



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:33 pm BST

PDB ID : 5AEU
Title : Crystal structure of II9 variant of Biphenyl dioxygenase from Burkholderia xenovorans LB400
Authors : Dhindwal, S.; Gomez-Gil, L.; Sylvestre, M.; Eltis, L.D.; Bolin, J.T.; Kumar, P.
Deposited on : 2015-01-10
Resolution : 2.49 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

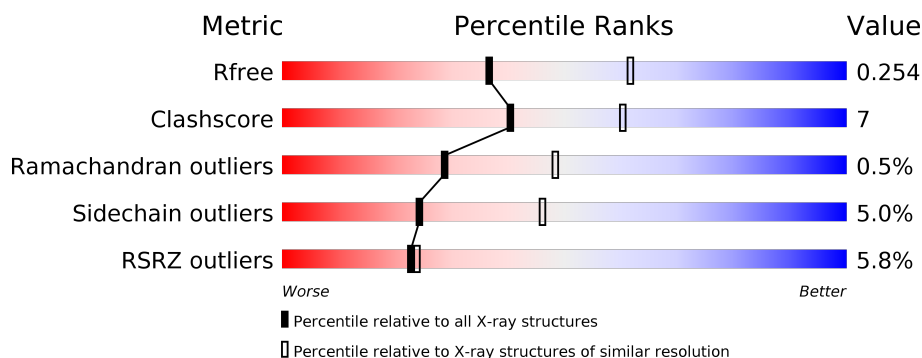
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	459	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>6%</div> </div> </div>
1	C	459	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>6%</div> </div> </div>
1	E	459	<div> <div>11%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>6%</div> </div> </div>
1	G	459	<div> <div>14%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>6%</div> </div> </div>
2	B	188	<div> <div></div> <div> <div></div> <div>86%</div> <div>11%</div> <div>• •</div> </div> </div>
2	D	188	<div> <div></div> <div> <div></div> <div>85%</div> <div>11%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	188	<div><div><div>2%</div><div></div><div>76%</div><div>20%</div><div></div><div>• •</div></div></div>
2	H	188	<div><div><div>2%</div><div></div><div>76%</div><div>21%</div><div></div><div>• •</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20136 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BIPHENYL DIOXYGENASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			
1	C	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			
1	E	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			
1	G	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			

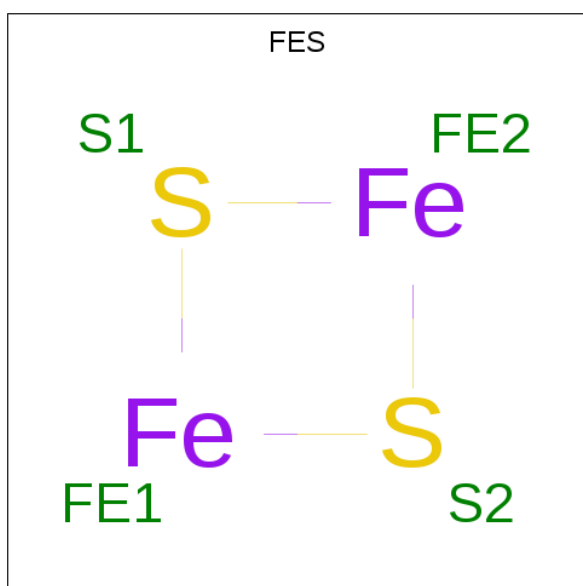
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	GLY	THR	engineered mutation	UNP P37333
A	336	ILE	PHE	engineered mutation	UNP P37333
A	338	THR	ASN	engineered mutation	UNP P37333
A	341	THR	ILE	engineered mutation	UNP P37333
C	335	GLY	THR	engineered mutation	UNP P37333
C	336	ILE	PHE	engineered mutation	UNP P37333
C	338	THR	ASN	engineered mutation	UNP P37333
C	341	THR	ILE	engineered mutation	UNP P37333
E	335	GLY	THR	engineered mutation	UNP P37333
E	336	ILE	PHE	engineered mutation	UNP P37333
E	338	THR	ASN	engineered mutation	UNP P37333
E	341	THR	ILE	engineered mutation	UNP P37333
G	335	GLY	THR	engineered mutation	UNP P37333
G	336	ILE	PHE	engineered mutation	UNP P37333
G	338	THR	ASN	engineered mutation	UNP P37333
G	341	THR	ILE	engineered mutation	UNP P37333

- Molecule 2 is a protein called BIPHENYL DIOXYGENASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	D	182	Total	C	N	O	S	0	0	0
			1517	963	269	281	4			
2	F	182	Total	C	N	O	S	0	0	0
			1517	963	269	281	4			
2	H	182	Total	C	N	O	S	0	0	0
			1517	963	269	281	4			

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Fe	0	0
			1	1		
4	A	1	Total	Fe	0	0
			1	1		

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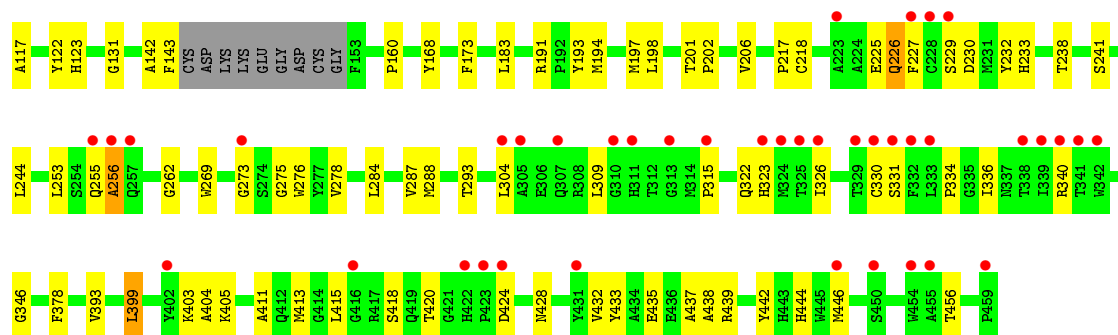
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Fe 1	0	0
4	E	1	Total 1	Fe 1	0	0

- Molecule 5 is water.

