



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:35 PM UTC

PDB ID : 6D3H / pdb_00006d3h
Title : FT_T dioxygenase with bound dichlorprop
Authors : Rydel, T.J.; Halls, C.E.
Deposited on : 2018-04-16
Resolution : 2.03 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

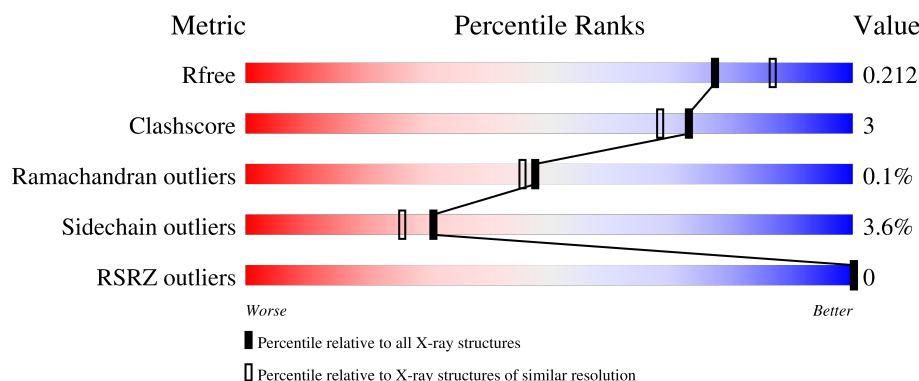
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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 $\leq 5\%$. 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	295	 86% 9% . .
1	B	295	 86% 8% . .
1	I	295	 86% 9% . .
1	M	295	 84% 9% . . .

2 Entry composition [i](#)

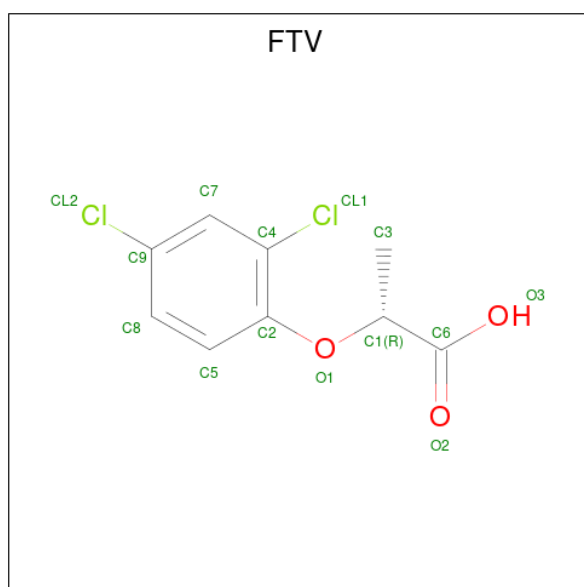
There are 6 unique types of molecules in this entry. The entry contains 10298 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FT_T dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	1	0
			2292	1457	394	430	11			
1	B	286	Total	C	N	O	S	0	1	0
			2292	1457	394	430	11			
1	I	286	Total	C	N	O	S	0	2	0
			2297	1461	394	430	12			
1	M	287	Total	C	N	O	S	0	2	0
			2305	1465	396	433	11			

- Molecule 2 is (2R)-2-(2,4-dichlorophenoxy)propanoic acid (CCD ID: FTV) (formula: C₉H₈Cl₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	O	0	0
			14	9	2	3		
2	B	1	Total	C	Cl	O	0	0
			14	9	2	3		

Continued on next page...

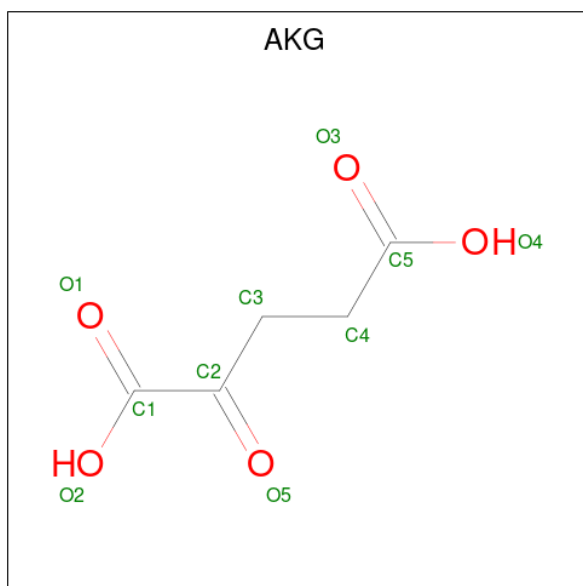
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total	C	Cl	O	0	0
			14	9	2	3		
2	M	1	Total	C	Cl	O	0	0
			14	9	2	3		

