEU	2.2
1	E	33	ILE	2.2
2	D	44	ILE	2.2
1	A	206	TYR	2.2
1	A	278	VAL	2.2
1	A	161	LEU	2.1
1	C	273	ASP	2.1
1	A	192	CYS	2.1
2	F	56	THR	2.1
1	A	34	PHE	2.1
1	C	192	CYS	2.1
1	A	229	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	429	VAL	2.1
1	C	211	THR	2.1
1	A	404	PHE	2.1
1	C	98	PHE	2.1
1	E	155	PRO	2.1
1	C	427	ALA	2.1
1	C	271	LEU	2.1
2	B	37	GLN	2.1
2	F	89	GLN	2.1
1	A	329	ILE	2.1
1	E	55	THR	2.1
2	F	66	ASP	2.1
1	E	331	PRO	2.1
1	C	34	PHE	2.1
1	E	54	ILE	2.1
1	E	64	ILE	2.1
1	A	336	PRO	2.0
1	E	96	LYS	2.0
1	E	131	LYS	2.0
2	B	135	VAL	2.0
1	E	166	TYR	2.0
1	E	290	TYR	2.0
2	D	66	ASP	2.0
1	C	416	PHE	2.0
1	C	440	PHE	2.0
1	A	190	LEU	2.0
2	B	78	LEU	2.0
2	D	78	LEU	2.0
1	A	105	TRP	2.0
1	C	446	TRP	2.0
1	A	149	CYS	2.0
1	C	80	CYS	2.0
1	A	299	PHE	2.0
1	C	73	PHE	2.0
2	D	116	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
5	OXY	E	457	2/2	0.98	0.17	2.14	24,24,24,26	2
5	OXY	C	457	2/2	0.93	0.16	1.77	29,29,29,29	2
4	FES	E	455	4/4	0.99	0.13	0.29	28,29,29,30	0
3	FE	C	456	1/1	1.00	0.13	-0.03	26,26,26,26	0
5	OXY	A	457	2/2	0.98	0.11	-0.81	21,21,21,22	2
4	FES	C	455	4/4	1.00	0.10	-1.40	23,24,25,25	0
3	FE	A	456	1/1	0.99	0.06	-3.24	37,37,37,37	0
4	FES	A	455	4/4	0.98	0.05	-3.86	37,38,38,39	0
3	FE	E	456	1/1	0.99	0.10	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.