Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2016 – 08:24 PM EST

PDB ID	:	3DHG
Title	:	Crystal Structure of Toluene 4-Monoxygenase Hydroxylase
Authors	:	Bailey, L.J.; Mccoy, J.G.; Phillips Jr., G.N.; Fox, B.G.
Deposited on	:	2008-06-17
Resolution	:	1.85 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

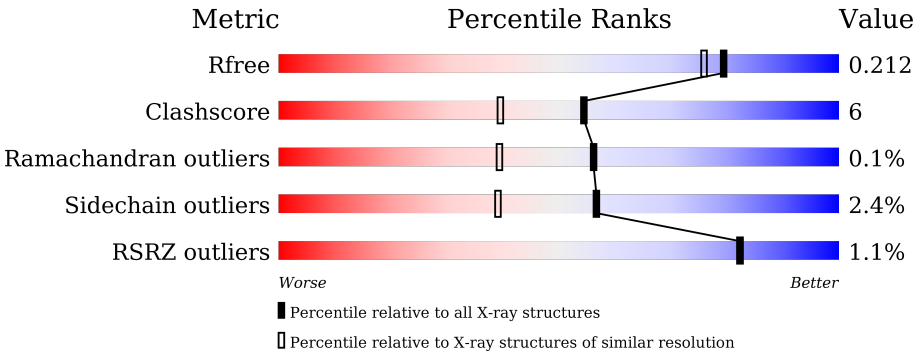
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	500	90% 8%
1	D	500	86% 12%
2	B	327	80% 12% 7%
2	E	327	82% 9% 7%
3	C	84	2% 82% 13%
3	F	84	6% 76% 19%

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
6	AZI	D	510	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16033 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 toluene 4-monooxygenase hydroxylase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	3	0
			4050	2599	683	745	23			
1	D	492	Total	C	N	O	S	0	10	0
			4101	2633	690	754	24			

- Molecule 2 is a protein called toluene 4-monooxygenase hydroxylase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	304	Total	C	N	O	S	0	4	0
			2547	1617	439	476	15			
2	E	304	Total	C	N	O	S	0	6	0
			2551	1617	439	479	16			

- Molecule 3 is a protein called toluene 4-monooxygenase hydroxylase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	82	Total	C	N	O	S	0	2	0
			664	420	117	123	4			
3	F	81	Total	C	N	O	S	0	0	0
			645	407	116	118	4			

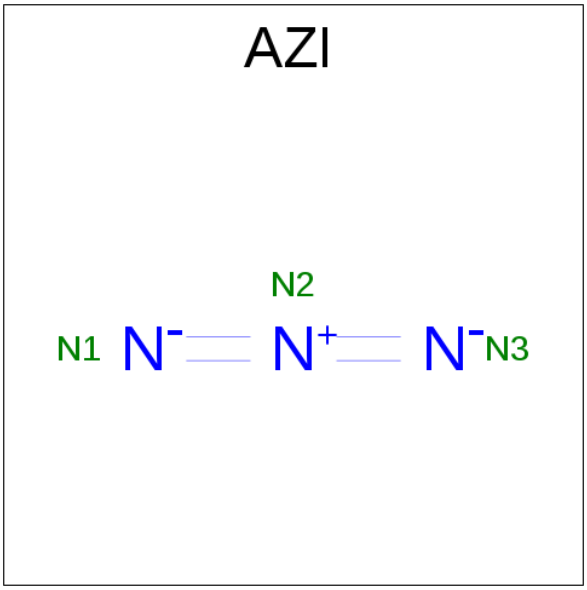
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Fe	0	0
			2	2		
4	D	2	Total	Fe	0	0
			2	2		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	5	Total Ca 5 5	0	0
5	C	1	Total Ca 1 1	0	0
5	F	1	Total Ca 1 1	0	0
5	E	2	Total Ca 2 2	0	0

- Molecule 6 is AZIDE ION (three-letter code: AZI) (formula: N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total N 3 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	352	Total O 352 352	0	0
7	B	302	Total O 302 302	0	0
7	C	42	Total O 42 42	0	0
7	D	408	Total O 408 408	0	0
7	E	306	Total O 306 306	0	0

