



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2016 – 02:42 PM EDT

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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
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) : rb-20027457

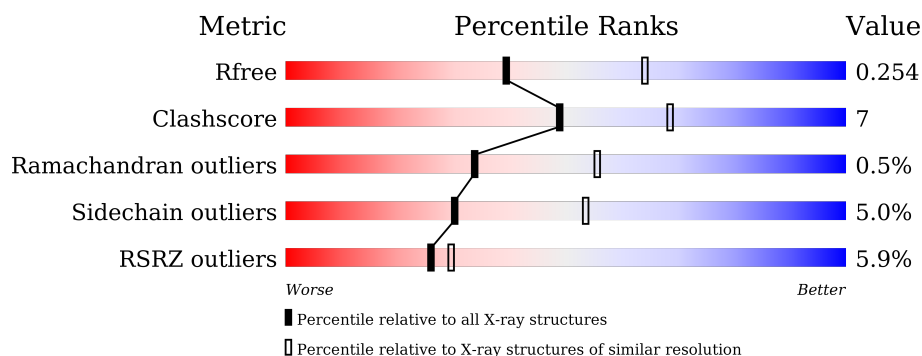
1 Overall quality at a glance

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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>

Continued on next page...

Continued from previous page...

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			

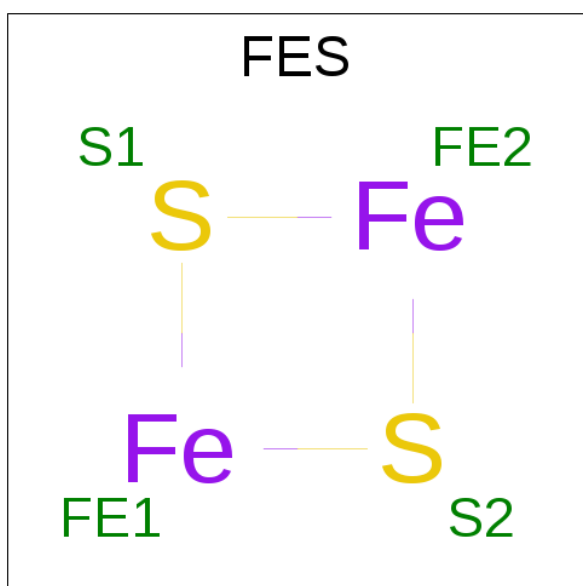
There are 16 discrepancies between the modelled and reference sequences:

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		

Continued on next page...

Continued from previous page...

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

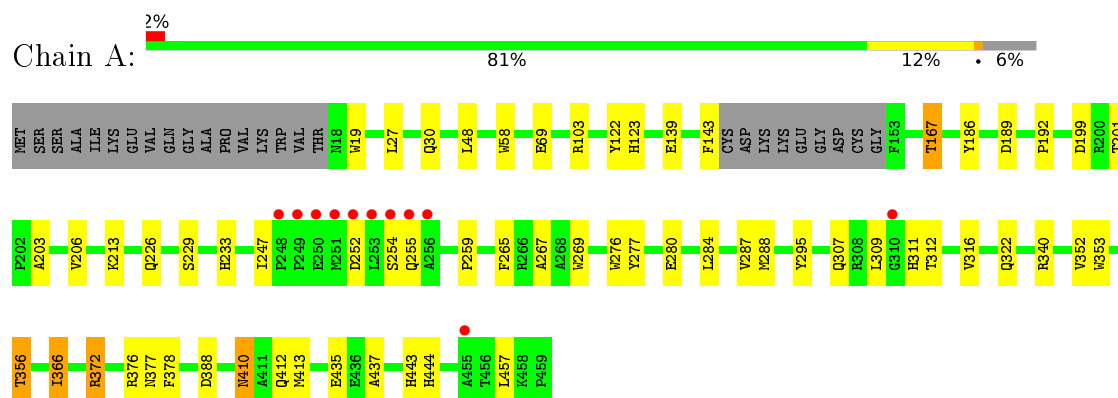
- Molecule 5 is water.