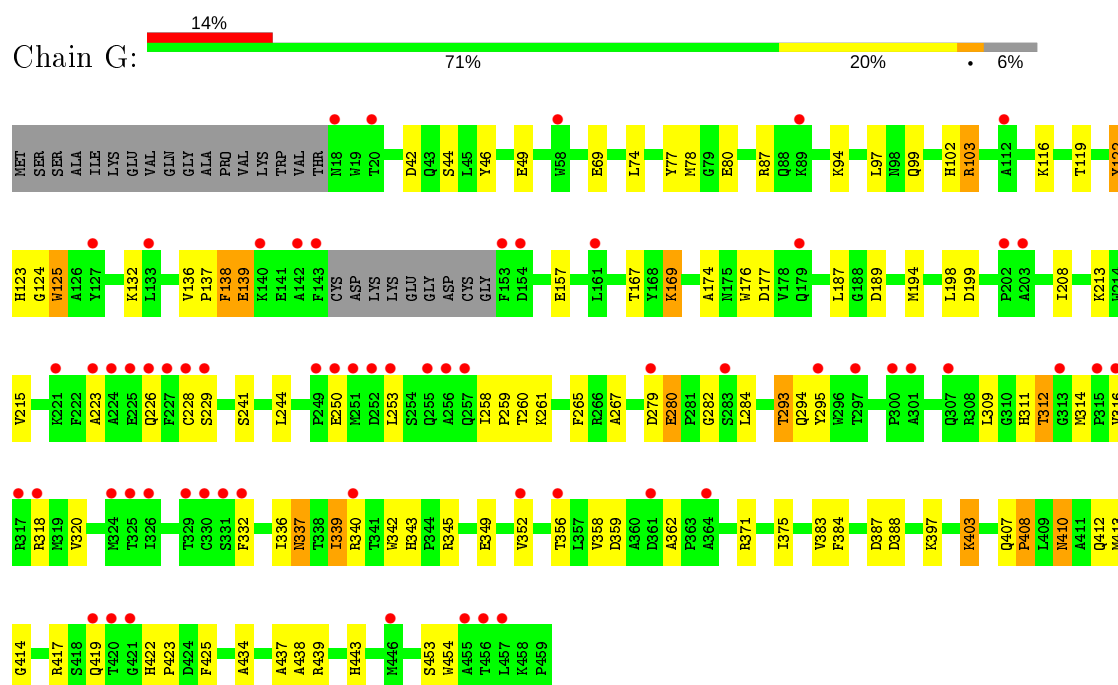
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total 105	O 105	0	0
5	B	56	Total 56	O 56	0	0
5	C	46	Total 46	O 46	0	0
5	D	50	Total 50	O 50	0	0
5	E	20	Total 20	O 20	0	0
5	F	26	Total 26	O 26	0	0
5	G	14	Total 14	O 14	0	0
5	H	12	Total 12	O 12	0	0

• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

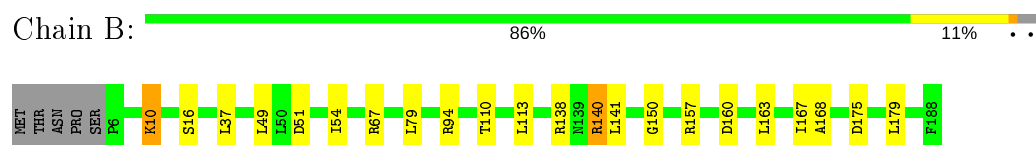




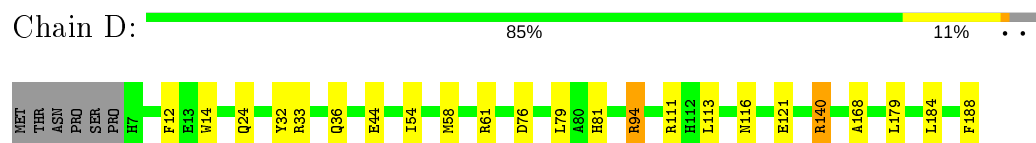
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



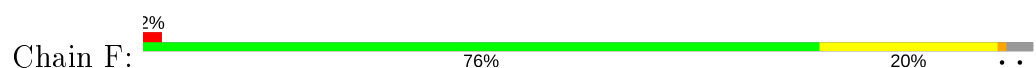
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

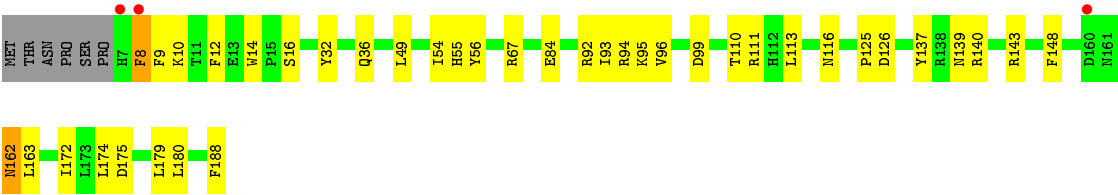


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

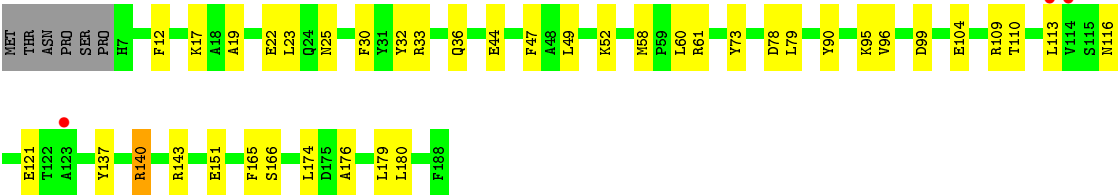
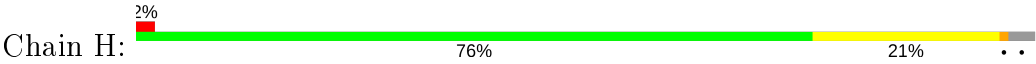


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA





● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	211.89Å 211.89Å 168.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.56 – 2.49 38.53 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.56-2.49) 99.3 (38.53-2.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.193 , 0.254 0.192 , 0.254	Depositor DCC
R_{free} test set	4865 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20136	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, FES