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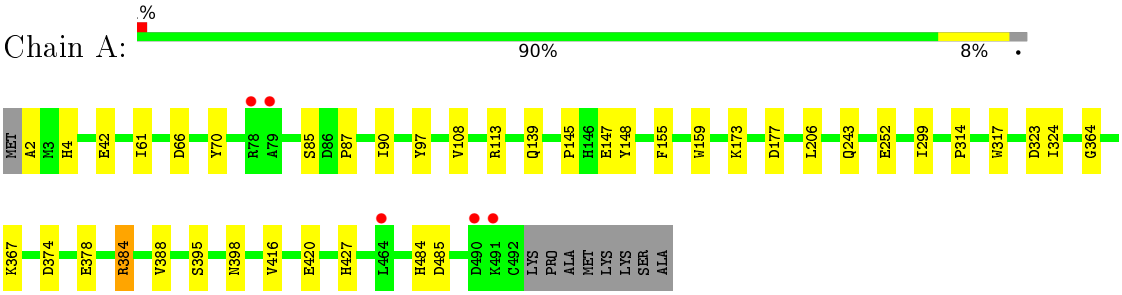
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	49	Total O 49 49	0	0

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.

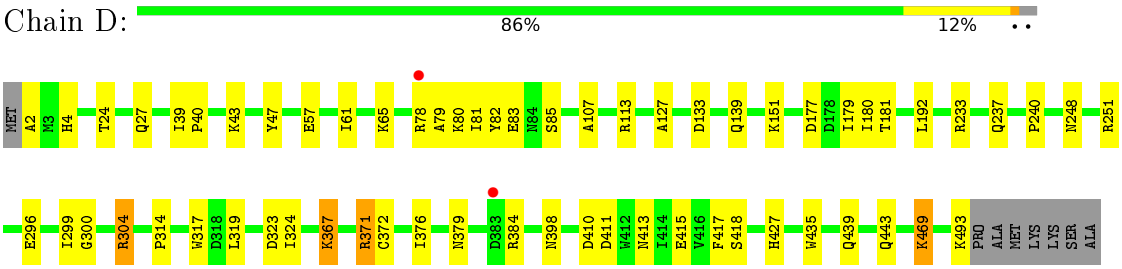
- Molecule 1: toluene 4-monooxygenase hydroxylase alpha subunit

Chain A:



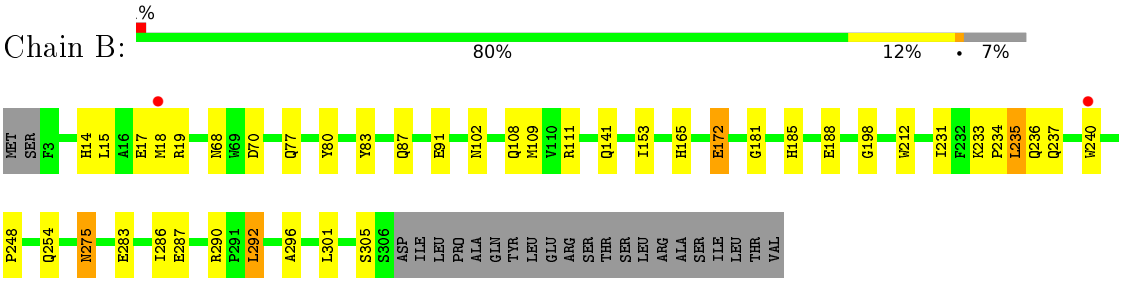
- Molecule 1: toluene 4-monooxygenase hydroxylase alpha subunit

Chain D:



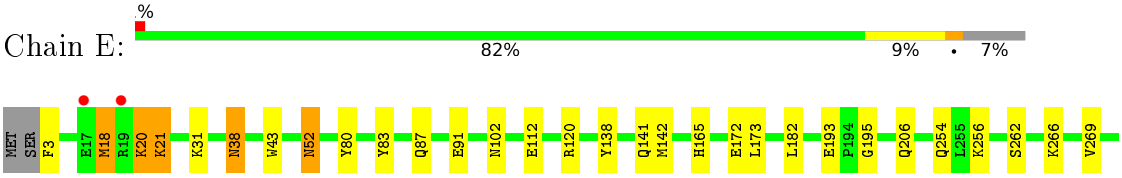
- Molecule 2: toluene 4-monooxygenase hydroxylase beta subunit

