



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:50 PM UTC

PDB ID : 3W04 / pdb_00003w04
Title : Crystal structure of Oryza sativa DWARF14 (D14)
Authors : Kagiya, M.; Hirano, Y.; Mori, T.; Kim, S.Y.; Kyojuka, J.; Seto, Y.; Yamaguchi, S.; Hakoshima, T.
Deposited on : 2012-10-19
Resolution : 1.45 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

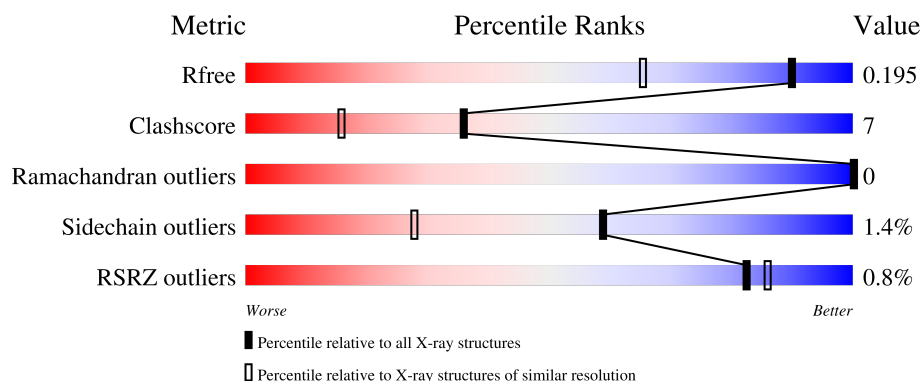
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	266	 84% 14% ..
1	B	266	 80% 18% ..

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
3	EDO	A	404	-	-	X	-
3	EDO	B	406	-	X	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4714 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.

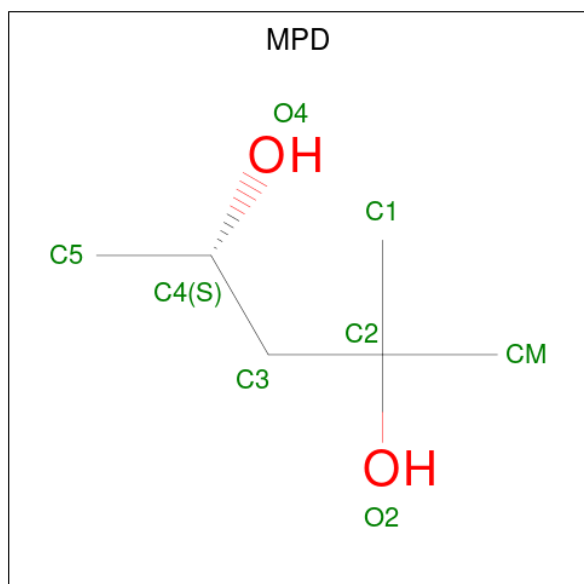
- Molecule 1 is a protein called Dwarf 88 esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	9	0
			2096	1336	372	378	10			
1	B	263	Total	C	N	O	S	0	11	0
			2107	1340	381	376	10			

There are 4 discrepancies between the modelled and reference sequences:

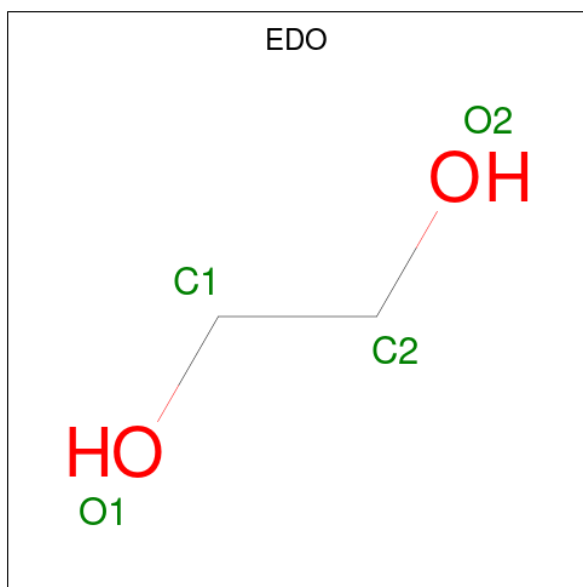
Chain	Residue	Modelled	Actual	Comment	Reference
A	53	GLY	-	expression tag	UNP Q10QA5
A	54	PRO	-	expression tag	UNP Q10QA5
B	53	GLY	-	expression tag	UNP Q10QA5
B	54	PRO	-	expression tag	UNP Q10QA5