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

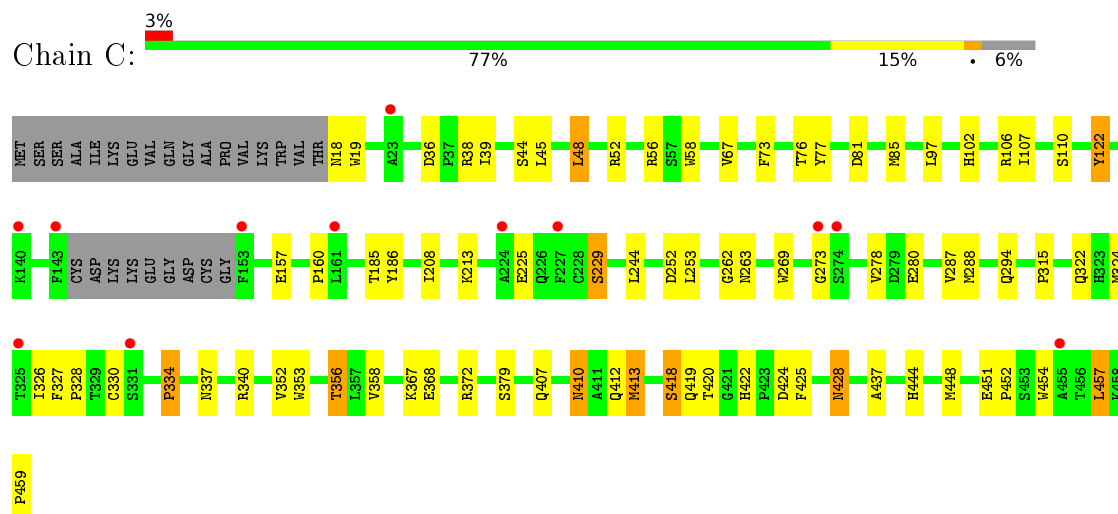
3 Residue-property plots

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.

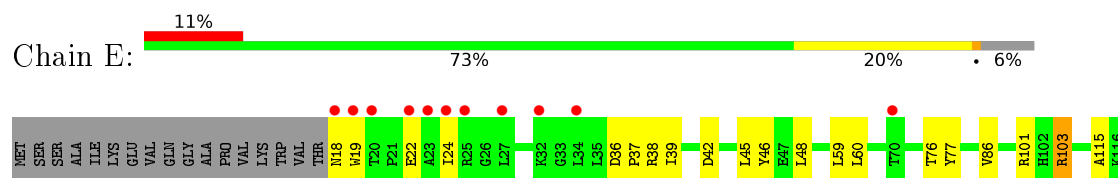
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