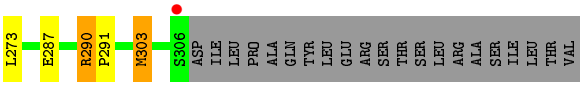
Chain B:



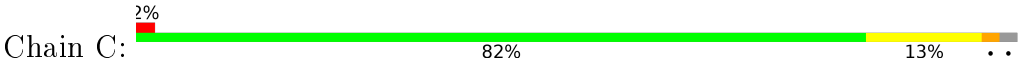
- Molecule 2: toluene 4-monooxygenase hydroxylase beta subunit

Chain E:

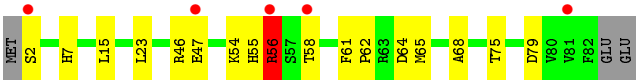




- Molecule 3: toluene 4-monooxygenase hydroxylase gamma subunit



- Molecule 3: toluene 4-monooxygenase hydroxylase gamma subunit



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.82Å 181.48Å 89.92Å 90.00° 107.62° 90.00°	Depositor
Resolution (Å)	49.45 – 1.85 49.42 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.45-1.85) 98.5 (49.42-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.164 , 0.214 0.163 , 0.212	Depositor DCC
R_{free} test set	7265 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	22.1	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16033	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: AZI, CA, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.75	0/4188	0.70	0/5686
1	D	0.79	0/4254	0.74	3/5774 (0.1%)
2	B	0.79	1/2636 (0.0%)	0.76	1/3584 (0.0%)
2	E	0.81	2/2644 (0.1%)	0.74	1/3593 (0.0%)
3	C	0.71	0/682	0.78	1/924 (0.1%)
3	F	0.70	0/657	0.77	0/890
All	All	0.78	3/15061 (0.0%)	0.74	6/20451 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	303[A]	MET	C-N	-5.47	1.21	1.34
2	E	303[B]	MET	C-N	-5.47	1.21	1.34
2	B	172	GLU	CD-OE2	-5.13	1.20	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	233	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	D	233	ARG	NE-CZ-NH2	5.54	123.07	120.30
2	B	235	LEU	CA-CB-CG	5.29	127.48	115.30
3	C	42	ARG	CG-CD-NE	-5.22	100.84	111.80
1	D	133	ASP	CB-CG-OD2	-5.11	113.70	118.30
2	E	112	GLU	C-N-CA	-5.08	111.63	122.30

There are no chirality outliers.

There are no planarity outliers.

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	4050	0	3820	36	0
1	D	4101	0	3882	58	0
2	B	2547	0	2428	45	0
2	E	2551	0	2439	39	0
3	C	664	0	664	13	0
3	F	645	0	643	18	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	B	5	0	0	0	0
5	C	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
6	D	3	0	0	0	0
7	A	352	0	0	5	0
7	B	302	0	0	14	0
7	C	42	0	0	1	0
7	D	408	0	0	7	0
7	E	306	0	0	6	0
7	F	49	0	0	2	0
All	All	16033	0	13876	182	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 6.