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



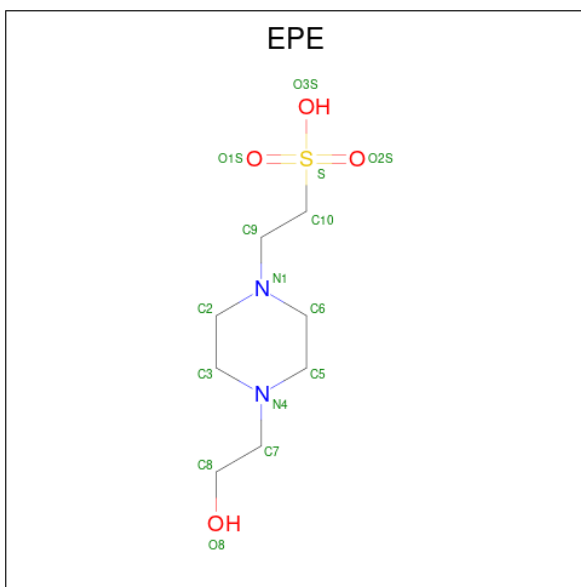
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

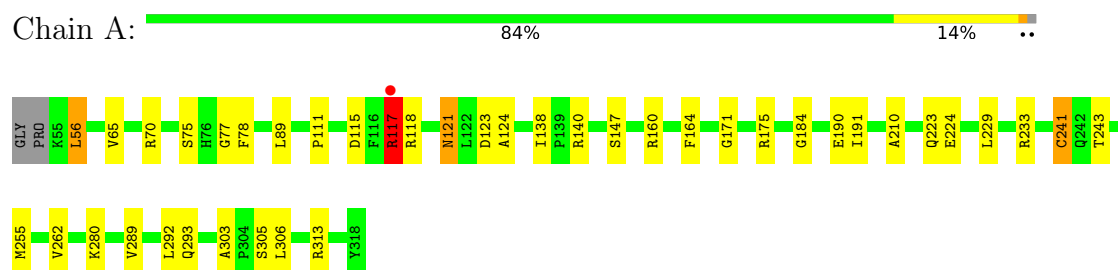
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	232	Total	O	0	0
			232	232		
5	B	220	Total	O	0	0
			220	220		

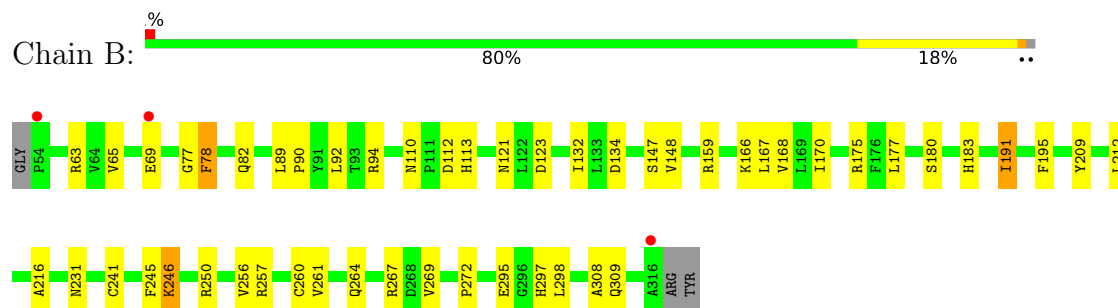
3 Residue-property plots

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: Dwarf 88 esterase



- Molecule 1: Dwarf 88 esterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.99Å 88.19Å 121.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.62 – 1.45 25.62 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.62-1.45) 99.7 (25.62-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.160 , 0.194 0.161 , 0.195	Depositor DCC
R_{free} test set	4597 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	10.9	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4714	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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, MPD, EPE

