Full wwPDB X-ray Structure Validation Report (i)

May 7, 2025 – 01:13 pm BST

PDB ID	:	9FYU / pdb_00009fyu
Title	:	Crystal structure of the engineered photoenzyme VEnT1.0
Authors	:	Hardy, F.J.; Roberts, G.W.
Deposited on	:	2024-07-04
Resolution	:	1.52 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 (i) 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 (1)) were used in the production of this report:

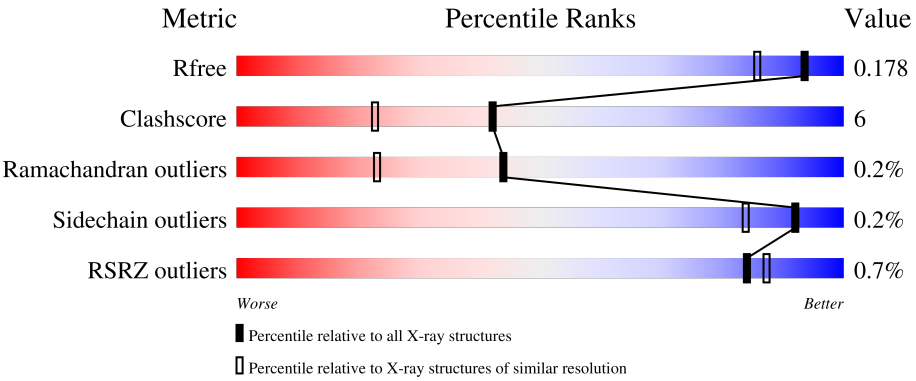
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 1.52 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}	164625	5293 (1.54-1.50)
Clashscore	180529	5759 (1.54-1.50)
Ramachandran outliers	177936	5653 (1.54-1.50)
Sidechain outliers	177891	5650 (1.54-1.50)
RSRZ outliers	164620	5293 (1.54-1.50)

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 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	326	% 87% 7% 6%
1	B	326	% 82% 12% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10758 atoms, of which 4973 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 Diisopropyl-fluorophosphatase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	308	Total	C	H	N	O	S	0	10	0
			4852	1578	2389	410	458	17			
1	B	309	Total	C	H	N	O	S	0	32	0
			5193	1687	2578	425	482	21			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	GLU	conflict	UNP Q7SIG4
A	37	TYR	GLU	conflict	UNP Q7SIG4
A	120	ALA	ASN	conflict	UNP Q7SIG4
A	121	TYR	ASP	conflict	UNP Q7SIG4
A	144	PHE	TYR	conflict	UNP Q7SIG4
A	146	ILE	ARG	conflict	UNP Q7SIG4
A	148	LEU	MET	conflict	UNP Q7SIG4
A	175	ALA	ASN	conflict	UNP Q7SIG4
A	195	GLN	THR	conflict	UNP Q7SIG4
A	225	LYS	GLU	conflict	UNP Q7SIG4
A	229	ALA	ASP	conflict	UNP Q7SIG4
A	272	ALA	ASN	conflict	UNP Q7SIG4
A	315	GLY	-	expression tag	UNP Q7SIG4
A	316	SER	-	expression tag	UNP Q7SIG4
A	317	LEU	-	expression tag	UNP Q7SIG4
A	318	GLU	-	expression tag	UNP Q7SIG4
A	319	TRP	-	expression tag	UNP Q7SIG4
A	320	SER	-	expression tag	UNP Q7SIG4
A	321	HIS	-	expression tag	UNP Q7SIG4
A	322	PRO	-	expression tag	UNP Q7SIG4
A	323	GLN	-	expression tag	UNP Q7SIG4
A	324	PHE	-	expression tag	UNP Q7SIG4
A	325	GLU	-	expression tag	UNP Q7SIG4
A	326	LYS	-	expression tag	UNP Q7SIG4
B	21	ALA	GLU	conflict	UNP Q7SIG4

