Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 12:31 AM EST

PDB ID	:	3DHI
Title	:	Crystal Structure of Reduced Toluene 4-Monoxygenase Hydroxylase Complexed with Effector Protein
Authors	:	Bailey, L.J.; Mccoy, J.G.; Phillips Jr., G.N.; Fox, B.G.
Deposited on	:	2008-06-17
Resolution	:	1.68 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

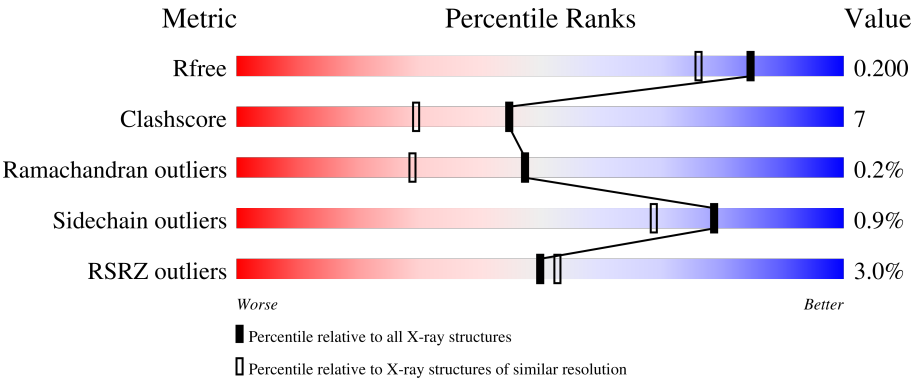
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.68 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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3% 88% 11%
2	B	327	2% 85% 9% 6%
3	C	84	7% 90% 7%
4	E	103	3% 79% 20%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 9198 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	498	Total	C	N	O	S	0	13	0
			4146	2670	692	758	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	306	Total	C	N	O	S	0	9	0
			2574	1628	446	485	15			

- 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
			654	412	117	121	4			

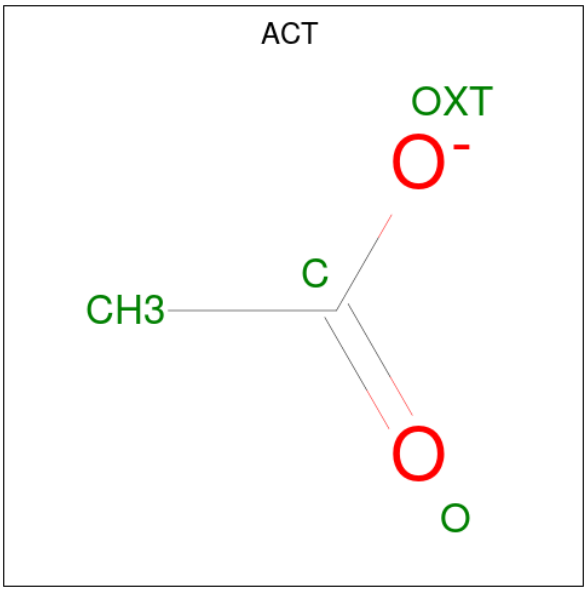
- Molecule 4 is a protein called Toluene-4-monooxygenase system effector protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	103	Total	C	N	O	S	0	5	0
			843	533	142	165	3			

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

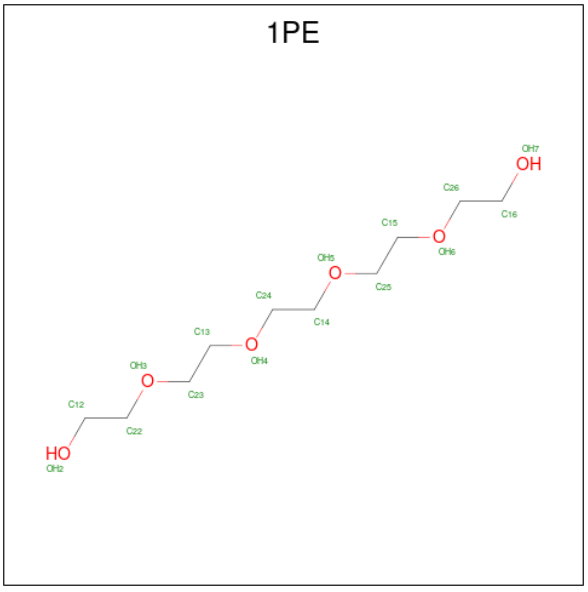
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Fe	0	0
			2	2		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0