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	1.68	19/2156 (0.9%)	1.44	8/2933 (0.3%)
1	B	1.66	16/2160 (0.7%)	1.40	9/2939 (0.3%)
All	All	1.67	35/4316 (0.8%)	1.42	17/5872 (0.3%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	256	VAL	CA-CB	6.79	1.61	1.54
1	A	124	ALA	CA-CB	6.64	1.63	1.53
1	A	255	MET	SD-CE	-6.58	1.63	1.79
1	A	117	ARG	N-CA	-6.54	1.38	1.46
1	B	298	LEU	N-CA	6.19	1.53	1.46
1	B	159	ARG	C-O	6.04	1.31	1.24
1	B	212	LEU	N-CA	-6.01	1.39	1.46
1	A	75	SER	N-CA	5.97	1.53	1.46
1	A	164	PHE	C-O	5.92	1.30	1.23
1	A	241[A]	CYS	C-O	5.87	1.30	1.24
1	A	241[B]	CYS	C-O	5.87	1.30	1.24
1	B	191	ILE	N-CA	5.73	1.53	1.46
1	A	210	ALA	N-CA	5.66	1.51	1.46
1	B	132	ILE	C-O	5.55	1.30	1.24
1	B	180	SER	N-CA	5.53	1.53	1.46
1	B	257	ARG	CA-CB	5.50	1.62	1.53
1	B	134	ASP	C-O	5.48	1.30	1.24
1	A	243	THR	C-O	5.45	1.30	1.24
1	B	168	VAL	C-O	5.43	1.29	1.24
1	B	209	TYR	N-CA	-5.40	1.39	1.46
1	B	148	VAL	N-CA	5.39	1.52	1.46
1	A	89	LEU	N-CA	-5.33	1.40	1.46
1	B	261	VAL	CA-C	-5.32	1.46	1.52
1	A	280	LYS	CA-C	5.28	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	ARG	CD-NE	5.27	1.53	1.46
1	B	166	LYS	N-CA	5.26	1.52	1.46
1	A	289	VAL	C-O	5.25	1.29	1.24
1	A	140	ARG	CB-CG	-5.22	1.36	1.52
1	A	191	ILE	CA-CB	5.14	1.61	1.54
1	A	56	LEU	CA-C	-5.12	1.45	1.52
1	A	184	GLY	N-CA	5.09	1.52	1.45
1	A	65	VAL	CA-CB	-5.04	1.47	1.54
1	B	245	PHE	N-CA	5.04	1.52	1.46
1	A	262	VAL	CA-CB	5.02	1.60	1.54
1	B	78	PHE	CA-CB	5.01	1.61	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ARG	CG-CD-NE	-8.56	93.17	112.00
1	A	160	ARG	NE-CZ-NH1	-6.98	114.52	121.50
1	A	171	GLY	O-C-N	6.11	128.12	122.57
1	B	250	ARG	O-C-N	5.61	128.06	122.12
1	B	297	HIS	CA-C-O	-5.55	112.77	119.27
1	A	313	ARG	CA-C-O	-5.34	115.21	120.82
1	B	308	ALA	N-CA-C	-5.33	105.64	111.82
1	A	117	ARG	CA-CB-CG	5.30	124.69	114.10
1	A	160	ARG	O-C-N	-5.23	117.00	121.23
1	B	170	ILE	O-C-N	-5.19	117.55	123.10
1	B	112	ASP	O-C-N	-5.18	115.65	122.39
1	A	138	ILE	CA-C-N	-5.16	114.95	120.47
1	A	138	ILE	C-N-CA	-5.16	114.95	120.47
1	B	92	LEU	N-CA-C	-5.12	107.69	114.04
1	B	69	GLU	CA-C-N	-5.10	114.21	121.50
1	B	69	GLU	C-N-CA	-5.10	114.21	121.50
1	B	134	ASP	CA-C-O	-5.03	115.09	120.42

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	2096	0	2109	18	0
1	B	2107	0	2120	42	0
2	A	8	0	14	0	0
2	B	8	0	14	0	0
3	A	12	0	18	7	0
3	B	16	0	24	8	0
4	B	15	0	17	1	0
5	A	232	0	0	8	0
5	B	220	0	0	5	0
All	All	4714	0	4316	63	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 7.