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	0.48	0/3530	0.67	0/4792
1	C	0.45	0/3530	0.61	0/4792
1	E	0.40	0/3530	0.59	0/4792
1	G	0.42	0/3530	0.59	0/4792
2	B	0.55	0/1561	0.74	0/2110
2	D	0.49	0/1553	0.68	0/2099
2	F	0.47	0/1553	0.66	0/2099
2	H	0.46	0/1553	0.66	0/2099
All	All	0.45	0/20340	0.64	0/27575

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	378	PHE	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	3428	0	3284	38	0
1	C	3428	0	3284	50	0
1	E	3428	0	3284	61	0
1	G	3428	0	3284	64	0
2	B	1524	0	1471	16	0
2	D	1517	0	1463	34	0
2	F	1517	0	1463	30	0
2	H	1517	0	1463	32	0
3	A	4	0	0	1	0
3	C	4	0	0	0	0
3	E	4	0	0	1	0
3	G	4	0	0	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	105	0	0	8	0
5	B	56	0	0	2	1
5	C	46	0	0	3	0
5	D	50	0	0	2	0
5	E	20	0	0	0	0
5	F	26	0	0	3	0
5	G	14	0	0	2	0
5	H	12	0	0	0	0
All	All	20136	0	18996	280	1

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 7.