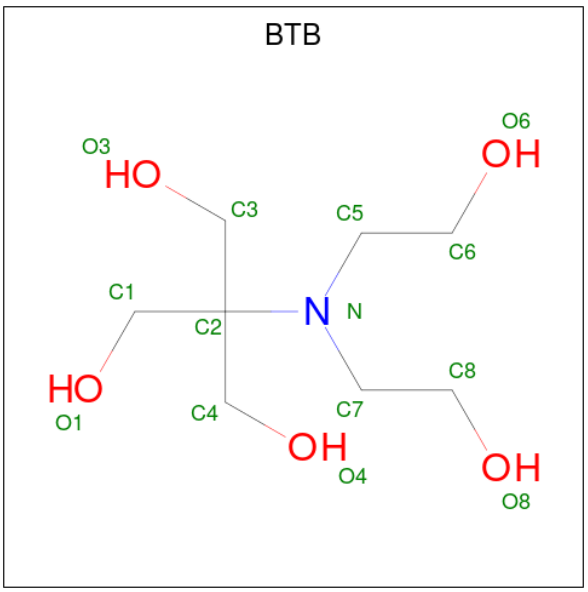
- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 16 10 6	0	0
7	B	1	Total C O 16 10 6	0	0

- Molecule 8 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN

E-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			14	8	1	5		

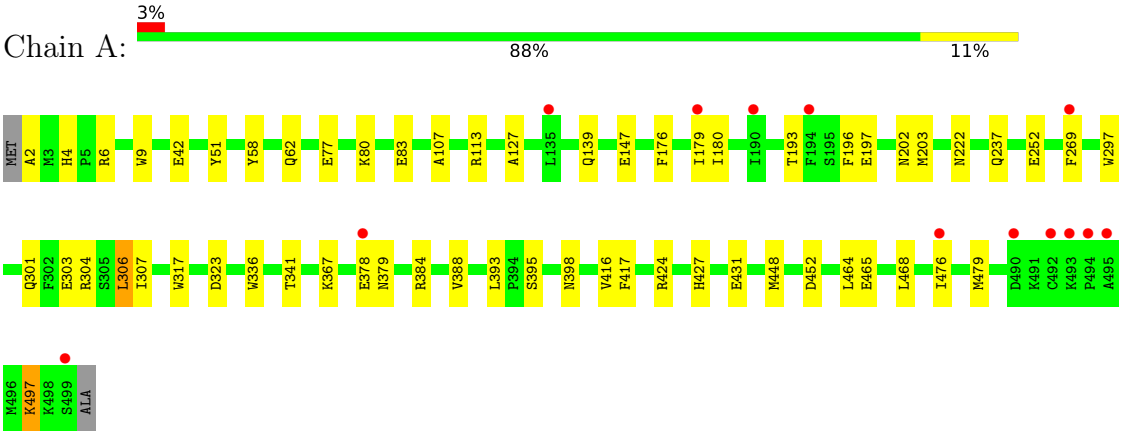
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	456	Total	O	0	0
			456	456		
9	B	277	Total	O	0	0
			277	277		
9	C	58	Total	O	0	0
			58	58		
9	E	138	Total	O	0	0
			138	138		

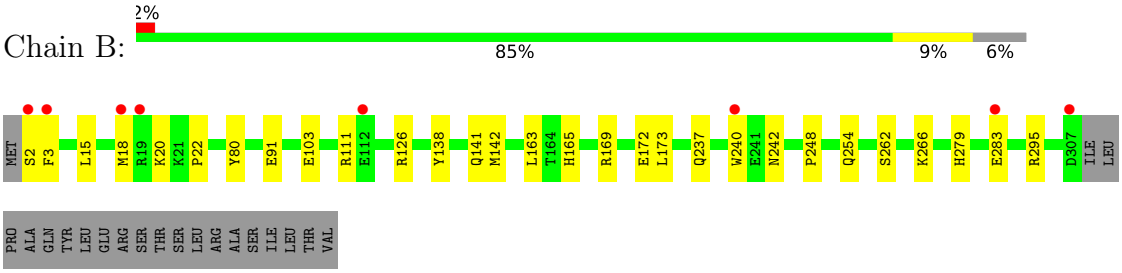
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