- Molecule 3 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Co	0	0
			1	1		
3	B	1	Total	Co	0	0
			1	1		
3	I	1	Total	Co	0	0
			1	1		
3	M	1	Total	Co	0	0
			1	1		

- Molecule 4 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		
4	B	1	Total	C	O	0	0
			10	5	5		
4	I	1	Total	C	O	0	0
			10	5	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	M	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		
5	I	1	Total	Cl	0	0
			1	1		
5	M	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

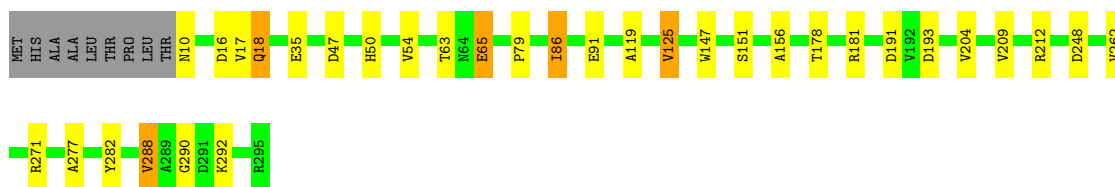
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	245	Total	O	0	0
			245	245		
6	B	260	Total	O	0	0
			260	260		
6	I	240	Total	O	0	0
			240	240		
6	M	263	Total	O	0	0
			263	263		

3 Residue-property plots

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.

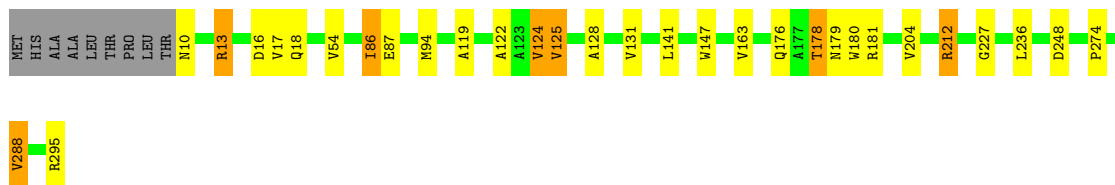
- Molecule 1: FT_T dioxygenase

Chain A: 



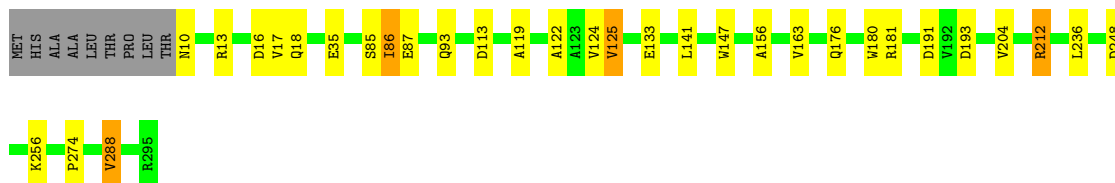
- Molecule 1: FT_T dioxygenase

Chain B: 



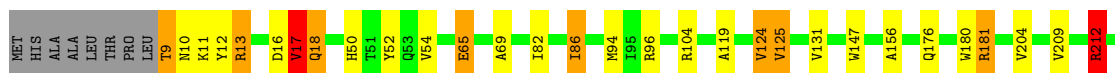
- Molecule 1: FT_T dioxygenase

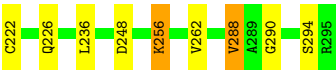
Chain I: 



- Molecule 1: FT_T dioxygenase

Chain M: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	138.16Å 138.16Å 148.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.60 – 2.03 46.60 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.60-2.03) 99.9 (46.60-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.170 , 0.211 0.172 , 0.212	Depositor DCC
R_{free} test set	5183 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10298	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0722e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: FTV, CO, AKG, CL