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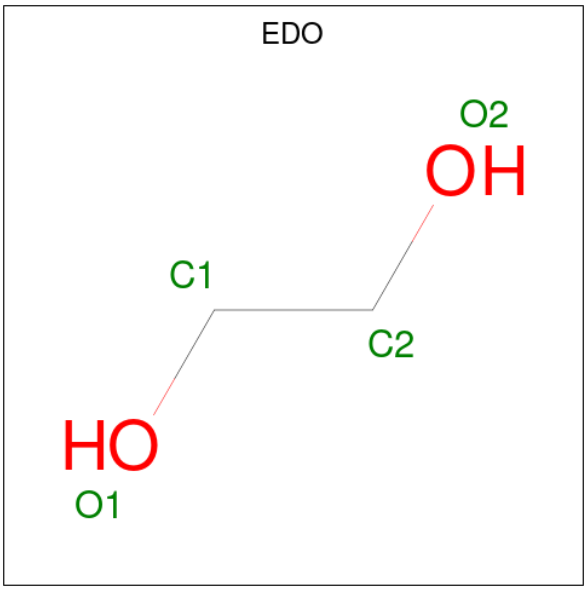
Chain	Residue	Modelled	Actual	Comment	Reference
B	37	TYR	GLU	conflict	UNP Q7SIG4
B	120	ALA	ASN	conflict	UNP Q7SIG4
B	121	TYR	ASP	conflict	UNP Q7SIG4
B	144	PHE	TYR	conflict	UNP Q7SIG4
B	146	ILE	ARG	conflict	UNP Q7SIG4
B	148	LEU	MET	conflict	UNP Q7SIG4
B	175	ALA	ASN	conflict	UNP Q7SIG4
B	195	GLN	THR	conflict	UNP Q7SIG4
B	225	LYS	GLU	conflict	UNP Q7SIG4
B	229	ALA	ASP	conflict	UNP Q7SIG4
B	272	ALA	ASN	conflict	UNP Q7SIG4
B	315	GLY	-	expression tag	UNP Q7SIG4
B	316	SER	-	expression tag	UNP Q7SIG4
B	317	LEU	-	expression tag	UNP Q7SIG4
B	318	GLU	-	expression tag	UNP Q7SIG4
B	319	TRP	-	expression tag	UNP Q7SIG4
B	320	SER	-	expression tag	UNP Q7SIG4
B	321	HIS	-	expression tag	UNP Q7SIG4
B	322	PRO	-	expression tag	UNP Q7SIG4
B	323	GLN	-	expression tag	UNP Q7SIG4
B	324	PHE	-	expression tag	UNP Q7SIG4
B	325	GLU	-	expression tag	UNP Q7SIG4
B	326	LYS	-	expression tag	UNP Q7SIG4

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 10 2 6 2	0	0

- Molecule 3 is water.

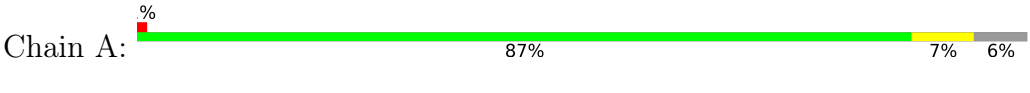
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	339	Total O 339 339	0	0
3	B	364	Total O 364 364	0	2

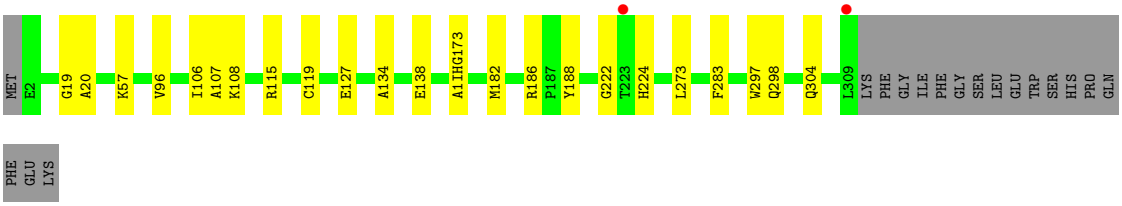
3 Residue-property plots (i)