All (182) 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:E:193:GLU:CG	2:E:303[A]:MET:HE2	1.79	1.11
3:C:23:LEU:HA	3:C:67[A]:ILE:HD11	1.36	1.07
1:D:61[A]:ILE:HD11	7:D:992:HOH:O	1.59	1.02
2:B:18:MET:HG2	7:B:1429:HOH:O	1.61	1.00
2:E:193:GLU:HG3	2:E:303[A]:MET:HE2	1.42	1.00
2:B:19:ARG:HG2	2:B:19:ARG:HH11	1.27	0.99
2:E:43:TRP:H	2:E:52:ASN:HD21	1.13	0.93
2:E:193:GLU:HG2	2:E:303[A]:MET:HE2	1.48	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:256:LYS:HE2	7:E:384:HOH:O	1.70	0.92
1:A:384:ARG:HH11	1:A:384:ARG:HG2	1.37	0.89
2:E:193:GLU:HG3	2:E:303[A]:MET:CE	2.05	0.86
1:D:371:ARG:CG	1:D:371:ARG:HH11	1.89	0.85
1:A:416:VAL:H	3:C:55:HIS:HE1	1.26	0.82
2:E:165:HIS:HD2	2:E:254:GLN:HE21	1.27	0.82
1:D:139:GLN:HE22	2:E:80:TYR:H	1.28	0.81
2:B:68[A]:ASN:OD1	2:B:70:ASP:OD1	2.00	0.80
1:D:413[B]:ASN:ND2	7:D:537:HOH:O	2.14	0.79
2:B:188[A]:GLU:HG3	7:B:1224:HOH:O	1.82	0.78
2:B:109:MET:HB2	7:B:1234:HOH:O	1.84	0.77
2:B:165:HIS:HD2	2:B:254:GLN:HE21	1.32	0.75
2:B:108:GLN:HG3	7:B:1374:HOH:O	1.87	0.73
2:B:19:ARG:NH1	2:B:19:ARG:HG2	1.98	0.73
2:E:165:HIS:CD2	2:E:254:GLN:HE21	2.05	0.72
1:A:420:GLU:HG2	7:A:983:HOH:O	1.87	0.72
1:A:139:GLN:HE22	2:B:80:TYR:H	1.37	0.71
1:D:415[B]:GLU:HG2	1:D:417:PHE:CZ	2.27	0.70
1:A:85:SER:HB2	1:A:90:ILE:HD11	1.73	0.69
1:D:43:LYS:HE2	1:D:248:ASN:HD21	1.58	0.69
1:D:398:ASN:HD22	1:D:427:HIS:H	1.39	0.69
1:A:398:ASN:HD22	1:A:427:HIS:H	1.41	0.69
2:E:21:LYS:O	7:E:1427:HOH:O	2.11	0.68
1:D:379:ASN:HD22	1:D:384:ARG:HH11	1.43	0.67
2:B:290:ARG:HD3	7:B:338:HOH:O	1.94	0.66
1:D:81:ILE:HG23	1:D:85:SER:OG	1.96	0.66
1:D:371:ARG:HG2	1:D:371:ARG:HH11	1.59	0.66
1:D:57:GLU:O	1:D:61[A]:ILE:HG12	1.95	0.66
2:B:165:HIS:CD2	2:B:254:GLN:HE21	2.14	0.66
3:C:23:LEU:HA	3:C:67[A]:ILE:CD1	2.22	0.65
1:A:113:ARG:HH11	2:B:141:GLN:HE21	1.45	0.65
3:F:62:PRO:HD2	3:F:65:MET:HE1	1.79	0.64
1:A:416:VAL:H	3:C:55:HIS:CE1	2.12	0.64
2:E:195:GLY:HA3	2:E:303[A]:MET:HE3	1.78	0.64
2:B:14:HIS:O	2:B:18:MET:HE2	1.97	0.64
3:C:55:HIS:HD2	3:C:79:ASP:OD1	1.82	0.63
2:B:15:LEU:HD23	2:B:18:MET:HE3	1.80	0.63
1:A:384:ARG:HH11	1:A:384:ARG:CG	2.11	0.62
1:A:299:ILE:HD11	1:A:324:ILE:HD13	1.82	0.62
2:B:287:GLU:HG2	7:B:851:HOH:O	2.00	0.62
1:D:80:LYS:HB3	1:D:83:GLU:CG	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ARG:HH11	2:E:141:GLN:HE21	1.50	0.60
2:E:195:GLY:HA3	2:E:303[A]:MET:CE	2.32	0.60
1:D:299:ILE:HD11	1:D:324:ILE:HD13	1.84	0.60
2:E:18:MET:HG3	2:E:20:LYS:HG2	1.83	0.59
3:F:61:PHE:HB3	3:F:65:MET:CE	2.33	0.59
1:D:47:TYR:CE1	1:D:240:PRO:HB2	2.38	0.59
1:D:418:SER:OG	1:D:427:HIS:HD2	1.86	0.59
1:D:80:LYS:HB3	1:D:83:GLU:HG2	1.85	0.58
3:F:61:PHE:HB3	3:F:65:MET:HE1	1.86	0.58
1:A:61[B]:ILE:HD11	7:A:695:HOH:O	2.02	0.58
1:D:2:ALA:N	2:E:102:ASN:HD22	2.02	0.57
2:E:31:LYS:HE3	7:E:923:HOH:O	2.04	0.57