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	1.47	12/2355 (0.5%)	1.25	8/3206 (0.2%)
1	B	1.48	8/2355 (0.3%)	1.28	7/3206 (0.2%)
1	I	1.48	6/2363 (0.3%)	1.28	8/3216 (0.2%)
1	M	1.47	11/2371 (0.5%)	1.24	7/3228 (0.2%)
All	All	1.48	37/9444 (0.4%)	1.26	30/12856 (0.2%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	119	ALA	CA-CB	7.84	1.64	1.53
1	B	122	ALA	CA-CB	7.10	1.65	1.53
1	B	274	PRO	CA-CB	7.01	1.57	1.53
1	A	119	ALA	CA-CB	6.90	1.62	1.53
1	M	124	VAL	CA-CB	6.74	1.64	1.54
1	A	156	ALA	CA-CB	6.62	1.64	1.53
1	M	290	GLY	N-CA	6.60	1.50	1.44
1	I	125	VAL	CA-CB	6.57	1.62	1.53
1	I	122	ALA	CA-CB	6.43	1.63	1.53
1	M	156	ALA	CA-CB	6.26	1.63	1.53
1	A	288	VAL	C-O	6.22	1.31	1.24
1	I	156	ALA	CA-CB	6.21	1.62	1.53
1	M	262	VAL	CA-CB	6.13	1.62	1.54
1	B	119	ALA	CA-CB	6.11	1.60	1.53
1	A	54	VAL	CA-CB	6.08	1.62	1.54
1	A	125	VAL	CA-CB	6.08	1.61	1.53
1	M	131	VAL	CA-CB	6.07	1.61	1.55
1	A	47	ASP	CA-C	6.00	1.60	1.52
1	I	274	PRO	CA-CB	5.99	1.57	1.53
1	B	128	ALA	CA-CB	5.97	1.61	1.53
1	M	54	VAL	CA-CB	5.82	1.61	1.54
1	A	290	GLY	N-CA	5.73	1.50	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	163	VAL	C-O	5.70	1.29	1.24
1	B	163	VAL	C-O	5.60	1.29	1.24
1	B	131	VAL	C-O	-5.48	1.20	1.24
1	A	151	SER	N-CA	5.46	1.53	1.45
1	M	222	CYS	N-CA	5.45	1.52	1.46
1	B	54	VAL	CA-CB	5.45	1.61	1.54
1	M	18	GLN	CG-CD	5.44	1.65	1.52
1	B	125	VAL	CA-CB	5.43	1.60	1.53
1	A	262	VAL	CA-CB	5.37	1.62	1.54
1	I	119	ALA	CA-CB	5.34	1.60	1.53
1	A	18	GLN	CG-CD	5.32	1.65	1.52
1	M	69	ALA	CA-CB	5.26	1.61	1.53
1	A	277	ALA	CA-CB	5.13	1.61	1.53
1	M	125	VAL	CA-CB	5.07	1.60	1.53
1	A	18	GLN	CD-OE1	5.02	1.33	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	86	ILE	CB-CA-C	-9.13	98.68	111.28
1	B	86	ILE	CB-CA-C	-8.76	99.20	111.28
1	A	86	ILE	CB-CA-C	-8.70	99.27	111.28
1	M	86	ILE	CB-CA-C	-8.32	99.79	111.28
1	A	65	GLU	CA-CB-CG	7.87	129.83	114.10
1	A	65	GLU	CB-CG-CD	6.50	123.64	112.60
1	A	63	THR	N-CA-C	-5.94	102.86	110.53
1	B	288	VAL	CB-CA-C	5.74	118.85	110.98
1	I	212	ARG	NE-CZ-NH2	-5.72	114.06	119.20
1	B	288	VAL	CA-CB-CG2	5.71	120.11	110.40
1	B	125	VAL	CG1-CB-CG2	5.63	123.19	110.80
1	A	212	ARG	CB-CG-CD	-5.48	98.70	111.30
1	I	125	VAL	CG1-CB-CG2	5.46	122.80	110.80
1	B	212	ARG	NE-CZ-NH2	-5.42	114.32	119.20
1	B	227	GLY	N-CA-C	-5.39	108.67	115.08
1	M	65	GLU	CA-CB-CG	5.34	124.77	114.10
1	A	35	GLU	CA-C-N	-5.27	114.53	119.85
1	A	35	GLU	C-N-CA	-5.27	114.53	119.85
1	A	125	VAL	CA-CB-CG1	5.21	119.25	110.40
1	I	288	VAL	CG1-CB-CG2	5.19	122.22	110.80
1	M	17	VAL	CG1-CB-CG2	5.19	122.21	110.80
1	B	124	VAL	CG1-CB-CG2	5.17	122.17	110.80
1	I	35	GLU	CA-C-N	-5.16	114.39	119.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	35	GLU	C-N-CA	-5.16	114.39	119.92
1	M	125	VAL	CG1-CB-CG2	5.16	122.15	110.80
1	I	212	ARG	CB-CG-CD	-5.16	99.44	111.30
1	M	124	VAL	CG1-CB-CG2	5.15	122.14	110.80
1	M	212	ARG	CB-CG-CD	-5.09	99.60	111.30
1	M	288	VAL	CA-CB-CG1	5.06	119.00	110.40
1	I	113	ASP	N-CA-C	5.02	117.71	110.28