All (280) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:PRO:HB3	1:A:280:GLU:HG2	1.50	0.94
2:B:140:ARG:HH11	2:B:140:ARG:HG2	1.39	0.87
1:G:123:HIS:HB2	3:G:500:FES:S1	2.15	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:162:ASN:H	2:F:162:ASN:ND2	1.76	0.83
2:D:36:GLN:HE21	2:F:12:PHE:H	1.32	0.77
1:A:201:THR:HG22	1:A:203:ALA:H	1.52	0.75
2:D:12:PHE:H	2:H:36:GLN:HE21	1.34	0.75
1:E:255:GLN:O	1:E:256:ALA:HB2	1.88	0.74
1:E:229:SER:OG	1:E:438:ALA:HB2	1.86	0.73
2:D:116:ASN:HA	2:H:32:TYR:CD1	2.24	0.72
2:B:16:SER:HB2	2:F:67:ARG:HH21	1.53	0.72
2:H:140:ARG:CG	2:H:140:ARG:HH11	2.03	0.71
2:B:140:ARG:NH1	2:B:140:ARG:HG2	2.05	0.70
1:E:262:GLY:HA2	1:E:278:VAL:HG23	1.73	0.70
2:F:36:GLN:HE21	2:H:12:PHE:H	1.39	0.70
1:E:411:ALA:HA	1:E:435:GLU:OE1	1.92	0.69
1:G:332:PHE:HB3	1:G:339:ILE:HB	1.73	0.69
2:D:140:ARG:HH11	2:D:140:ARG:CG	2.07	0.68
2:D:94:ARG:HD2	5:D:2024:HOH:O	1.94	0.67
1:G:336:ILE:O	1:G:337:ASN:HB2	1.94	0.67
1:C:334:PRO:O	1:C:337:ASN:OD1	2.13	0.66
1:G:226:GLN:NE2	1:G:388:ASP:OD1	2.29	0.65
2:D:36:GLN:NE2	2:F:12:PHE:H	1.94	0.65
2:D:58:MET:HE1	2:D:184:LEU:HD13	1.78	0.65
1:E:230:ASP:OD2	1:G:123:HIS:HE1	1.79	0.64
1:C:454:TRP:CE3	1:C:457:LEU:HB3	2.32	0.64
1:E:241:SER:HB2	2:F:95:LYS:HG3	1.78	0.64
1:E:123:HIS:HB2	3:E:500:FES:S1	2.37	0.64
2:D:140:ARG:HH11	2:D:140:ARG:HG3	1.62	0.64
1:C:106:ARG:HD2	5:C:2008:HOH:O	1.98	0.63
1:A:167:THR:HG22	5:A:2036:HOH:O	1.97	0.63
1:C:269:TRP:CZ2	1:C:444:HIS:HE1	2.17	0.62
1:E:131:GLY:O	1:E:160:PRO:HD2	1.98	0.62
1:C:36:ASP:OD2	1:C:38:ARG:HB2	1.99	0.62
2:D:113:LEU:HD22	2:H:113:LEU:HD21	1.81	0.62
2:B:141:LEU:HD23	5:B:2043:HOH:O	2.00	0.62
2:D:140:ARG:NH1	2:D:140:ARG:CG	2.63	0.62
1:E:322:GLN:HB3	1:E:334:PRO:HD2	1.82	0.62
1:A:410:ASN:HD21	1:A:412:GLN:HB2	1.65	0.62
1:A:376:ARG:HD3	5:A:2091:HOH:O	2.00	0.61
1:A:413:MET:HE3	1:A:435:GLU:HG3	1.82	0.61
2:H:44:GLU:H	2:H:44:GLU:CD	2.01	0.60
1:C:422:HIS:CD2	1:C:424:ASP:H	2.18	0.60
1:E:418:SER:HB3	1:E:428:ASN:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:VAL:HG12	1:E:288:MET:HE3	1.85	0.59
2:D:111:ARG:HB2	2:F:175:ASP:OD2	2.01	0.59
2:D:58:MET:HE1	2:D:184:LEU:CD1	2.32	0.59
1:E:255:GLN:O	1:E:256:ALA:CB	2.51	0.59
1:E:411:ALA:O	1:E:439:ARG:NH1	2.36	0.59
1:E:269:TRP:CZ2	1:E:444:HIS:HE1	2.21	0.59
1:A:259:PRO:HB3	1:A:280:GLU:CG	2.28	0.58
1:C:413:MET:HG2	1:E:142:ALA:HB1	1.85	0.58
1:E:42:ASP:HB3	1:E:45:LEU:HB2	1.85	0.58
1:C:18:ASN:HA	1:C:19:TRP:HB2	1.85	0.58
2:F:9:PHE:O	2:F:10:LYS:HB3	2.03	0.58
1:C:422:HIS:HD2	1:C:424:ASP:H	1.50	0.57
1:G:208:ILE:HD12	1:G:356:THR:HG23	1.85	0.57
1:G:371:ARG:HD2	2:H:78:ASP:O	2.03	0.57
1:E:435:GLU:OE2	1:G:102:HIS:NE2	2.28	0.56
2:D:54:ILE:HA	2:D:168:ALA:O	2.06	0.56
2:F:162:ASN:HD22	2:F:162:ASN:H	1.51	0.56
2:F:36:GLN:NE2	2:H:12:PHE:H	2.04	0.56
2:D:58:MET:HE2	2:D:81:HIS:CB	2.36	0.55
2:H:140:ARG:HG2	2:H:140:ARG:NH1	2.21	0.55
1:C:262:GLY:HA2	1:C:278:VAL:HG23	1.88	0.55
2:D:24:GLN:HG2	2:H:25:ASN:HD21	1.71	0.55
1:E:315:PRO:HD3	1:E:424:ASP:HB3	1.87	0.55
2:H:30:PHE:CD1	2:H:165:PHE:HB2	2.42	0.55
1:A:189:ASP:O	1:A:192:PRO:HD2	2.07	0.55
1:E:432:VAL:HG13	1:E:433:TYR:CD2	2.41	0.54
2:F:49:LEU:HD21	2:F:163:LEU:HD13	1.88	0.54
2:B:150:GLY:HA2	2:B:175:ASP:OD2	2.07	0.54
2:H:19:ALA:HB1	2:H:23:LEU:HD23	1.90	0.54
1:E:230:ASP:OD2	1:G:123:HIS:CE1	2.58	0.54
2:F:162:ASN:HB3	5:F:2026:HOH:O	2.07	0.54
2:D:58:MET:CE	2:D:81:HIS:CB	2.86	0.54
1:A:356:THR:HG23	2:B:79:LEU:HD21	1.89	0.54
1:E:36:ASP:O	1:E:39:ILE:HG12	2.08	0.54
1:C:76:THR:OG1	1:C:77:TYR:N	2.39	0.54
2:D:58:MET:CE	2:D:81:HIS:HB2	2.37	0.54
2:D:12:PHE:H	2:H:36:GLN:NE2	2.02	0.53
2:F:111:ARG:NH1	2:H:151:GLU:HB3	2.24	0.53
2:H:140:ARG:CG	2:H:140:ARG:NH1	2.65	0.53
1:C:273:GLY:O	1:C:324:MET:HG3	2.09	0.53
1:G:124:GLY:O	1:G:125:TRP:C	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:2016:HOH:O	2:D:81:HIS:HD2	1.92	0.53
1:E:194:MET:SD	1:E:326:ILE:HD11	2.48	0.53
1:G:80:GLU:OE2	1:G:345:ARG:HA	2.09	0.53
2:D:32:TYR:CD1	2:F:116:ASN:HA	2.44	0.53
1:C:56:ARG:NH2	1:C:448:MET:O	2.42	0.53
1:A:269:TRP:CZ2	1:A:444:HIS:HE1	2.26	0.52
2:D:44:GLU:OE1	5:D:2022:HOH:O	2.19	0.52
2:F:56:TYR:HB3	2:F:84:GLU:HB2	1.91	0.52
1:G:42:ASP:OD2	1:G:44:SER:HB2	2.09	0.52
1:C:326:ILE:HB	1:C:330:CYS:HB3	1.91	0.52
2:D:58:MET:HE2	2:D:81:HIS:HB2	1.92	0.52
1:E:226:GLN:HG3	1:G:122:TYR:OH	2.09	0.52
1:G:332:PHE:HB3	1:G:339:ILE:CB	2.39	0.52
1:G:375:ILE:HG13	2:H:79:LEU:HD22	1.92	0.52
1:G:413:MET:HB3	1:G:434:ALA:HA	1.92	0.52
1:E:287:VAL:HG12	1:E:288:MET:CE	2.40	0.51
1:G:383:VAL:HG23	1:G:384:PHE:CD1	2.45	0.51
1:G:208:ILE:HD12	1:G:356:THR:CG2	2.40	0.51
1:C:36:ASP:O	1:C:39:ILE:HG12	2.11	0.51
1:C:356:THR:CG2	2:D:79:LEU:HD11	2.41	0.51
1:A:167:THR:HG23	5:A:2010:HOH:O	2.10	0.51
1:C:410:ASN:C	1:C:410:ASN:HD22	2.14	0.51
1:A:123:HIS:HB2	3:A:500:FES:S1	2.51	0.51
1:E:225:GLU:OE1	1:G:103:ARG:NE	2.39	0.51
1:C:327:PHE:CG	1:C:328:PRO:HA	2.46	0.50
2:F:93:ILE:HA	2:F:96:VAL:HG12	1.93	0.50
1:A:247:ILE:O	2:B:94:ARG:NH1	2.44	0.50
1:G:213:LYS:HA	1:G:352:VAL:O	2.11	0.50
1:G:279:ASP:HA	1:G:318:ARG:HG3	1.93	0.50
1:C:160:PRO:O	5:C:2010:HOH:O	2.18	0.50
1:E:244:LEU:HD13	1:E:253:LEU:HG	1.93	0.50
2:D:116:ASN:HA	2:H:32:TYR:CG	2.47	0.50
1:C:18:ASN:CA	1:C:19:TRP:HB2	2.41	0.49
1:E:201:THR:HB	1:E:202:PRO:HD2	1.94	0.49
5:B:2001:HOH:O	1:C:252:ASP:HB2	2.13	0.49
1:E:232:TYR:CE2	1:G:123:HIS:HB3	2.47	0.49
1:G:280:GLU:O	1:G:320:VAL:HG21	2.12	0.49
1:G:414:GLY:HA2	1:G:417:ARG:HD2	1.94	0.49
1:G:241:SER:HB2	2:H:95:LYS:HG2	1.94	0.49
1:C:322:GLN:CD	1:C:334:PRO:HG2	2.33	0.49
1:C:229:SER:HB2	1:C:437:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:MET:HB2	1:E:435:GLU:HG3	1.95	0.49
1:C:358:VAL:HG21	1:C:367:LYS:HD3	1.92	0.49
1:E:217:PRO:HD2	1:E:393:VAL:HG22	1.94	0.48
1:E:288:MET:HE3	1:E:336:ILE:HG12	1.95	0.48
1:C:225:GLU:OE2	1:E:103:ARG:NH2	2.36	0.48
1:A:69:GLU:HA	1:A:69:GLU:OE1	2.13	0.48
1:C:287:VAL:HG12	1:C:288:MET:CE	2.43	0.48
2:B:16:SER:HB2	2:F:67:ARG:NH2	2.27	0.48
1:E:76:THR:OG1	1:E:77:TYR:N	2.39	0.48
2:F:143:ARG:HD3	1:G:215:VAL:HG21	1.95	0.48
1:C:81:ASP:HB3	1:C:97:LEU:HD11	1.95	0.48
1:A:311:HIS:HE1	5:A:2043:HOH:O	1.97	0.48
2:B:51:ASP:OD2	2:B:157:ARG:NH1	2.46	0.48
1:E:168:TYR:OH	1:E:191:ARG:HG2	2.14	0.48