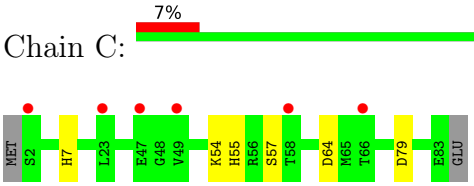
• Molecule 1: toluene 4-monooxygenase hydroxylase alpha subunit



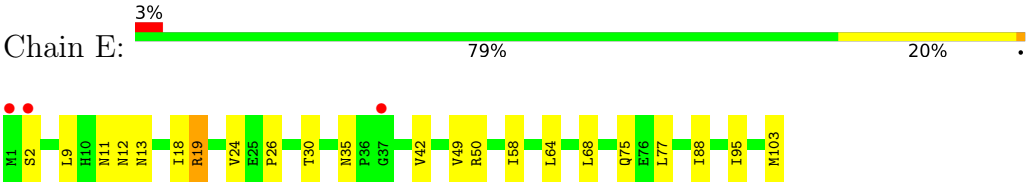
• Molecule 2: toluene 4-monooxygenase hydroxylase beta subunit



• Molecule 3: toluene 4-monooxygenase hydroxylase gamma subunit



• Molecule 4: Toluene-4-monooxygenase system effector protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	97.66Å 115.30Å 180.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.85 – 1.68 48.83 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.85-1.68) 99.7 (48.83-1.68)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.44 (at 1.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.167 , 0.202 0.166 , 0.200	Depositor DCC
R_{free} test set	5782 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	19.0	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9198	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: FE, BTB, 1PE, ACT

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	0.64	0/4311	0.66	0/5849
2	B	0.56	0/2662	0.66	1/3618 (0.0%)
3	C	0.61	0/666	0.59	0/902
4	E	0.75	0/865	0.76	1/1169 (0.1%)
All	All	0.63	0/8504	0.66	2/11538 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	E	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	18	ILE	C-N-CA	5.11	134.47	121.70
2	B	169	ARG	NE-CZ-NH1	-5.00	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	19	ARG	Mainchain