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: Diisopropyl-fluorophosphatase

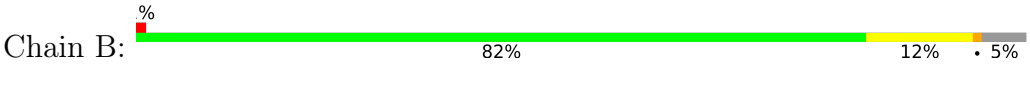
Chain A:

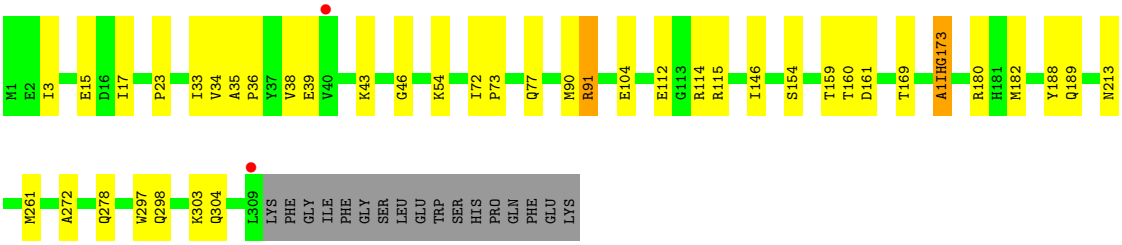




- Molecule 1: Diisopropyl-fluorophosphatase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.73Å 73.44Å 74.12Å 90.00° 94.16° 90.00°	Depositor
Resolution (Å)	50.60 – 1.52 50.60 – 1.52	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.60-1.52) 95.0 (50.60-1.52)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 1.52Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.143 , 0.174 0.148 , 0.178	Depositor DCC
R_{free} test set	1870 reflections (2.36%)	wwPDB-VP
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	10758	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% 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: EDO, A1IHG

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	0.40	0/2533	0.57	0/3428
1	B	0.40	0/2703	0.57	0/3662
All	All	0.40	0/5236	0.57	0/7090

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	B	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	B	91	ARG	Sidechain

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	2463	2389	2391	18	1
1	B	2615	2578	2553	44	4
2	A	4	6	6	0	0
3	A	339	0	0	7	2
3	B	364	0	0	11	3
All	All	5785	4973	4950	62	5