There are no chirality outliers.

There are no planarity outliers.

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	2292	0	2224	11	0
1	B	2292	0	2224	16	0
1	I	2297	0	2233	15	0
1	M	2305	0	2239	19	0
2	A	14	0	0	0	0
2	B	14	0	0	0	0
2	I	14	0	0	0	0
2	M	14	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	I	1	0	0	0	0
3	M	1	0	0	0	0
4	A	10	0	4	0	0
4	B	10	0	4	0	0
4	I	10	0	4	0	0
4	M	10	0	4	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	I	1	0	0	0	0
5	M	1	0	0	0	0
6	A	245	0	0	4	0
6	B	260	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	240	0	0	5	0
6	M	263	0	0	9	0
All	All	10298	0	8936	59	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 3.

All (59) 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:M:13:ARG:NH1	6:M:401:HOH:O	1.67	1.28
1:I:180:TRP:CD1	6:I:440:HOH:O	2.01	1.11
1:B:180:TRP:HE3	6:B:639:HOH:O	1.47	0.96
1:I:180:TRP:HD1	6:I:440:HOH:O	1.40	0.95
1:M:248:ASP:CG	6:M:415:HOH:O	2.09	0.94
1:B:16:ASP:HB3	1:B:18:GLN:HE22	1.49	0.78
1:M:9:THR:HG21	1:M:52:TYR:OH	1.88	0.73
1:I:248:ASP:CG	6:I:407:HOH:O	2.30	0.73
1:I:16:ASP:HB3	1:I:18:GLN:HE22	1.55	0.72
1:B:248:ASP:CG	6:B:421:HOH:O	2.34	0.70
1:M:212:ARG:HD3	6:M:572:HOH:O	1.92	0.69
1:M:16:ASP:HB3	1:M:18:GLN:HE22	1.59	0.67
1:I:212:ARG:NH2	6:I:402:HOH:O	2.27	0.66
1:A:16:ASP:HB3	1:A:18:GLN:HE22	1.61	0.65
1:M:248:ASP:CB	6:M:415:HOH:O	2.41	0.65
1:M:256:LYS:HE2	6:M:479:HOH:O	1.97	0.64
1:I:256:LYS:HE3	6:I:501:HOH:O	1.97	0.62
1:M:11:LYS:O	6:M:402:HOH:O	2.15	0.62
1:I:176:GLN:NE2	1:I:181:ARG:HH22	2.01	0.58
1:B:212:ARG:NH2	6:B:408:HOH:O	2.40	0.54
1:B:178:THR:CG2	6:B:423:HOH:O	2.56	0.53
1:A:292:LYS:HG3	6:A:631:HOH:O	2.08	0.53
1:B:178:THR:OG1	6:B:401:HOH:O	2.00	0.52
1:M:226:GLN:OE1	6:M:403:HOH:O	2.19	0.51
1:A:178:THR:O	1:A:181:ARG:NH1	2.44	0.51
1:M:248:ASP:HB2	6:M:415:HOH:O	2.08	0.51
1:A:271:ARG:NH2	6:A:405:HOH:O	2.35	0.50
6:A:483:HOH:O	1:I:13:ARG:HD3	2.11	0.50
1:A:50:HIS:CE1	1:A:209:VAL:HG11	2.48	0.49