2:H:140:ARG:HG2	2:H:140:ARG:HH11	1.78	0.48
2:D:58:MET:CE	2:D:184:LEU:HD13	2.41	0.48
1:G:187:LEU:HD22	1:G:194:MET:SD	2.53	0.48
1:C:315:PRO:HD2	1:C:425:PHE:CE1	2.50	0.47
1:G:229:SER:OG	1:G:438:ALA:N	2.47	0.47
1:A:410:ASN:ND2	1:A:412:GLN:H	2.12	0.47
1:G:422:HIS:CG	1:G:423:PRO:HD2	2.50	0.47
1:A:199:ASP:HB3	1:A:309:LEU:HD11	1.96	0.47
1:E:60:LEU:HD22	1:E:330:CYS:SG	2.55	0.47
1:E:273:GLY:HA3	1:E:437:ALA:HB1	1.95	0.47
1:G:383:VAL:HG23	1:G:384:PHE:HD1	1.79	0.47
1:G:284:LEU:HD23	1:G:293:THR:HG23	1.97	0.47
1:G:97:LEU:HD21	1:G:99:GLN:OE1	2.15	0.47
1:C:263:ASN:ND2	1:C:425:PHE:CE2	2.83	0.47
1:E:19:TRP:HB3	1:E:24:ILE:HD11	1.97	0.47
1:E:46:TYR:CE2	1:E:346:GLY:HA2	2.49	0.47
1:G:439:ARG:O	1:G:443:HIS:HB2	2.15	0.47
1:C:67:VAL:HG23	1:C:67:VAL:O	2.15	0.47
1:C:263:ASN:ND2	1:C:425:PHE:HE2	2.14	0.46
1:G:78:MET:SD	1:G:174:ALA:HB3	2.55	0.46
1:G:46:TYR:O	1:G:49:GLU:HB2	2.15	0.46
2:B:140:ARG:HH11	2:B:140:ARG:CG	2.20	0.46
1:E:115:ALA:HB1	1:E:117:ALA:O	2.16	0.46
1:E:201:THR:HG22	1:E:304:LEU:HD23	1.98	0.46
1:E:227:PHE:CD2	1:E:331:SER:HB3	2.51	0.46
1:E:284:LEU:HD23	1:E:293:THR:HG23	1.97	0.46
1:G:167:THR:HG22	5:G:2001:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:GLU:HA	1:C:452:PRO:HD3	1.80	0.46
1:G:422:HIS:HB3	1:G:425:PHE:O	2.15	0.46
1:E:275:GLY:HA3	1:E:323:HIS:CE1	2.50	0.46
1:E:19:TRP:HH2	1:E:38:ARG:HH21	1.62	0.46
1:E:37:PRO:HG2	1:E:405:LYS:O	2.15	0.46
2:F:162:ASN:CB	5:F:2026:HOH:O	2.62	0.46
1:A:30:GLN:NE2	1:A:443:HIS:CE1	2.84	0.46
2:B:54:ILE:HA	2:B:168:ALA:O	2.16	0.46
1:G:314:MET:HB3	1:G:316:VAL:HG13	1.98	0.46
2:D:116:ASN:HA	2:H:32:TYR:CE1	2.49	0.45
2:F:110:THR:HA	2:F:137:TYR:O	2.15	0.45
2:H:110:THR:HA	2:H:137:TYR:O	2.15	0.45
1:A:226:GLN:NE2	1:A:388:ASP:OD1	2.49	0.45
2:F:172:ILE:HD13	2:F:188:PHE:HB2	1.98	0.45
1:G:359:ASP:HB2	1:G:362:ALA:HB2	1.98	0.45
1:C:208:ILE:HD13	1:C:208:ILE:HA	1.84	0.45
2:F:139:ASN:OD1	2:H:176:ALA:HA	2.16	0.45
1:G:410:ASN:HD21	1:G:412:GLN:HB2	1.82	0.45
2:H:49:LEU:O	2:H:166:SER:HB2	2.16	0.45
1:E:336:ILE:HG21	1:E:378:PHE:CE2	2.52	0.45
1:A:167:THR:CG2	5:A:2010:HOH:O	2.64	0.45
1:C:407:GLN:HG3	1:E:101:ARG:NH2	2.32	0.45
2:H:140:ARG:HH11	2:H:140:ARG:HG3	1.77	0.45
1:A:192:PRO:HB3	1:A:312:THR:HG21	1.97	0.45
1:C:356:THR:HG22	2:D:79:LEU:HD11	1.98	0.44
1:A:229:SER:HB2	1:A:437:ALA:HB3	1.99	0.44
2:D:188:PHE:CD1	2:D:188:PHE:N	2.85	0.44
2:D:33:ARG:HG2	2:F:14:TRP:CD2	2.53	0.44
2:H:96:VAL:HG23	2:H:104:GLU:HG3	2.00	0.44
1:A:356:THR:CG2	2:B:79:LEU:HD21	2.48	0.44
1:G:223:ALA:HB1	1:G:342:TRP:CE2	2.52	0.44
1:A:259:PRO:HB2	1:A:277:TYR:CE1	2.52	0.44
1:A:287:VAL:O	1:A:377:ASN:ND2	2.49	0.44
2:D:58:MET:CE	2:D:184:LEU:CD1	2.96	0.44
2:D:58:MET:HE2	2:D:81:HIS:HB3	1.98	0.44
1:E:193:TYR:HE2	1:E:276:TRP:CH2	2.36	0.44
1:G:312:THR:HG23	5:G:2008:HOH:O	2.17	0.44
1:C:418:SER:HB3	1:C:428:ASN:HD21	1.82	0.44
2:H:61:ARG:HG2	2:H:73:TYR:CE2	2.53	0.44
1:C:213:LYS:HA	1:C:352:VAL:O	2.18	0.44
1:C:244:LEU:HD13	1:C:253:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:LEU:HG	1:C:52:ARG:HH12	1.83	0.44
1:E:229:SER:HB3	1:E:437:ALA:HB3	1.99	0.44
1:G:403:LYS:HA	1:G:403:LYS:HD3	1.80	0.44
1:A:233:HIS:CE1	5:A:2059:HOH:O	2.71	0.43
1:G:138:PHE:CD1	1:G:138:PHE:N	2.86	0.43
1:E:230:ASP:CG	1:G:123:HIS:HE1	2.21	0.43
1:E:233:HIS:HD2	1:E:238:THR:HG21	1.84	0.43
1:C:413:MET:HG3	1:E:143:PHE:CZ	2.53	0.43
1:C:368:GLU:OE2	1:C:372:ARG:NE	2.50	0.43
1:A:372:ARG:HG3	5:A:2089:HOH:O	2.18	0.43
2:F:8:PHE:N	5:F:2001:HOH:O	2.42	0.43
2:F:84:GLU:CD	2:F:92:ARG:HE	2.22	0.43
1:E:403:LYS:HG3	1:G:176:TRP:CD2	2.53	0.43
1:A:284:LEU:HD13	5:A:2078:HOH:O	2.18	0.43
1:C:410:ASN:ND2	1:C:412:GLN:H	2.16	0.43
2:F:143:ARG:NH2	1:G:349:GLU:OE2	2.52	0.43
1:A:295:TYR:CD1	1:A:366:ILE:HD13	2.54	0.43
1:E:232:TYR:HA	1:E:433:TYR:HD1	1.83	0.43
1:E:225:GLU:HG3	1:E:442:TYR:CE2	2.54	0.43
1:C:45:LEU:HA	1:C:45:LEU:HD23	1.89	0.42
1:C:410:ASN:ND2	1:C:410:ASN:C	2.73	0.42
1:E:59:LEU:O	1:E:173:PHE:HA	2.19	0.42
1:G:229:SER:OG	1:G:437:ALA:HB3	2.19	0.42
2:H:58:MET:HE1	2:H:174:LEU:HD22	2.01	0.42
2:B:10:LYS:HA	2:B:10:LYS:HD3	1.97	0.42
1:C:185:THR:HG22	1:C:459:PRO:HG2	2.01	0.42
1:G:309:LEU:C	1:G:311:HIS:H	2.23	0.42
1:G:241:SER:OG	1:G:387:ASP:OD2	2.37	0.42
1:G:199:ASP:HB3	1:G:309:LEU:HD11	2.01	0.42
1:C:294:GLN:HA	1:C:294:GLN:OE1	2.19	0.42
1:G:169:LYS:HB3	1:G:198:LEU:HB3	2.01	0.42
2:H:47:PHE:CZ	2:H:90:TYR:HB2	2.55	0.42
1:A:287:VAL:HG12	1:A:288:MET:HE2	2.02	0.42
1:C:58:TRP:HB2	1:C:186:TYR:CE2	2.55	0.42
1:G:136:VAL:HB	1:G:139:GLU:HG3	2.02	0.42
1:C:73:PHE:HA	1:C:85:MET:O	2.19	0.42
2:F:125:PRO:O	2:F:126:ASP:HB2	2.19	0.42
1:A:287:VAL:HG12	1:A:288:MET:CE	2.50	0.42
1:C:18:ASN:HA	1:C:19:TRP:CB	2.47	0.42
2:H:17:LYS:HB3	2:H:17:LYS:HE2	1.93	0.42
2:B:110:THR:HG22	2:B:138:ARG:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:GLU:O	1:G:87:ARG:HG2	2.20	0.41
1:E:404:ALA:HA	1:G:97:LEU:HD21	2.01	0.41
2:D:61:ARG:NH2	2:H:109:ARG:HG2	2.35	0.41
1:A:139:GLU:HA	1:A:143:PHE:HD1	1.85	0.41
1:C:213:LYS:HE2	1:C:353:TRP:CZ3	2.55	0.41
1:E:232:TYR:HA	1:E:433:TYR:CD1	2.55	0.41
1:G:177:ASP:OD2	1:G:454:TRP:CD1	2.73	0.41
1:G:265:PHE:CZ	1:G:267:ALA:HA	2.55	0.41
1:G:77:TYR:HB2	1:G:343:HIS:ND1	2.35	0.41
1:A:276:TRP:HB3	1:A:322:GLN:HG3	2.03	0.41
2:B:37:LEU:HD12	2:B:49:LEU:HD11	2.02	0.41
1:G:407:GLN:HA	1:G:408:PRO:HD2	1.71	0.41
2:F:54:ILE:HG13	2:F:55:HIS:N	2.36	0.41
1:G:132:LYS:HB2	1:G:132:LYS:HE3	1.91	0.41
2:F:148:PHE:HB3	2:F:174:LEU:HD11	2.02	0.41
1:G:293:THR:C	1:G:295:TYR:H	2.24	0.41
1:E:399:LEU:O	1:E:405:LYS:HE3	2.21	0.40
1:A:213:LYS:HE2	1:A:353:TRP:CE3	2.57	0.40
1:G:124:GLY:HA3	1:G:137:PRO:HG2	2.04	0.40
1:G:244:LEU:HB2	1:G:253:LEU:HD22	2.02	0.40
2:F:32:TYR:CD1	2:H:116:ASN:HA	2.56	0.40
2:D:58:MET:HE3	2:D:81:HIS:CB	2.51	0.40
1:G:258:ILE:HA	1:G:259:PRO:HD2	1.80	0.40
1:A:58:TRP:HD1	1:A:186:TYR:CD2	2.39	0.40
1:A:213:LYS:HA	1:A:352:VAL:O	2.20	0.40
1:E:168:TYR:HB2	1:E:183:LEU:HD21	2.04	0.40
1:E:197:MET:HE3	1:E:198:LEU:HD21	2.04	0.40
2:D:14:TRP:CD2	2:H:33:ARG:HG2	2.56	0.40
1:A:265:PHE:CZ	1:A:267:ALA:HA	2.57	0.40
1:A:19:TRP:CZ3	1:A:27:LEU:HD21	2.56	0.40
2:B:54:ILE:HD13	2:B:167:ILE:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2008:HOH:O	5:B:2008:HOH:O[3_565]	1.90	0.30