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 (62) 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:B:36[B]:PRO:O	3:B:501:HOH:O	1.80	0.99
1:B:104[A]:GLU:OE2	3:B:502[A]:HOH:O	1.82	0.97
1:B:115:ARG:NH2	3:B:503:HOH:O	2.03	0.92
1:A:186:ARG:NH2	3:A:603:HOH:O	2.05	0.88
1:A:304:GLN:OE1	3:A:601:HOH:O	1.89	0.88
1:A:138:GLU:OE1	3:A:602:HOH:O	1.91	0.88
1:B:17:ILE:CD1	1:B:33[A]:ILE:HD11	2.15	0.77
1:B:304:GLN:NE2	3:B:505:HOH:O	2.20	0.72
1:B:17:ILE:HD12	1:B:33[A]:ILE:HD11	1.72	0.71
1:A:108:LYS:HD2	1:A:108:LYS:N	2.08	0.69
1:B:161[A]:ASP:OD1	3:B:504:HOH:O	2.12	0.67
1:A:107:ALA:O	3:A:604:HOH:O	2.14	0.64
1:B:35[B]:ALA:O	1:B:38[B]:VAL:HG12	1.98	0.64
1:B:112:GLU:OE1	1:B:114:ARG:NH2	2.31	0.63
1:B:154:SER:OG	1:B:169[B]:THR:HG22	2.03	0.59
1:A:222:GLY:O	3:A:605:HOH:O	2.17	0.58
1:B:17:ILE:HD13	1:B:33[A]:ILE:HD11	1.87	0.56
1:B:38[B]:VAL:HG13	1:B:46:GLY:HA2	1.87	0.55
1:B:77[B]:GLN:NE2	3:B:512:HOH:O	2.39	0.55
1:B:3[B]:ILE:HG22	3:B:654:HOH:O	2.06	0.54
1:A:127:GLU:OE2	1:A:186:ARG:NH1	2.44	0.50
1:B:90[B]:MET:HE1	1:B:146[B]:ILE:CD1	2.41	0.50
1:A:115:ARG:HG3	3:A:818:HOH:O	2.11	0.49
1:A:108:LYS:HD2	1:A:108:LYS:H	1.77	0.49
1:B:77[B]:GLN:NE2	1:B:77[B]:GLN:HA	2.27	0.49
1:B:304:GLN:NE2	3:B:511:HOH:O	2.36	0.48
1:A:96[A]:VAL:CG2	1:A:106:ILE:HD11	2.44	0.48
1:B:77[B]:GLN:HA	1:B:77[B]:GLN:HE21	1.78	0.48
1:A:182:MET:HG2	1:A:188:TYR:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90[B]:MET:HE1	1:B:146[B]:ILE:HD13	1.95	0.48
1:B:38[B]:VAL:CG1	1:B:46:GLY:HA2	2.43	0.48
1:B:36[B]:PRO:HB3	1:B:73:PRO:O	2.14	0.48
1:B:15:GLU:HB2	3:B:510:HOH:O	2.14	0.47
1:B:17:ILE:HD12	1:B:33[A]:ILE:CD1	2.44	0.47
1:A:297:TRP:CG	1:A:298:GLN:H	2.33	0.46
1:B:278:GLN:NE2	1:B:303:LYS:NZ	2.63	0.46
1:B:34[B]:VAL:HG11	1:B:73:PRO:C	2.40	0.46
1:B:72:ILE:HD12	1:B:91:ARG:HG2	1.97	0.46
1:A:19:GLY:O	1:A:20:ALA:C	2.58	0.46
1:B:34[B]:VAL:HG12	1:B:36[B]:PRO:HD3	1.97	0.45
1:B:38[B]:VAL:HA	3:B:700:HOH:O	2.16	0.45
1:B:278:GLN:HE22	1:B:303:LYS:NZ	2.14	0.45
1:B:213:ASN:OD1	3:B:506:HOH:O	2.21	0.43
1:B:3[B]:ILE:HG12	1:B:261:MET:HA	1.98	0.43
1:B:146[B]:ILE:HG12	1:B:173[B]:A1IHG:CE1	2.49	0.42
1:B:23:PRO:HD2	1:B:272[B]:ALA:HB1	2.01	0.42
1:A:119:CYS:HA	1:A:134:ALA:HA	2.02	0.42
1:A:297:TRP:CG	1:A:298:GLN:N	2.89	0.41
1:B:182[B]:MET:HG3	1:B:188:TYR:CD1	2.55	0.41
1:B:34[A]:VAL:HB	1:B:73:PRO:HB2	2.02	0.41
1:B:159:THR:OG1	1:B:161[A]:ASP:OD1	2.38	0.41
1:B:297:TRP:CG	1:B:298:GLN:N	2.89	0.41
1:A:127:GLU:OE2	3:A:606:HOH:O	2.22	0.41
1:A:273:LEU:HA	1:A:283:PHE:O	2.21	0.41
1:B:46:GLY:HA3	1:B:73:PRO:HD2	2.03	0.41
1:B:297:TRP:CG	1:B:298:GLN:H	2.39	0.41
1:B:34[B]:VAL:CG1	1:B:73:PRO:O	2.69	0.40
1:A:96[A]:VAL:HG23	1:A:106:ILE:HD11	2.04	0.40
1:B:180:ARG:HB3	1:B:189:GLN:HB3	2.03	0.40
1:B:278:GLN:NE2	1:B:303:LYS:HZ3	2.19	0.40