1:A:206:LEU:HD13	1:D:304[A]:ARG:NH2	2.19	0.57
2:E:287:GLU:HG3	7:E:401:HOH:O	2.05	0.57
2:B:292:LEU:HD23	7:B:961:HOH:O	2.05	0.56
2:B:283:GLU:HG2	7:B:543:HOH:O	2.06	0.56
1:D:300:GLY:O	1:D:304[A]:ARG:HD2	2.06	0.56
1:A:87:PRO:HG2	1:A:484:HIS:CD2	2.41	0.55
2:B:286:ILE:HG22	2:B:290:ARG:HE	1.70	0.55
2:E:266:LYS:HE2	7:E:375:HOH:O	2.06	0.55
1:D:415[B]:GLU:OE1	3:F:56:ARG:HD2	2.06	0.55
1:D:107:ALA:HA	1:D:180:ILE:HG21	1.87	0.55
1:D:371:ARG:HG3	1:D:371:ARG:HH11	1.71	0.54
1:D:314:PRO:HD2	1:D:317:TRP:CE3	2.43	0.53
2:E:120:ARG:NH2	2:E:193:GLU:OE2	2.41	0.53
1:A:314:PRO:HD2	1:A:317:TRP:CE3	2.44	0.52
1:A:139:GLN:NE2	2:B:80:TYR:H	2.06	0.52
2:B:68[A]:ASN:ND2	7:B:879:HOH:O	2.40	0.52
3:C:28:ASP:OD1	3:C:63:ARG:HD2	2.10	0.52
1:D:415[B]:GLU:HG2	1:D:417:PHE:CE2	2.45	0.52
3:F:55:HIS:HD2	3:F:79:ASP:OD1	1.92	0.52
1:D:415[B]:GLU:CD	3:F:56:ARG:HD2	2.30	0.52
2:B:234:PRO:HG2	2:B:301:LEU:HD21	1.91	0.51
1:A:147:GLU:HB3	7:A:1262:HOH:O	2.09	0.51
7:D:666:HOH:O	3:F:7:HIS:HE1	1.94	0.51
2:B:286:ILE:HG22	2:B:290:ARG:NE	2.26	0.50
3:F:2:SER:CB	7:F:649:HOH:O	2.59	0.50
1:A:395:SER:OG	3:C:7:HIS:HD2	1.95	0.50
2:E:193:GLU:CG	2:E:303[A]:MET:CE	2.66	0.49
2:E:269:VAL:O	2:E:273:LEU:HG	2.13	0.49
3:C:53:ARG:HD2	3:C:57:SER:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304[A]:ARG:HD3	7:D:965:HOH:O	2.13	0.49
1:A:395:SER:OG	3:C:7:HIS:CD2	2.67	0.48
1:D:469:LYS:HE3	2:E:3:PHE:CE1	2.47	0.48
2:E:173:LEU:HB3	2:E:182:LEU:HD13	1.94	0.48
2:B:181:GLY:HA3	2:B:185:HIS:HD2	1.77	0.48
2:B:91:GLU:OE1	2:B:165:HIS:HE1	1.97	0.47
1:D:372:CYS:O	1:D:376[A]:ILE:HG12	2.14	0.47
1:D:411:ASP:HB2	7:D:693:HOH:O	2.14	0.47
1:D:79:ALA:O	1:D:80:LYS:C	2.52	0.47
2:E:262:SER:O	2:E:266:LYS:HG3	2.14	0.47
1:D:367:LYS:HA	1:D:371:ARG:NH1	2.29	0.47
1:A:364:GLY:O	1:A:367:LYS:HG2	2.14	0.47
1:D:61[A]:ILE:HG23	7:D:636:HOH:O	2.14	0.47
2:B:111:ARG:HD2	7:B:837:HOH:O	2.16	0.46
2:E:38:ASN:C	2:E:38:ASN:HD22	2.18	0.46
2:B:275:ASN:HD22	2:B:275:ASN:C	2.19	0.46
2:E:91:GLU:OE1	2:E:165:HIS:HE1	1.99	0.46
2:B:14:HIS:O	2:B:18:MET:CE	2.63	0.46
1:D:371:ARG:HD2	7:F:372:HOH:O	2.16	0.46
1:D:78:ARG:HG2	7:D:611:HOH:O	2.15	0.46
2:E:266:LYS:CE	7:E:375:HOH:O	2.62	0.46
2:E:83:TYR:CZ	2:E:87:GLN:HG3	2.51	0.46
1:D:415[B]:GLU:CG	1:D:417:PHE:CE2	2.98	0.46
1:A:4:HIS:HE1	2:B:172:GLU:HG3	1.81	0.46
1:A:108:VAL:HG11	2:B:153:ILE:HD11	1.98	0.46
2:B:236:GLN:HG2	2:B:248:PRO:HA	1.97	0.46
2:E:195:GLY:CA	2:E:303[A]:MET:HE3	2.46	0.46
1:D:371:ARG:NH1	1:D:410:ASP:CG	2.70	0.45
1:D:427:HIS:HE1	3:F:75:THR:O	1.99	0.45
1:A:113:ARG:HH11	2:B:141:GLN:NE2	2.14	0.45
2:B:198:GLY:HA3	2:B:296:ALA:HA	1.99	0.45
1:D:81:ILE:HG23	1:D:85:SER:HG	1.79	0.45
1:A:66:ASP:O	1:A:70:TYR:HD2	1.99	0.45
1:A:252:GLU:HG3	7:A:585:HOH:O	2.17	0.45
1:A:2:ALA:N	2:B:102:ASN:HD22	2.15	0.45