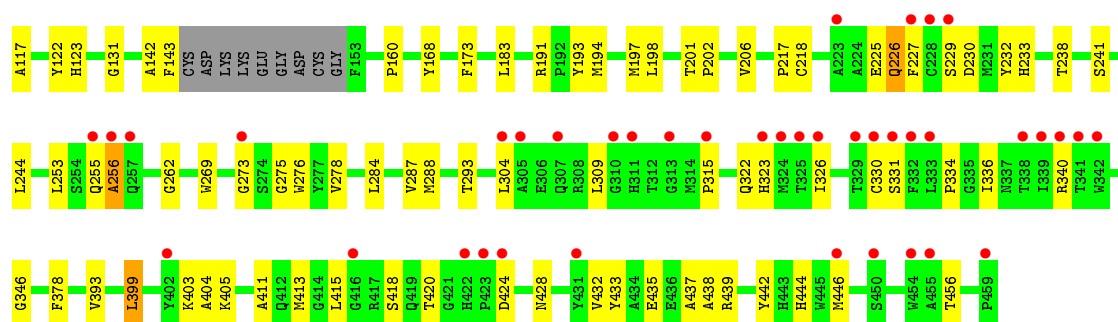


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

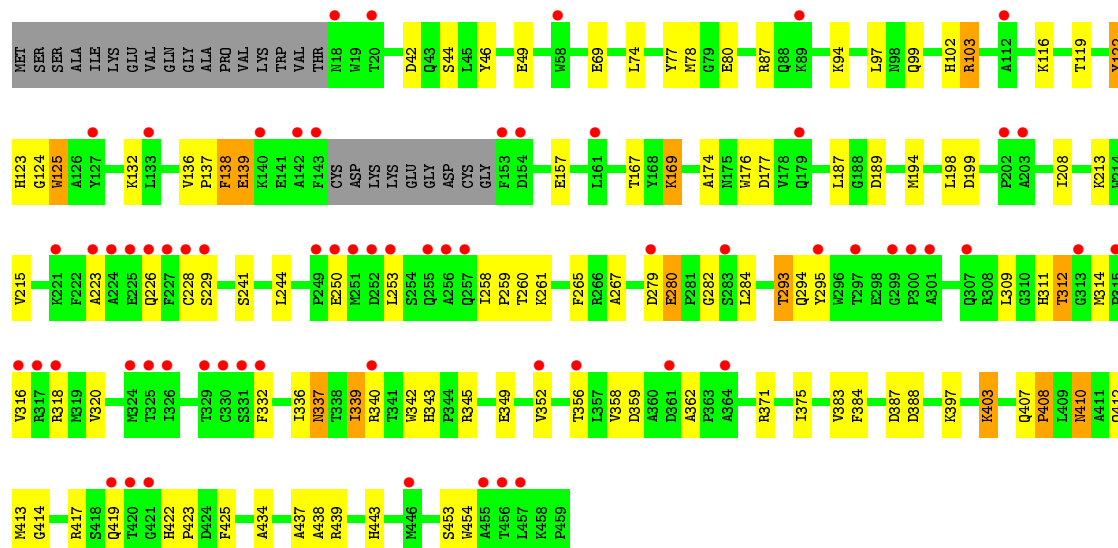


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

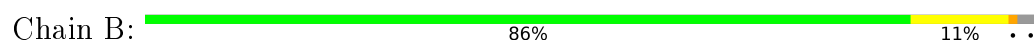




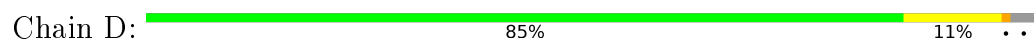
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



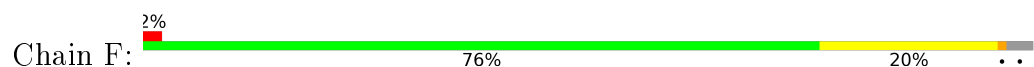
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

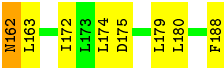


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

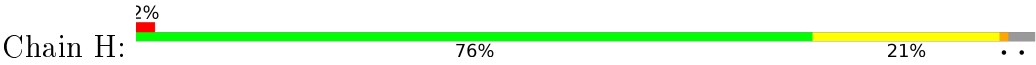


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA





● 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 (5.25%)	DCC
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, 0.375 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: 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:269:TRP:CZ2	1:E:444:HIS:HE1	2.21	0.59
1:E:411:ALA:O	1:E:439:ARG:NH1	2.36	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

Continued on next page...

Continued from previous page...

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:356:THR:CG2	2:D:79:LEU:HD11	2.41	0.51
1:C:36:ASP:O	1:C:39:ILE:HG12	2.11	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
2:D:116:ASN:HA	2:H:32:TYR:CG	2.47	0.50
1:E:244:LEU:HD13	1:E:253:LEU:HG	1.93	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

Continued on next page...

Continued from previous page...

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:288:MET:HE3	1:E:336:ILE:HG12	1.95	0.48
1:E:217:PRO:HD2	1:E:393:VAL:HG22	1.94	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:46:TYR:O	1:G:49:GLU:HB2	2.15	0.46
1:G:78:MET:SD	1:G:174:ALA:HB3	2.55	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:284:LEU:HD23	1:E:293:THR:HG23	1.97	0.46
1:E:227:PHE:CD2	1:E:331:SER:HB3	2.51	0.46
1:G:167:THR:HG22	5:G:2001:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
1:E:403:LYS:HG3	1:G:176:TRP:CD2	2.53	0.43
2:F:84:GLU:CD	2:F:92:ARG:HE	2.22	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:199:ASP:HB3	1:G:309:LEU:HD11	2.01	0.42
1:G:241:SER:OG	1:G:387:ASP:OD2	2.37	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:GLU:O	1:G:87:ARG:HG2	2.20	0.41
2:D:61:ARG:NH2	2:H:109:ARG:HG2	2.35	0.41
1:E:404:ALA:HA	1:G:97:LEU:HD21	2.01	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%)	52	75
1	C	429/459 (94%)	406 (95%)	21 (5%)	2 (0%)	34	55
1	E	429/459 (94%)	397 (92%)	30 (7%)	2 (0%)	34	55
1	G	429/459 (94%)	382 (89%)	42 (10%)	5 (1%)	16	29
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%)	30	50
2	H	180/188 (96%)	168 (93%)	11 (6%)	1 (1%)	30	50
All	All	2437/2588 (94%)	2272 (93%)	153 (6%)	12 (0%)	34	55