1:B:178:THR:HG22	6:B:423:HOH:O	2.13	0.49
1:I:176:GLN:HE22	1:I:181:ARG:HH22	1.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ILE:CD1	1:B:94:MET:HG2	2.43	0.48
1:B:176:GLN:NE2	1:B:181:ARG:HH22	2.12	0.48
1:B:180:TRP:CE3	6:B:639:HOH:O	2.36	0.48
1:A:191:ASP:OD2	1:A:193:ASP:HB2	2.14	0.46
1:M:9:THR:C	6:M:450:HOH:O	2.58	0.46
1:B:13:ARG:NH1	1:M:96:ARG:HH22	2.14	0.45
1:I:141:LEU:C	1:I:141:LEU:HD12	2.42	0.45
1:B:147:TRP:CZ3	1:B:204:VAL:HG21	2.52	0.44
1:M:12:TYR:CD2	1:M:17:VAL:HG13	2.52	0.44
1:A:79:PRO:HD3	1:A:91:GLU:OE1	2.17	0.44
1:B:86:ILE:HG22	1:B:87:GLU:N	2.32	0.44
1:B:141:LEU:C	1:B:141:LEU:HD12	2.43	0.43
1:I:85:SER:HA	1:I:93:GLN:HA	2.00	0.43
1:I:256:LYS:HA	1:I:256:LYS:HD3	1.83	0.43
1:I:191:ASP:OD2	1:I:193:ASP:HB2	2.19	0.43
1:A:86:ILE:CD1	1:A:282:TYR:OH	2.67	0.43
1:A:292:LYS:HB3	1:A:292:LYS:HE3	1.87	0.42
1:B:86:ILE:N	1:B:86:ILE:HD13	2.33	0.42
1:I:86:ILE:HG22	1:I:87:GLU:N	2.33	0.42
1:B:13:ARG:HH12	1:M:96:ARG:HH22	1.67	0.42
1:M:147:TRP:CZ3	1:M:204:VAL:HG21	2.56	0.41
1:I:147:TRP:CZ3	1:I:204:VAL:HG21	2.55	0.41
1:M:86:ILE:CD1	1:M:94:MET:HG2	2.51	0.41
1:M:176:GLN:NE2	1:M:181:ARG:HH22	2.19	0.41
1:A:271:ARG:NE	6:A:405:HOH:O	2.39	0.41
1:A:147:TRP:CZ3	1:A:204:VAL:HG21	2.57	0.40
1:M:50:HIS:CE1	1:M:209:VAL:HG11	2.57	0.40
1:M:104:ARG:HD2	1:M:180:TRP:CE3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/295 (97%)	278 (98%)	7 (2%)	0	100	100
1	B	285/295 (97%)	279 (98%)	6 (2%)	0	100	100
1	I	286/295 (97%)	281 (98%)	5 (2%)	0	100	100
1	M	287/295 (97%)	282 (98%)	4 (1%)	1 (0%)	36	31
All	All	1143/1180 (97%)	1120 (98%)	22 (2%)	1 (0%)	48	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	10	ASN

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	250/256 (98%)	244 (98%)	6 (2%)	43	41
1	B	250/256 (98%)	240 (96%)	10 (4%)	28	22
1	I	251/256 (98%)	244 (97%)	7 (3%)	38	35
1	M	252/256 (98%)	239 (95%)	13 (5%)	21	13
All	All	1003/1024 (98%)	967 (96%)	36 (4%)	31	26