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	4146	0	3943	71	0
2	B	2574	0	2451	27	0
3	C	654	0	649	7	0
4	E	843	0	858	22	0
5	A	2	0	0	0	0
6	A	4	0	3	0	0
7	A	16	0	22	4	0
7	B	16	0	22	3	0
8	C	14	0	19	0	0
9	A	456	0	0	8	1
9	B	277	0	0	2	0
9	C	58	0	0	0	0
9	E	138	0	0	0	0
All	All	9198	0	7967	106	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 (106) 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:196:PHE:HA	9:A:876:HOH:O	1.48	1.13
1:A:448[B]:MET:HE2	1:A:452:ASP:HB3	1.44	0.95
1:A:203:MET:CB	1:A:269[B]:PHE:CZ	2.54	0.91
4:E:12:ASN:HD21	4:E:103:MET:H	1.17	0.90
4:E:88:ILE:HD11	4:E:95[A]:ILE:HD11	1.54	0.89
1:A:203:MET:CB	1:A:269[B]:PHE:HZ	1.89	0.86
1:A:416:VAL:H	3:C:55:HIS:HE1	1.22	0.86
1:A:448[B]:MET:HE2	1:A:452:ASP:CB	2.07	0.85
4:E:11:ASN:HD22	4:E:13:ASN:H	1.26	0.84
1:A:203:MET:HB2	1:A:269[B]:PHE:CE1	2.15	0.82
2:B:18:MET:HE1	2:B:22:PRO:HB3	1.60	0.81
4:E:35:ASN:HD21	4:E:58:ILE:H	1.27	0.79
1:A:196:PHE:HE1	1:A:269[A]:PHE:CE1	2.02	0.78
1:A:416:VAL:H	3:C:55:HIS:CE1	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLU:OE2	9:A:554:HOH:O	2.01	0.78
1:A:203:MET:HB3	1:A:269[B]:PHE:HZ	1.48	0.77
1:A:139:GLN:HE22	2:B:80:TYR:H	1.32	0.76
2:B:165:HIS:HD2	2:B:254:GLN:HE21	1.33	0.74
1:A:301:GLN:HE21	4:E:50:ARG:HH12	1.36	0.74
1:A:196:PHE:CE1	1:A:269[A]:PHE:CE1	2.76	0.73
1:A:203:MET:HG3	1:A:269[B]:PHE:CZ	2.25	0.71
1:A:398:ASN:HD22	1:A:427:HIS:H	1.37	0.71
1:A:203:MET:HB2	1:A:269[B]:PHE:CZ	2.25	0.70
1:A:304:ARG:HH11	4:E:12:ASN:HD22	1.39	0.70
1:A:196:PHE:CE1	1:A:269[A]:PHE:HE1	2.09	0.70
1:A:424:ARG:NH2	1:A:448[B]:MET:HE3	2.08	0.69
1:A:367:LYS:NZ	9:A:886:HOH:O	2.26	0.68
1:A:203:MET:CG	1:A:269[B]:PHE:CZ	2.76	0.68
1:A:113:ARG:HH11	2:B:141:GLN:HE21	1.42	0.67
2:B:295:ARG:NH1	9:B:555:HOH:O	2.21	0.66
1:A:468:LEU:HD13	1:A:479:MET:SD	2.36	0.65
1:A:464:LEU:HD13	7:A:603:1PE:H231	1.79	0.64
1:A:448[B]:MET:CE	1:A:452:ASP:HB3	2.25	0.63
1:A:476:ILE:O	9:A:560:HOH:O	2.16	0.62
3:C:55:HIS:HD2	3:C:79:ASP:OD1	1.83	0.61
2:B:165:HIS:CD2	2:B:254:GLN:HE21	2.16	0.59
1:A:193:THR:HA	1:A:197:GLU:OE1	2.02	0.58
1:A:196:PHE:HE1	1:A:269[A]:PHE:HE1	1.43	0.58
4:E:77:LEU:HD23	4:E:95[B]:ILE:HD12	1.85	0.58
1:A:304:ARG:HH11	4:E:12:ASN:ND2	2.02	0.57
1:A:203:MET:HB3	1:A:269[B]:PHE:CZ	2.29	0.57
1:A:393:LEU:HG	7:A:603:1PE:H241	1.87	0.56
1:A:203:MET:CG	1:A:269[B]:PHE:HZ	2.18	0.56
2:B:262:SER:O	2:B:266:LYS:HG2	2.07	0.54
4:E:24:VAL:HG13	4:E:49[B]:VAL:HG21	1.90	0.53
1:A:367:LYS:HD3	9:A:736:HOH:O	2.09	0.52
4:E:88:ILE:CD1	4:E:95[A]:ILE:HD11	2.36	0.50
2:B:18:MET:CE	2:B:22:PRO:HB3	2.36	0.50
4:E:26:PRO:HG2	4:E:68[B]:LEU:HD23	1.94	0.50