All (5) 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)
1:A:115:ARG:HH12	1:B:104[A]:GLU:OE1[2_655]	1.55	0.05
1:B:43[B]:LYS:NZ	3:B:521:HOH:O[1_655]	2.16	0.04
1:B:54:LYS:NZ	3:A:625:HOH:O[1_545]	2.18	0.02
3:A:693:HOH:O	3:B:568:HOH:O[1_465]	2.18	0.02
1:B:43[B]:LYS:HZ3	3:B:521:HOH:O[1_655]	1.58	0.02

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	315/326 (97%)	307 (98%)	7 (2%)	1 (0%)	37 18
1	B	337/326 (103%)	325 (96%)	12 (4%)	0	100 100
All	All	652/652 (100%)	632 (97%)	19 (3%)	1 (0%)	44 23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	HIS

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	261/268 (97%)	260 (100%)	1 (0%)	89 80
1	B	280/268 (104%)	280 (100%)	0	100 100
All	All	541/536 (101%)	540 (100%)	1 (0%)	92 84

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	304	GLN
1	B	278	GLN
1	B	304	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	A1IHG	B	173[B]	-	21,22,23	2.29	8 (38%)	28,31,33	3.05	12 (42%)
1	A1IHG	B	173[A]	-	21,22,23	2.59	9 (42%)	28,31,33	3.06	9 (32%)
1	A1IHG	A	173	1	21,22,23	2.05	6 (28%)	28,31,33	2.97	9 (32%)

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
1	A1IHG	B	173[B]	-	-	2/5/6/8	0/3/3/3
1	A1IHG	B	173[A]	-	-	4/5/6/8	0/3/3/3
1	A1IHG	A	173	1	-	4/5/6/8	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	173[A]	A1IHG	C15-S16	8.06	1.90	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	173[B]	A1IHG	C15-S16	5.63	1.86	1.76
1	B	173[B]	A1IHG	CZ-S16	4.89	1.84	1.76
1	A	173	A1IHG	C15-S16	4.81	1.84	1.76
1	B	173[A]	A1IHG	C10-C09	4.06	1.57	1.48
1	A	173	A1IHG	CZ-S16	3.86	1.83	1.76
1	B	173[B]	A1IHG	C10-C09	3.43	1.55	1.48
1	A	173	A1IHG	C10-C09	3.36	1.55	1.48
1	B	173[A]	A1IHG	CZ-S16	3.22	1.81	1.76
1	B	173[A]	A1IHG	C11-C10	2.86	1.44	1.39
1	A	173	A1IHG	C11-C10	2.56	1.44	1.39
1	B	173[A]	A1IHG	O-C	2.48	1.29	1.19
1	B	173[B]	A1IHG	O-C	2.48	1.29	1.19
1	B	173[A]	A1IHG	C14-C15	2.43	1.44	1.39
1	A	173	A1IHG	O-C	2.40	1.29	1.19
1	B	173[A]	A1IHG	CE2-C09	2.32	1.53	1.48
1	B	173[A]	A1IHG	O17-C09	2.23	1.26	1.22
1	B	173[B]	A1IHG	CE1-CD1	2.19	1.42	1.38
1	B	173[A]	A1IHG	CD1-CG	2.12	1.43	1.38
1	B	173[B]	A1IHG	C14-C15	2.10	1.43	1.39
1	B	173[B]	A1IHG	CB-CA	2.09	1.58	1.53
1	A	173	A1IHG	CD1-CG	2.07	1.43	1.38
1	B	173[B]	A1IHG	O17-C09	2.04	1.26	1.22