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	17	VAL
1	A	65	GLU
1	A	125	VAL
1	A	248	ASP
1	A	288	VAL
1	B	10	ASN
1	B	13	ARG
1	B	17	VAL
1	B	124	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	125	VAL
1	B	178	THR
1	B	179	ASN
1	B	236	LEU
1	B	288	VAL
1	B	295	ARG
1	I	10	ASN
1	I	17	VAL
1	I	124	VAL
1	I	125	VAL
1	I	133	GLU
1	I	236	LEU
1	I	288	VAL
1	M	9	THR
1	M	13	ARG
1	M	17	VAL
1	M	65	GLU
1	M	82	ILE
1	M	124	VAL
1	M	125	VAL
1	M	181	ARG
1	M	212	ARG
1	M	236	LEU
1	M	256	LYS
1	M	288	VAL
1	M	294	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	50	HIS
1	A	64	ASN
1	A	176	GLN
1	A	226	GLN
1	B	18	GLN
1	B	50	HIS
1	B	64	ASN
1	B	176	GLN
1	I	18	GLN
1	I	50	HIS
1	I	176	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	18	GLN
1	M	50	HIS
1	M	64	ASN
1	M	176	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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$
2	FTV	M	301	-	14,14,14	1.40	1 (7%)	19,19,19	1.66	4 (21%)
4	AKG	I	303	3	9,9,9	2.15	3 (33%)	11,11,11	2.14	5 (45%)
2	FTV	B	301	-	14,14,14	1.10	1 (7%)	19,19,19	1.44	4 (21%)
4	AKG	B	303	3	9,9,9	2.19	3 (33%)	11,11,11	1.37	2 (18%)
4	AKG	A	303	3	9,9,9	2.11	3 (33%)	11,11,11	2.05	4 (36%)
2	FTV	A	301	-	14,14,14	1.46	3 (21%)	19,19,19	1.95	7 (36%)
2	FTV	I	301	-	14,14,14	1.12	0	19,19,19	1.54	3 (15%)
4	AKG	M	303	3	9,9,9	1.64	2 (22%)	11,11,11	2.09	2 (18%)

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
2	FTV	M	301	-	-	6/8/8/8	0/1/1/1
4	AKG	I	303	3	-	3/9/9/9	-
2	FTV	B	301	-	-	6/8/8/8	0/1/1/1
4	AKG	B	303	3	-	2/9/9/9	-
4	AKG	A	303	3	-	1/9/9/9	-
2	FTV	A	301	-	-	6/8/8/8	0/1/1/1
2	FTV	I	301	-	-	6/8/8/8	0/1/1/1
4	AKG	M	303	3	-	1/9/9/9	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	303	AKG	C2-C1	-4.94	1.46	1.53
4	I	303	AKG	C2-C1	-4.66	1.46	1.53
4	A	303	AKG	C2-C1	-4.11	1.47	1.53
4	M	303	AKG	C2-C1	-3.36	1.48	1.53
4	A	303	AKG	O1-C1	3.32	1.30	1.22
2	M	301	FTV	C4-CL1	2.70	1.80	1.73
4	B	303	AKG	O3-C5	2.68	1.30	1.22
4	M	303	AKG	O3-C5	2.67	1.30	1.22
4	A	303	AKG	O2-C1	-2.61	1.23	1.30
4	I	303	AKG	C3-C2	2.51	1.53	1.51
2	B	301	FTV	C9-CL2	2.43	1.80	1.74
4	I	303	AKG	O1-C1	2.38	1.28	1.22
2	A	301	FTV	C4-CL1	2.26	1.79	1.73
2	A	301	FTV	C8-C9	2.19	1.42	1.38
2	A	301	FTV	O2-C6	2.06	1.28	1.22
4	B	303	AKG	O1-C1	2.03	1.27	1.22

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	303	AKG	C3-C2-C1	5.01	124.37	115.86
2	A	301	FTV	C7-C9-CL2	-4.27	113.82	119.17
4	A	303	AKG	C3-C2-C1	3.82	122.35	115.86
4	I	303	AKG	C3-C2-C1	3.68	122.11	115.86
2	A	301	FTV	C4-C7-C9	-3.44	114.83	118.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	303	AKG	O3-C5-C4	-3.29	112.64	123.09
2	M	301	FTV	O1-C1-C6	-3.24	107.24	111.34
2	I	301	FTV	C7-C9-CL2	-3.23	115.11	119.17
4	B	303	AKG	C3-C2-C1	3.19	121.28	115.86
2	I	301	FTV	C4-C7-C9	-3.11	115.20	118.72
2	M	301	FTV	C7-C9-CL2	-3.08	115.30	119.17
4	A	303	AKG	O5-C2-C1	-2.96	115.43	119.67
4	A	303	AKG	O3-C5-C4	-2.95	113.73	123.09
2	B	301	FTV	C3-C1-C6	2.77	114.62	109.42
2	A	301	FTV	C3-C1-C6	2.65	114.40	109.42
2	M	301	FTV	C4-C7-C9	-2.62	115.76	118.72
2	I	301	FTV	C3-C1-C6	2.57	114.23	109.42
2	B	301	FTV	C7-C9-CL2	-2.48	116.05	119.17
4	M	303	AKG	O2-C1-C2	2.45	120.38	113.59
4	I	303	AKG	O4-C5-C4	2.36	121.44	114.00
2	B	301	FTV	C4-C7-C9	-2.34	116.07	118.72
4	I	303	AKG	O2-C1-C2	2.32	120.01	113.59
4	A	303	AKG	O4-C5-C4	2.30	121.28	114.00
4	I	303	AKG	O1-C1-C2	-2.29	118.96	121.81
2	A	301	FTV	O1-C1-C6	-2.26	108.48	111.34
2	M	301	FTV	C7-C4-C2	2.13	123.71	121.01
2	A	301	FTV	C7-C4-C2	2.10	123.68	121.01
4	B	303	AKG	C3-C4-C5	-2.07	108.17	113.67
2	B	301	FTV	O1-C1-C6	-2.05	108.74	111.34
2	A	301	FTV	O3-C6-O2	-2.04	119.44	124.08
2	A	301	FTV	O3-C6-C1	2.03	121.35	113.96