1:A:417:PHE:CE1	1:A:431:GLU:HG2	2.47	0.50
2:B:15:LEU:HB3	2:B:18:MET:CE	2.41	0.50
1:A:393:LEU:HG	7:A:603:1PE:H132	1.93	0.49
2:B:126:ARG:HB2	2:B:163:LEU:CD1	2.42	0.49
1:A:306:LEU:C	1:A:306:LEU:HD23	2.33	0.49
2:B:138:TYR:CZ	2:B:142:MET:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:HIS:CE1	2:B:283:GLU:OE2	2.66	0.48
1:A:341:THR:HG21	7:A:603:1PE:H142	1.95	0.48
1:A:424:ARG:CZ	1:A:448[B]:MET:HE3	2.44	0.48
4:E:42:VAL:HG13	4:E:49[A]:VAL:CG1	2.44	0.48
1:A:379:ASN:HD22	1:A:384:ARG:NE	2.13	0.47
1:A:203:MET:HB2	1:A:269[B]:PHE:HE1	1.75	0.47
1:A:139:GLN:NE2	2:B:80:TYR:H	2.07	0.46
1:A:303[B]:GLU:HG3	1:A:317:TRP:CZ3	2.50	0.46
1:A:127:ALA:HB2	1:A:237:GLN:HE22	1.81	0.46
2:B:18:MET:HE2	2:B:18:MET:HB2	1.79	0.46
3:C:54:LYS:O	3:C:57:SER:HB2	2.16	0.46
1:A:4:HIS:HE1	2:B:172:GLU:OE1	1.99	0.45
1:A:113:ARG:HH11	2:B:141:GLN:NE2	2.12	0.45
1:A:497:LYS:H	1:A:497:LYS:HE2	1.81	0.45
1:A:58:TYR:CZ	1:A:62:GLN:HG3	2.51	0.45
4:E:77:LEU:HD23	4:E:95[B]:ILE:CD1	2.47	0.45
1:A:2:ALA:N	2:B:103:GLU:OE1	2.50	0.44
1:A:107:ALA:HA	1:A:180:ILE:HG21	2.00	0.44
2:B:248:PRO:HB3	7:B:604:1PE:H241	1.99	0.44
2:B:15:LEU:HB3	2:B:18:MET:HE1	1.99	0.44
1:A:176[B]:PHE:CD1	1:A:180:ILE:HD12	2.52	0.44
2:B:91:GLU:OE1	2:B:165:HIS:HE1	2.01	0.44
1:A:301:GLN:NE2	4:E:50:ARG:HH12	2.10	0.43
2:B:126:ARG:HB2	2:B:163:LEU:HD13	2.00	0.43
2:B:237:GLN:HA	7:B:604:1PE:H152	2.00	0.43
1:A:303[B]:GLU:HB3	4:E:9:LEU:HD13	2.01	0.43
1:A:147:GLU:HB3	9:A:836:HOH:O	2.17	0.43
1:A:80:LYS:HB3	1:A:83:GLU:HG2	2.00	0.43
1:A:465:GLU:OE2	2:B:2:SER:N	2.52	0.43
1:A:222:ASN:OD1	4:E:19:ARG:NH2	2.52	0.42
1:A:179:ILE:HG13	1:A:180:ILE:HG13	2.00	0.42
1:A:301:GLN:NE2	4:E:50:ARG:HH22	2.17	0.42
2:B:240:TRP:CG	7:B:604:1PE:H262	2.55	0.42
4:E:30:THR:HG21	4:E:64[B]:LEU:HG	2.00	0.42
1:A:6:ARG:HH12	4:E:75:GLN:HE22	1.68	0.41
1:A:77:GLU:OE2	1:A:147:GLU:OE2	2.38	0.41
1:A:203:MET:CB	1:A:269[B]:PHE:CE1	2.87	0.41
1:A:336:TRP:HH2	1:A:388[A]:VAL:CG1	2.32	0.41
1:A:336:TRP:CH2	1:A:388[A]:VAL:CG1	3.03	0.41
2:B:111:ARG:HB3	2:B:242:ASN:HD22	1.85	0.41
1:A:202:ASN:HB3	1:A:297:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:HIS:ND1	2:B:283:GLU:OE2	2.54	0.41
1:A:378:GLU:HG3	9:A:679:HOH:O	2.21	0.40
1:A:395:SER:OG	3:C:7:HIS:CD2	2.75	0.40
9:A:937:HOH:O	3:C:7:HIS:HE1	2.03	0.40
1:A:307:ILE:HD12	4:E:9:LEU:HD11	2.04	0.40
1:A:395:SER:OG	3:C:7:HIS:HD2	2.05	0.40
2:B:240:TRP:HA	9:B:427:HOH:O	2.22	0.40
4:E:77:LEU:CD2	4:E:95[B]:ILE:HD12	2.50	0.40
1:A:6:ARG:HH12	4:E:75:GLN:NE2	2.19	0.40
1:A:6:ARG:HA	1:A:9:TRP:CE2	2.57	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)
9:A:856:HOH:O	9:A:856:HOH:O[4_545]	2.08	0.12