2:B:68[A]:ASN:OD1	7:B:879:HOH:O	2.21	0.45
1:D:179:ILE:HG13	1:D:180:ILE:HG13	1.99	0.45
1:D:82:TYR:HB3	1:D:151:LYS:HE3	1.98	0.44
2:B:231:ILE:O	2:B:235:LEU:HB2	2.17	0.44
3:C:2:SER:HB2	3:C:23:LEU:HB3	1.99	0.44
2:E:52:ASN:HA	2:E:52:ASN:HD22	1.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:HD13	1:D:304[B]:ARG:HD2	2.00	0.44
1:A:416:VAL:N	3:C:55:HIS:HE1	2.06	0.44
1:D:139:GLN:NE2	2:E:80:TYR:H	2.07	0.43
1:A:384:ARG:HD3	7:A:622:HOH:O	2.17	0.43
1:D:61[B]:ILE:HG12	1:D:65:LYS:HE3	2.00	0.43
1:A:388:VAL:O	1:A:388:VAL:HG12	2.17	0.43
1:D:435:TRP:O	1:D:439:GLN:HG2	2.18	0.43
1:A:97:TYR:CE1	1:A:145:PRO:HD3	2.54	0.43
1:A:299:ILE:HD11	1:A:324:ILE:CD1	2.48	0.43
2:B:77:GLN:NE2	7:B:361:HOH:O	2.52	0.43
1:D:39:ILE:HA	1:D:40:PRO:HD3	1.87	0.43
2:E:195:GLY:CA	2:E:303[A]:MET:CE	2.97	0.43
2:B:19:ARG:NH1	2:B:19:ARG:CG	2.74	0.43
3:C:55:HIS:O	3:C:56:ARG:HB2	2.19	0.43
1:D:177:ASP:HA	1:D:181:THR:OG1	2.18	0.43
1:D:299:ILE:HD11	1:D:324:ILE:CD1	2.49	0.43
2:E:18:MET:CG	2:E:20:LYS:HG2	2.48	0.43
2:B:83:TYR:CZ	2:B:87:GLN:HG3	2.54	0.43
1:D:127:ALA:HB2	1:D:237:GLN:HE22	1.84	0.42
1:D:427:HIS:CE1	3:F:75:THR:O	2.72	0.42
1:D:24:THR:OG1	1:D:27:GLN:HG3	2.19	0.42
1:A:384:ARG:NH1	1:A:384:ARG:CG	2.77	0.42
3:F:62:PRO:HD2	3:F:65:MET:CE	2.48	0.42
2:B:233:LYS:O	2:B:237:GLN:NE2	2.53	0.42
2:B:240[A]:TRP:HH2	7:B:1288:HOH:O	1.99	0.42
1:D:177:ASP:HB3	2:E:43:TRP:HB3	2.02	0.42
1:D:371:ARG:NH1	1:D:410:ASP:OD1	2.53	0.41
1:D:107:ALA:HA	1:D:180:ILE:CG2	2.51	0.41
2:B:240[A]:TRP:HA	2:B:240[A]:TRP:CE3	2.55	0.41
1:A:173:LYS:O	1:A:177:ASP:HB2	2.20	0.41
1:D:4:HIS:HE1	2:E:172:GLU:OE1	2.03	0.41
2:E:138:TYR:CZ	2:E:142:MET:HG3	2.56	0.41
2:E:290:ARG:HB3	2:E:291:PRO:HD3	2.02	0.41
3:F:23:LEU:HG	3:F:68:ALA:HB2	2.03	0.41
3:F:65:MET:HE2	3:F:65:MET:HB3	1.30	0.41
1:D:379:ASN:ND2	1:D:384:ARG:HH11	2.12	0.40
1:D:4:HIS:HE1	2:E:172:GLU:HG3	1.86	0.40
2:B:14:HIS:CE1	2:B:15:LEU:HG	2.56	0.40
1:A:374:ASP:O	1:A:378:GLU:HG3	2.21	0.40
1:A:159:TRP:CE2	2:B:14:HIS:CD2	3.09	0.40
2:B:237:GLN:HG3	7:B:852:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:ILE:HG12	1:D:192:LEU:HD13	2.02	0.40
1:A:148:TYR:HB3	1:A:155:PHE:CD2	2.56	0.40
2:B:301:LEU:HA	2:B:301:LEU:HD23	1.92	0.40
3:C:2:SER:HB3	7:C:527:HOH:O	2.21	0.40
2:E:195:GLY:HA3	2:E:303[B]:MET:SD	2.62	0.40
3:F:54:LYS:HE2	3:F:54:LYS:HB3	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	492/500 (98%)	477 (97%)	15 (3%)	0	100	100
1	D	500/500 (100%)	486 (97%)	14 (3%)	0	100	100
2	B	306/327 (94%)	301 (98%)	5 (2%)	0	100	100
2	E	308/327 (94%)	302 (98%)	6 (2%)	0	100	100
3	C	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
3	F	79/84 (94%)	75 (95%)	3 (4%)	1 (1%)	15	3
All	All	1767/1822 (97%)	1718 (97%)	48 (3%)	1 (0%)	56	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	56	ARG