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	429/459 (94%)	406 (95%)	22 (5%)	1 (0%)	47	68
1	C	429/459 (94%)	406 (95%)	21 (5%)	2 (0%)	29	48
1	E	429/459 (94%)	397 (92%)	30 (7%)	2 (0%)	29	48
1	G	429/459 (94%)	382 (89%)	42 (10%)	5 (1%)	13	24
2	B	181/188 (96%)	174 (96%)	7 (4%)	0	100	100
2	D	180/188 (96%)	171 (95%)	9 (5%)	0	100	100
2	F	180/188 (96%)	168 (93%)	11 (6%)	1 (1%)	25	43
2	H	180/188 (96%)	168 (93%)	11 (6%)	1 (1%)	25	43
All	All	2437/2588 (94%)	2272 (93%)	153 (6%)	12 (0%)	29	48

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	SER
1	E	256	ALA
2	F	8	PHE
2	H	99	ASP
1	C	122	TYR
1	E	399	LEU
1	G	294	GLN
1	G	337	ASN
1	G	125	TRP
1	G	408	PRO
1	C	102	HIS
1	G	282	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	351/372 (94%)	336 (96%)	15 (4%)	29	53
1	C	351/372 (94%)	332 (95%)	19 (5%)	22	42
1	E	351/372 (94%)	336 (96%)	15 (4%)	29	53
1	G	351/372 (94%)	325 (93%)	26 (7%)	13	27
2	B	162/167 (97%)	155 (96%)	7 (4%)	29	53
2	D	161/167 (96%)	156 (97%)	5 (3%)	40	67
2	F	161/167 (96%)	153 (95%)	8 (5%)	24	46
2	H	161/167 (96%)	153 (95%)	8 (5%)	24	46
All	All	2049/2156 (95%)	1946 (95%)	103 (5%)	24	46