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	507/500 (101%)	493 (97%)	14 (3%)	0	100 100
2	B	310/327 (95%)	307 (99%)	2 (1%)	1 (0%)	41 23
3	C	80/84 (95%)	77 (96%)	3 (4%)	0	100 100
4	E	106/103 (103%)	102 (96%)	3 (3%)	1 (1%)	17 4
All	All	1003/1014 (99%)	979 (98%)	22 (2%)	2 (0%)	47 29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3	PHE
4	E	2	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	433/423 (102%)	428 (99%)	5 (1%)	71	57
2	B	283/296 (96%)	281 (99%)	2 (1%)	84	76
3	C	73/75 (97%)	72 (99%)	1 (1%)	67	51
4	E	92/87 (106%)	92 (100%)	0	100	100
All	All	881/881 (100%)	873 (99%)	8 (1%)	78	69

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	51	TYR
1	A	306	LEU
1	A	323	ASP
1	A	497	LYS
2	B	20	LYS
2	B	173	LEU
3	C	64[A]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) 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	204	GLN
1	A	237	GLN
1	A	248	ASN

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Mol	Chain	Res	Type
1	A	301	GLN
1	A	379	ASN
1	A	398	ASN
2	B	84	ASN
2	B	102	ASN
2	B	141	GLN
2	B	150	ASN
2	B	165	HIS
2	B	242	ASN
3	C	7	HIS
3	C	55	HIS
4	E	11	ASN
4	E	12	ASN
4	E	13	ASN
4	E	35	ASN
4	E	75	GLN
4	E	87	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 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	$\#\|Z\|>2$
8	BTB	C	605	-	13,13,13	0.42	0	7,16,16	0.65	0
7	1PE	B	604	-	15,15,15	0.44	0	14,14,14	0.32	0
7	1PE	A	603	-	15,15,15	0.47	0	14,14,14	0.26	0
6	ACT	A	602	5	3,3,3	0.79	0	3,3,3	1.53	0

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
7	1PE	B	604	-	-	7/13/13/13	-
7	1PE	A	603	-	-	9/13/13/13	-
8	BTB	C	605	-	-	3/21/21/21	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	605	BTB	C4-C2-C3-O3
7	B	604	1PE	OH6-C15-C25-OH5
7	B	604	1PE	OH5-C14-C24-OH4
7	A	603	1PE	OH5-C14-C24-OH4
7	B	604	1PE	OH4-C13-C23-OH3
7	A	603	1PE	OH2-C12-C22-OH3
7	A	603	1PE	OH7-C16-C26-OH6
7	A	603	1PE	OH4-C13-C23-OH3
7	A	603	1PE	C14-C24-OH4-C13
7	A	603	1PE	C23-C13-OH4-C24
7	B	604	1PE	C25-C15-OH6-C26
7	A	603	1PE	C15-C25-OH5-C14
7	B	604	1PE	C13-C23-OH3-C22
7	B	604	1PE	C12-C22-OH3-C23
8	C	605	BTB	C1-C2-C3-O3
8	C	605	BTB	C4-C2-N-C7
7	A	603	1PE	OH6-C15-C25-OH5
7	A	603	1PE	C16-C26-OH6-C15
7	B	604	1PE	C24-C14-OH5-C25

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	604	1PE	3	0
7	A	603	1PE	4	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, 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	498/500 (99%)	-0.05	13 (2%)	56	58	12, 18, 32, 48	0
2	B	306/327 (93%)	-0.09	8 (2%)	56	58	13, 20, 33, 52	0
3	C	82/84 (97%)	0.46	6 (7%)	15	16	19, 27, 38, 43	1 (1%)
4	E	103/103 (100%)	-0.05	3 (2%)	51	54	12, 19, 30, 49	0
All	All	989/1014 (97%)	-0.02	30 (3%)	50	53	12, 20, 34, 52	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	1	MET	8.2
4	E	2	SER	5.1
1	A	269[A]	PHE	4.9
2	B	307	ASP	4.6
2	B	2	SER	4.2
2	B	240	TRP	4.2
3	C	23	LEU	3.9
2	B	3	PHE	3.6
4	E	37	GLY	3.6
1	A	494	PRO	3.4
3	C	47	GLU	3.0
3	C	2	SER	2.9
1	A	492	CYS	2.9
1	A	499	SER	2.9
1	A	493	LYS	2.9
1	A	135	LEU	2.8
3	C	58	THR	2.8
1	A	190[A]	ILE	2.7
2	B	19	ARG	2.5
1	A	490	ASP	2.5
1	A	495	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	194	PHE	2.3
3	C	66	THR	2.2
1	A	378	GLU	2.2
2	B	283	GLU	2.2
1	A	179	ILE	2.1
1	A	476	ILE	2.1
2	B	18	MET	2.1
2	B	112	GLU	2.1
3	C	49	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
7	1PE	B	604	16/16	0.79	0.18	53,57,62,63	0
8	BTB	C	605	14/14	0.82	0.23	36,39,39,40	0
7	1PE	A	603	16/16	0.85	0.20	42,50,56,57	0
6	ACT	A	602	4/4	0.90	0.19	27,29,29,30	0
5	FE	A	601	1/1	0.99	0.06	17,17,17,17	0
5	FE	A	600	1/1	1.00	0.07	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.