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	419/423 (99%)	414 (99%)	5 (1%)	78 69
1	D	427/423 (101%)	416 (97%)	11 (3%)	54 36
2	B	279/296 (94%)	274 (98%)	5 (2%)	66 52
2	E	281/296 (95%)	274 (98%)	7 (2%)	55 37
3	C	75/75 (100%)	72 (96%)	3 (4%)	38 18
3	F	72/75 (96%)	66 (92%)	6 (8%)	14 3
All	All	1553/1588 (98%)	1516 (98%)	37 (2%)	57 39

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	243	GLN
1	A	323	ASP
1	A	384	ARG
1	A	485	ASP
2	B	17	GLU
2	B	212	TRP
2	B	275	ASN
2	B	292	LEU
2	B	305	SER
3	C	42	ARG
3	C	56	ARG
3	C	58	THR
1	D	251	ARG
1	D	296	GLU
1	D	304[A]	ARG
1	D	304[B]	ARG
1	D	319	LEU
1	D	323	ASP
1	D	367	LYS
1	D	371	ARG
1	D	443	GLN
1	D	469	LYS
1	D	493	LYS
2	E	18	MET
2	E	20	LYS

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Mol	Chain	Res	Type
2	E	21	LYS
2	E	38	ASN
2	E	52	ASN
2	E	206	GLN
2	E	290	ARG
3	F	15	LEU
3	F	46	ARG
3	F	47	GLU
3	F	56	ARG
3	F	58	THR
3	F	64	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	123	ASN
1	A	139	GLN
1	A	141	GLN
1	A	237	GLN
1	A	248	ASN
1	A	379	ASN
1	A	398	ASN
1	A	484	HIS
2	B	77	GLN
2	B	84	ASN
2	B	141	GLN
2	B	150	ASN
2	B	165	HIS
2	B	236	GLN
2	B	242	ASN
2	B	275	ASN
3	C	7	HIS
3	C	55	HIS
1	D	4	HIS
1	D	123	ASN
1	D	139	GLN
1	D	237	GLN
1	D	248	ASN
1	D	379	ASN
1	D	382	ASN
1	D	398	ASN