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%)	35	61
1	C	351/372 (94%)	332 (95%)	19 (5%)	27	49
1	E	351/372 (94%)	336 (96%)	15 (4%)	35	61
1	G	351/372 (94%)	325 (93%)	26 (7%)	17	31
2	B	162/167 (97%)	155 (96%)	7 (4%)	35	61
2	D	161/167 (96%)	156 (97%)	5 (3%)	47	75
2	F	161/167 (96%)	153 (95%)	8 (5%)	30	53
2	H	161/167 (96%)	153 (95%)	8 (5%)	30	53
All	All	2049/2156 (95%)	1946 (95%)	103 (5%)	30	53

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	A	500	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	C	500	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	E	500	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	G	500	1	0,4,4	0.00	-	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	A	500	1	-	0/0/4/4	0/1/1/1
3	FES	C	500	1	-	0/0/4/4	0/1/1/1
3	FES	E	500	1	-	0/0/4/4	0/1/1/1
3	FES	G	500	1	-	0/0/4/4	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	A	500	FES	1	0
3	E	500	FES	1	0
3	G	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%) 61 65	31, 44, 67, 178	5 (1%)
1	C	433/459 (94%)	-0.01	12 (2%) 56 61	35, 55, 78, 108	2 (0%)
1	E	433/459 (94%)	0.55	51 (11%) 6 6	43, 71, 107, 129	10 (2%)
1	G	433/459 (94%)	0.76	64 (14%) 3 3	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%) 74 78	35, 50, 72, 124	1 (0%)
2	H	182/188 (96%)	-0.21	3 (1%) 74 78	39, 55, 82, 119	0
All	All	2461/2588 (95%)	0.07	144 (5%) 26 29	27, 56, 97, 178	31 (1%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	PRO	9.0
1	A	251	MET	7.8
1	E	256	ALA	6.6
1	A	252	ASP	5.9
1	A	255	GLN	5.9
1	A	253	LEU	5.4
1	G	256	ALA	5.3
1	G	255	GLN	5.2
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	24	ILE	4.3
1	G	249	PRO	4.3
1	E	273	GLY	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	251	MET	4.2
1	E	331	SER	4.2
1	C	153	PHE	4.2
1	E	23	ALA	4.1
1	G	257	GLN	4.1
1	G	456	THR	4.1
1	E	255	GLN	4.1
1	E	338	THR	4.0
1	E	339	ILE	4.0
1	A	248	PRO	4.0
1	E	324	MET	4.0
1	E	332	PHE	4.0
1	C	140	LYS	4.0
2	H	123	ALA	4.0
1	E	454	TRP	3.9
1	E	330	CYS	3.9
1	G	317	ARG	3.8
1	E	257	GLN	3.7
1	E	325	THR	3.7
1	C	273	GLY	3.6
1	G	142	ALA	3.6
1	G	313	GLY	3.6
1	E	19	TRP	3.5
1	G	58	TRP	3.5
1	A	455	ALA	3.5
1	G	331	SER	3.4
1	E	27	LEU	3.4
1	G	153	PHE	3.4
1	E	333	LEU	3.4
1	G	325	THR	3.4
1	G	301	ALA	3.3
1	G	318	ARG	3.3
1	G	224	ALA	3.2
1	G	330	CYS	3.2
1	G	421	GLY	3.2
1	E	340	ARG	3.2
1	G	227	PHE	3.2
1	G	455	ALA	3.1
2	F	7	HIS	3.1
1	E	342	TRP	3.1
1	E	329	THR	3.1
1	E	326	ILE	3.1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	224	ALA	2.0
1	G	299	GLY	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
3	FES	E	500	4/4	0.99	0.10	-0.75	42,45,46,47	0
3	FES	G	500	4/4	0.99	0.09	-0.98	70,73,75,78	0
3	FES	C	500	4/4	0.98	0.09	-1.57	62,68,68,78	0
3	FES	A	500	4/4	0.99	0.08	-1.88	40,41,42,46	0
4	FE2	G	501	1/1	0.99	0.15	-	69,69,69,69	0
4	FE2	C	501	1/1	1.00	0.15	-	43,43,43,43	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

6.5 Other polymers [i](#)

There are no such residues in this entry.