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	103	ARG
1	A	122	TYR
1	A	167	THR
1	A	206	VAL
1	A	252	ASP
1	A	255	GLN
1	A	307	GLN
1	A	316	VAL
1	A	340	ARG
1	A	356	THR
1	A	366	ILE
1	A	372	ARG
1	A	410	ASN
1	A	457	LEU
2	B	10	LYS
2	B	67	ARG
2	B	113	LEU
2	B	140	ARG
2	B	160	ASP
2	B	163	LEU
2	B	179	LEU
1	C	44	SER

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Mol	Chain	Res	Type
1	C	48	LEU
1	C	107	ILE
1	C	110	SER
1	C	122	TYR
1	C	157	GLU
1	C	229	SER
1	C	280	GLU
1	C	334	PRO
1	C	340	ARG
1	C	356	THR
1	C	379	SER
1	C	410	ASN
1	C	413	MET
1	C	418	SER
1	C	419	GLN
1	C	420	THR
1	C	428	ASN
1	C	457	LEU
2	D	76	ASP
2	D	94	ARG
2	D	121	GLU
2	D	140	ARG
2	D	179	LEU
1	E	18	ASN
1	E	22	GLU
1	E	48	LEU
1	E	86	VAL
1	E	103	ARG
1	E	122	TYR
1	E	206	VAL
1	E	218	CYS
1	E	226	GLN
1	E	309	LEU
1	E	340	ARG
1	E	415	LEU
1	E	420	THR
1	E	446	MET
1	E	456	THR
2	F	16	SER
2	F	94	ARG
2	F	99	ASP
2	F	113	LEU

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Mol	Chain	Res	Type
2	F	140	ARG
2	F	162	ASN
2	F	179	LEU
2	F	180	LEU
1	G	74	LEU
1	G	94	LYS
1	G	103	ARG
1	G	116	LYS
1	G	119	THR
1	G	122	TYR
1	G	138	PHE
1	G	139	GLU
1	G	157	GLU
1	G	169	LYS
1	G	189	ASP
1	G	228	CYS
1	G	250	GLU
1	G	260	THR
1	G	261	LYS
1	G	280	GLU
1	G	293	THR
1	G	312	THR
1	G	339	ILE
1	G	340	ARG
1	G	358	VAL
1	G	397	LYS
1	G	403	LYS
1	G	410	ASN
1	G	419	GLN
1	G	453	SER
2	H	22	GLU
2	H	52	LYS
2	H	60	LEU
2	H	121	GLU
2	H	140	ARG
2	H	143	ARG
2	H	179	LEU
2	H	180	LEU