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	173[B]	A1IHG	C10-C09-CE2	8.52	131.90	117.60
1	B	173[A]	A1IHG	C10-C09-CE2	8.19	131.34	117.60
1	B	173[A]	A1IHG	C15-C10-C09	-8.07	118.34	123.72
1	A	173	A1IHG	C10-C09-CE2	8.07	131.15	117.60
1	A	173	A1IHG	C15-C10-C09	-8.07	118.35	123.72
1	B	173[B]	A1IHG	C15-C10-C09	-7.15	118.96	123.72
1	B	173[B]	A1IHG	CZ-CE2-C09	-5.01	120.39	123.72
1	B	173[A]	A1IHG	C15-S16-CZ	4.99	112.41	100.44
1	B	173[B]	A1IHG	C15-S16-CZ	4.96	112.33	100.44
1	B	173[B]	A1IHG	O17-C09-C10	-4.77	113.92	120.91
1	A	173	A1IHG	CZ-CE2-C09	-4.64	120.63	123.72
1	B	173[A]	A1IHG	O17-C09-C10	-4.64	114.11	120.91
1	B	173[B]	A1IHG	O17-C09-CE2	-4.59	114.17	120.91
1	A	173	A1IHG	O17-C09-CE2	-4.56	114.22	120.91
1	A	173	A1IHG	C15-S16-CZ	4.45	111.10	100.44
1	B	173[A]	A1IHG	CZ-CE2-C09	-4.43	120.77	123.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	173[A]	A1IHG	O17-C09-CE2	-4.35	114.53	120.91
1	A	173	A1IHG	O17-C09-C10	-4.28	114.63	120.91
1	A	173	A1IHG	C11-C10-C09	3.28	124.58	119.25
1	B	173[A]	A1IHG	C11-C10-C09	3.19	124.44	119.25
1	B	173[B]	A1IHG	C11-C10-C09	3.08	124.26	119.25
1	B	173[A]	A1IHG	CE1-CZ-CE2	2.78	122.66	119.14
1	B	173[B]	A1IHG	C14-C15-C10	2.63	122.46	119.14
1	A	173	A1IHG	CE1-CZ-CE2	2.40	122.18	119.14
1	A	173	A1IHG	C14-C15-C10	2.25	121.99	119.14
1	B	173[B]	A1IHG	CE1-CZ-CE2	2.18	121.90	119.14
1	B	173[A]	A1IHG	CD2-CE2-C09	2.18	122.91	119.13
1	B	173[B]	A1IHG	CE2-CZ-S16	-2.09	117.90	122.27
1	B	173[B]	A1IHG	C10-C15-S16	-2.03	118.04	122.27
1	B	173[B]	A1IHG	CD2-CE2-C09	2.01	122.61	119.13

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	173[A]	A1IHG	C-CA-CB-CG
1	B	173[B]	A1IHG	N-CA-CB-CG
1	B	173[B]	A1IHG	C-CA-CB-CG
1	A	173	A1IHG	N-CA-CB-CG
1	B	173[A]	A1IHG	N-CA-CB-CG
1	A	173	A1IHG	C-CA-CB-CG
1	A	173	A1IHG	CA-CB-CG-CD1
1	A	173	A1IHG	CA-CB-CG-CD2
1	B	173[A]	A1IHG	CA-CB-CG-CD1
1	B	173[A]	A1IHG	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	173[B]	A1IHG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	EDO	A	501	-	3,3,3	0.27	0	2,2,2	0.30	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
2	EDO	A	501	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	EDO	O1-C1-C2-O2

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

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	307/326 (94%)	-0.37	2 (0%)	84	87	8, 24, 45, 92	9 (2%)
1	B	308/326 (94%)	-0.44	2 (0%)	85	88	9, 22, 40, 97	29 (9%)
All	All	615/652 (94%)	-0.41	4 (0%)	84	87	8, 23, 42, 97	38 (6%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	LEU	4.9
1	B	40[A]	VAL	3.6
1	A	223	THR	3.5
1	A	309	LEU	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	A1IHG	A	173	20/21	0.95	0.09	17,29,51,62	0
1	A1IHG	B	173[A]	20/21	0.96	0.10	14,26,44,48	26
1	A1IHG	B	173[B]	20/21	0.96	0.10	13,26,40,43	26

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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
2	EDO	A	501	4/4	0.82	0.14	38,49,58,61	0

6.5 Other polymers

There are no such residues in this entry.