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	FTV	O1-C1-C6-O3
2	B	301	FTV	O1-C1-C6-O2
2	B	301	FTV	C3-C1-C6-O3
2	B	301	FTV	C3-C1-C6-O2
2	I	301	FTV	O1-C1-C6-O3
2	M	301	FTV	O1-C1-C6-O3
2	M	301	FTV	O1-C1-C6-O2
2	M	301	FTV	C3-C1-C6-O3
2	M	301	FTV	C3-C1-C6-O2
4	A	303	AKG	C1-C2-C3-C4
4	B	303	AKG	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	I	303	AKG	C1-C2-C3-C4
4	M	303	AKG	C1-C2-C3-C4
2	A	301	FTV	C3-C1-C6-O3
2	A	301	FTV	C3-C1-C6-O2
2	I	301	FTV	C3-C1-C6-O3
2	I	301	FTV	C3-C1-C6-O2
2	A	301	FTV	O1-C1-C6-O3
2	I	301	FTV	O1-C1-C6-O2
2	B	301	FTV	C3-C1-O1-C2
2	I	301	FTV	C3-C1-O1-C2
2	B	301	FTV	C6-C1-O1-C2
2	I	301	FTV	C6-C1-O1-C2
2	M	301	FTV	C6-C1-O1-C2
4	B	303	AKG	O5-C2-C3-C4
2	A	301	FTV	C3-C1-O1-C2
2	A	301	FTV	C6-C1-O1-C2
2	A	301	FTV	O1-C1-C6-O2
2	M	301	FTV	C3-C1-O1-C2
4	I	303	AKG	C3-C4-C5-O4
4	I	303	AKG	O5-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	286/295 (96%)	-1.33	0 100 100	17, 24, 37, 61	1 (0%)
1	B	286/295 (96%)	-1.35	0 100 100	16, 24, 36, 61	1 (0%)
1	I	286/295 (96%)	-1.33	0 100 100	16, 24, 36, 60	2 (0%)
1	M	287/295 (97%)	-1.32	0 100 100	15, 24, 38, 66	2 (0%)
All	All	1145/1180 (97%)	-1.33	0 100 100	15, 24, 37, 66	6 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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
2	FTV	A	301	14/14	0.99	0.04	25,27,33,40	0
2	FTV	B	301	14/14	0.99	0.03	21,26,32,40	0
2	FTV	I	301	14/14	0.99	0.04	22,26,30,39	0
2	FTV	M	301	14/14	0.99	0.03	24,29,33,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AKG	A	303	10/10	0.99	0.03	20,23,26,26	0
4	AKG	B	303	10/10	0.99	0.03	19,20,24,25	0
4	AKG	M	303	10/10	0.99	0.03	20,24,26,26	0
3	CO	M	302	1/1	1.00	0.00	20,20,20,20	0
3	CO	A	302	1/1	1.00	0.01	21,21,21,21	0
3	CO	B	302	1/1	1.00	0.01	20,20,20,20	0
4	AKG	I	303	10/10	1.00	0.02	18,20,23,24	0
3	CO	I	302	1/1	1.00	0.01	19,19,19,19	0
5	CL	A	304	1/1	1.00	0.03	25,25,25,25	0
5	CL	B	304	1/1	1.00	0.04	24,24,24,24	0
5	CL	I	304	1/1	1.00	0.04	25,25,25,25	0
5	CL	M	304	1/1	1.00	0.03	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.