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Mol	Chain	Res	Type
1	D	427	HIS
1	D	439	GLN
1	D	443	GLN
1	D	445	GLN
1	D	474	GLN
2	E	38	ASN
2	E	52	ASN
2	E	77	GLN
2	E	84	ASN
2	E	100	GLN
2	E	108	GLN
2	E	141	GLN
2	E	150	ASN
2	E	165	HIS
2	E	185	HIS
2	E	206	GLN
2	E	237	GLN
2	E	238	GLN
2	E	242	ASN
3	F	7	HIS
3	F	55	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 14 ligands modelled in this entry, 13 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
6	AZI	D	510	4	0,2,2	0.00	-	0,1,1	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
6	AZI	D	510	4	-	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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	491/500 (98%)	-0.34	5 (1%)	84	84	14, 23, 39, 52	0
1	D	492/500 (98%)	-0.41	2 (0%)	93	92	14, 21, 34, 50	0
2	B	304/327 (92%)	-0.39	2 (0%)	89	88	15, 21, 33, 46	0
2	E	304/327 (92%)	-0.45	3 (0%)	84	84	13, 20, 32, 43	0
3	C	82/84 (97%)	-0.15	2 (2%)	62	60	22, 31, 41, 48	0
3	F	81/84 (96%)	-0.10	5 (6%)	24	22	20, 30, 44, 49	0
All	All	1754/1822 (96%)	-0.37	19 (1%)	82	82	13, 22, 38, 52	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	18	MET	4.9
2	E	17	GLU	3.3
1	A	464	LEU	3.2
2	B	240[A]	TRP	3.0
3	F	56	ARG	2.9
2	E	306	SER	2.8
3	F	58	THR	2.6
1	D	78	ARG	2.6
3	F	81	VAL	2.6
2	E	19	ARG	2.5
1	A	79	ALA	2.4
1	A	491	LYS	2.3
3	C	58	THR	2.3
1	A	78	ARG	2.2
1	A	490	ASP	2.1
3	C	59	GLU	2.1
1	D	383	ASP	2.0
3	F	47	GLU	2.0
3	F	2	SER	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, 95^{th} 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
6	AZI	D	510	3/3	0.91	0.23	7.22	33,33,41,42	0
4	FE	A	501	1/1	1.00	0.11	0.66	20,20,20,20	0
5	CA	B	504	1/1	0.97	0.12	0.24	39,39,39,39	0
4	FE	D	508	1/1	1.00	0.10	-0.49	18,18,18,18	0
4	FE	A	502	1/1	1.00	0.10	-0.90	23,23,23,23	0
4	FE	D	507	1/1	0.99	0.10	-1.31	23,23,23,23	0
5	CA	E	512	1/1	0.99	0.06	-2.02	29,29,29,29	0
5	CA	B	505	1/1	0.99	0.04	-2.93	28,28,28,28	0
5	CA	C	506	1/1	0.99	0.05	-3.51	38,38,38,38	0
5	CA	F	513	1/1	0.99	0.07	-	38,38,38,38	0
5	CA	B	511	1/1	0.97	0.11	-	49,49,49,49	0
5	CA	E	509	1/1	0.99	0.08	-	33,33,33,33	0
5	CA	B	502	1/1	0.99	0.10	-	31,31,31,31	0
5	CA	B	503	1/1	0.99	0.03	-	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.