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

Mol	Chain	Res	Type
1	A	294	GLN
1	A	410	ASN
1	A	422	HIS
1	A	444	HIS
2	B	25	ASN
2	B	55	HIS
2	B	77	GLN
2	B	131	ASN
1	C	18	ASN
1	C	88	GLN
1	C	263	ASN
1	C	410	ASN
1	C	422	HIS
1	C	428	ASN
1	C	444	HIS
2	D	25	ASN
2	D	36	GLN
1	E	263	ASN
1	E	444	HIS
2	F	25	ASN
2	F	36	GLN
2	F	81	HIS
2	F	131	ASN
2	F	162	ASN
1	G	123	HIS
1	G	257	GLN
1	G	322	GLN
1	G	337	ASN
1	G	391	ASN
1	G	410	ASN
1	G	422	HIS
2	H	25	ASN
2	H	36	GLN
2	H	81	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
3	FES	G	500	1	0,4,4	0.00	-	-		
3	FES	E	500	1	0,4,4	0.00	-	-		
3	FES	C	500	1	0,4,4	0.00	-	-		
3	FES	A	500	1	0,4,4	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
3	FES	G	500	1	-	-	0/1/1/1
3	FES	E	500	1	-	-	0/1/1/1
3	FES	C	500	1	-	-	0/1/1/1
3	FES	A	500	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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	500	FES	1	0
3	E	500	FES	1	0
3	A	500	FES	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	433/459 (94%)	-0.13	11 (2%) 57 61	31, 44, 67, 178	5 (1%)
1	C	433/459 (94%)	-0.01	12 (2%) 53 56	35, 55, 78, 108	2 (0%)
1	E	433/459 (94%)	0.55	51 (11%) 4 4	43, 71, 107, 129	10 (2%)
1	G	433/459 (94%)	0.76	63 (14%) 2 2	49, 79, 109, 139	10 (2%)
2	B	183/188 (97%)	-0.65	0 100 100	27, 35, 63, 85	1 (0%)
2	D	182/188 (96%)	-0.49	0 100 100	32, 42, 63, 94	2 (1%)
2	F	182/188 (96%)	-0.42	3 (1%) 72 74	35, 50, 72, 124	1 (0%)
2	H	182/188 (96%)	-0.21	3 (1%) 72 74	39, 55, 82, 119	0
All	All	2461/2588 (95%)	0.07	143 (5%) 23 24	27, 56, 97, 178	31 (1%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	PRO	8.9
1	A	251	MET	7.8
1	E	256	ALA	6.7
1	A	255	GLN	5.9
1	A	252	ASP	5.8
1	A	253	LEU	5.5
1	G	256	ALA	5.3
1	G	255	GLN	5.3
1	G	420	THR	5.2
1	A	254	SER	5.1
1	E	227	PHE	4.6
1	A	250	GLU	4.4
1	G	228	CYS	4.4
1	E	273	GLY	4.4
1	E	24	ILE	4.3
1	G	249	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	153	PHE	4.2
1	E	331	SER	4.2
1	G	251	MET	4.1
1	E	23	ALA	4.1
1	E	255	GLN	4.1
1	E	338	THR	4.1
1	G	257	GLN	4.1
1	E	339	ILE	4.0
1	E	324	MET	4.0
1	C	140	LYS	4.0
1	G	456	THR	4.0
1	A	248	PRO	4.0
1	E	332	PHE	4.0
2	H	123	ALA	4.0
1	E	454	TRP	3.9
1	E	330	CYS	3.9
1	G	317	ARG	3.9
1	E	257	GLN	3.7
1	E	325	THR	3.7
1	C	273	GLY	3.7
1	G	142	ALA	3.6
1	G	313	GLY	3.6
1	E	19	TRP	3.5
1	A	455	ALA	3.5
1	G	58	TRP	3.5
1	G	331	SER	3.4
1	G	153	PHE	3.4
1	E	27	LEU	3.4
1	E	333	LEU	3.3
1	G	325	THR	3.3
1	G	301	ALA	3.3
1	G	421	GLY	3.3
1	G	318	ARG	3.3
1	G	455	ALA	3.2
1	G	330	CYS	3.2
1	G	224	ALA	3.2
1	E	340	ARG	3.2
2	F	7	HIS	3.2
1	G	227	PHE	3.1
1	E	342	TRP	3.1
1	E	329	THR	3.1
1	E	326	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	446	MET	3.0
1	E	304	LEU	3.0
1	G	161	LEU	3.0
1	E	423	PRO	3.0
1	A	256	ALA	3.0
1	G	419	GLN	2.9
1	E	455	ALA	2.9
1	E	32	LYS	2.9
1	G	179	GLN	2.8
1	E	459	PRO	2.8
1	E	22	GLU	2.8
1	E	311	HIS	2.8
1	G	326	ILE	2.8
1	G	364	ALA	2.8
1	E	307	GLN	2.8
1	E	416	GLY	2.8
1	E	25	ARG	2.7
1	C	331	SER	2.7
1	G	329	THR	2.7
1	G	446	MET	2.7
1	E	424	ASP	2.7
1	C	455	ALA	2.6
1	C	325	THR	2.6
1	G	18	ASN	2.6
1	G	202	PRO	2.6
1	G	315	PRO	2.6
1	G	127	TYR	2.6
1	G	143	PHE	2.6
1	G	223	ALA	2.5
1	E	229	SER	2.5
1	G	203	ALA	2.5
1	G	133	LEU	2.5
1	G	253	LEU	2.5
1	G	112	ALA	2.5
1	G	356	THR	2.5
1	E	310	GLY	2.5
1	E	228	CYS	2.5
1	E	450	SER	2.5
1	E	18	ASN	2.5
1	G	226	GLN	2.4
1	G	229	SER	2.4
1	C	143	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	23	ALA	2.4
1	G	295	TYR	2.4
1	G	300	PRO	2.4
1	E	20	THR	2.4
1	G	352	VAL	2.4
1	E	431	TYR	2.4
1	G	140	LYS	2.4
1	G	20	THR	2.4
1	E	422	HIS	2.4
1	G	324	MET	2.3
2	F	8	PHE	2.3
1	G	89	LYS	2.3
1	E	323	HIS	2.3
1	G	283	SER	2.3
1	G	361	ASP	2.3
1	E	315	PRO	2.3
1	G	154	ASP	2.3
1	E	34	LEU	2.3
1	E	223	ALA	2.3
1	E	402	TYR	2.3
1	G	316	VAL	2.3
1	A	310	GLY	2.2
1	G	332	PHE	2.2
1	G	457	LEU	2.2
1	G	307	GLN	2.2
1	E	70	THR	2.2
2	H	113	LEU	2.2
1	G	279	ASP	2.1
1	E	341	THR	2.1
1	C	227	PHE	2.1
1	G	340	ARG	2.1
1	G	225	GLU	2.1
1	E	305	ALA	2.1
1	G	297	THR	2.1
1	G	252	ASP	2.1
1	E	313	GLY	2.1
2	H	114	VAL	2.1
1	G	250	GLU	2.1
1	C	274	SER	2.0
1	G	221	LYS	2.0
2	F	160	ASP	2.0
1	C	161	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	224	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	FES	C	500	4/4	0.98	0.09	62,68,68,78	0
4	FE2	G	501	1/1	0.99	0.15	69,69,69,69	0
3	FES	E	500	4/4	0.99	0.10	42,45,46,47	0
3	FES	A	500	4/4	0.99	0.08	40,41,42,46	0
3	FES	G	500	4/4	0.99	0.09	70,73,75,78	0
4	FE2	A	501	1/1	1.00	0.12	39,39,39,39	0
4	FE2	E	501	1/1	1.00	0.20	71,71,71,71	0
4	FE2	C	501	1/1	1.00	0.15	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.