All (63) 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:177[A]:LEU:HD21	1:B:191:ILE:CD1	1.59	1.31
1:B:63[B]:ARG:HE	1:B:82:GLN:NE2	1.45	1.15
1:B:177[A]:LEU:CD2	1:B:191:ILE:CD1	2.27	1.12
1:B:177[A]:LEU:CD2	1:B:191:ILE:HD12	1.81	1.09
1:B:177[A]:LEU:HD21	1:B:191:ILE:HD12	0.98	0.97
1:B:231:ASN:HB2	5:B:626:HOH:O	1.67	0.94
1:B:177[A]:LEU:CD2	1:B:191:ILE:HD11	2.04	0.85
1:B:121[B]:ASN:HD22	1:B:123:ASP:H	1.24	0.82
1:A:115:ASP:OD1	1:A:117:ARG:HG2	1.80	0.82
1:B:63[B]:ARG:NE	1:B:82:GLN:NE2	2.29	0.80
1:B:63[B]:ARG:HE	1:B:82:GLN:HE22	1.26	0.80
1:B:183:HIS:HD2	5:B:640:HOH:O	1.63	0.80
1:B:267[B]:ARG:NH2	3:B:406:EDO:H11	1.97	0.78
1:B:267[B]:ARG:NH2	3:B:406:EDO:O1	2.16	0.78
1:B:267[A]:ARG:HB3	1:B:295:GLU:HG3	1.70	0.73
1:B:267[B]:ARG:NH2	3:B:406:EDO:C1	2.52	0.72
1:B:231:ASN:CB	5:B:626:HOH:O	2.29	0.71
1:A:111:PRO:HA	5:A:698:HOH:O	1.92	0.68
1:B:177[A]:LEU:HD23	1:B:191:ILE:HD11	1.75	0.67
1:B:267[B]:ARG:HH22	3:B:406:EDO:H11	1.57	0.67
1:B:63[B]:ARG:NE	1:B:82:GLN:HE22	1.91	0.66
5:A:681:HOH:O	1:B:309:GLN:HG3	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121[B]:ASN:ND2	1:B:123:ASP:H	1.97	0.61
1:A:224:GLU:OE2	5:A:629:HOH:O	2.16	0.61
1:A:293:GLN:NE2	5:A:690:HOH:O	2.26	0.60
1:A:303:ALA:C	3:A:404:EDO:H11	2.27	0.60
1:A:305[B]:SER:HB2	3:A:404:EDO:H12	1.83	0.59
1:A:117:ARG:HG3	1:A:117:ARG:HH11	1.67	0.59
1:B:231:ASN:CG	5:B:626:HOH:O	2.46	0.58
1:B:267[B]:ARG:HG3	1:B:267[B]:ARG:HH11	1.69	0.58
1:A:117:ARG:HH11	1:A:117:ARG:CG	2.21	0.54
1:B:77:GLY:HA3	1:B:147:SER:HB3	1.89	0.54
1:B:177[A]:LEU:HD23	1:B:191:ILE:CD1	2.27	0.54
1:B:267[B]:ARG:CZ	3:B:406:EDO:O1	2.57	0.53
1:B:267[B]:ARG:HH22	3:B:406:EDO:C1	2.17	0.52
1:B:272:PRO:HG3	3:B:406:EDO:H12	1.93	0.50
1:A:292:LEU:HD22	1:A:306:LEU:HG	1.93	0.49
1:A:77:GLY:HA3	1:A:147:SER:HB3	1.96	0.48
1:A:190[B]:GLU:OE2	5:A:685:HOH:O	2.20	0.47
5:A:681:HOH:O	1:B:309:GLN:CG	2.59	0.47
1:B:89:LEU:HB3	1:B:90:PRO:HD3	1.96	0.47
1:A:121:ASN:ND2	1:A:123:ASP:H	2.13	0.46
1:B:267[B]:ARG:HH11	1:B:267[B]:ARG:CG	2.28	0.46
1:B:216:ALA:CB	4:B:401:EPE:H82	2.45	0.46
1:A:70:ARG:HG2	5:A:677:HOH:O	2.16	0.46
1:B:269:VAL:O	3:B:406:EDO:H22	2.15	0.45
1:B:63[A]:ARG:HG2	1:B:65:VAL:HG13	1.99	0.45
1:A:121:ASN:HD21	1:A:123:ASP:CG	2.25	0.45
1:A:233:ARG:HG2	1:B:90:PRO:HG2	1.99	0.44
1:B:78:PHE:CE1	1:B:241[B]:CYS:SG	3.11	0.43
1:B:191:ILE:HG22	1:B:195:PHE:CE2	2.55	0.42
1:B:246:LYS:HB3	1:B:246:LYS:HE3	1.54	0.42
1:B:175:ARG:NH2	1:B:177[B]:LEU:HD23	2.35	0.42
1:B:110:ASN:HB3	1:B:113:HIS:CD2	2.55	0.41
1:A:223[A]:GLN:HG3	5:A:708:HOH:O	2.20	0.41
1:A:305[B]:SER:HB2	3:A:404:EDO:C1	2.49	0.41
1:B:167:LEU:O	1:B:260[B]:CYS:HA	2.21	0.41
1:A:78:PHE:CZ	1:A:241[B]:CYS:SG	3.14	0.40
1:B:94:ARG:HD2	5:B:561:HOH:O	2.21	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	271/266 (102%)	266 (98%)	5 (2%)	0	100	100
1	B	272/266 (102%)	265 (97%)	7 (3%)	0	100	100
All	All	543/532 (102%)	531 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	227/219 (104%)	223 (98%)	4 (2%)	51	19
1	B	227/219 (104%)	225 (99%)	2 (1%)	70	46
All	All	454/438 (104%)	448 (99%)	6 (1%)	59	31

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	117	ARG
1	A	121	ASN
1	A	229	LEU
1	B	246	LYS
1	B	264	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	239	HIS
1	B	58	GLN
1	B	61	ASN
1	B	82	GLN
1	B	183	HIS
1	B	264	GLN
1	B	282	HIS

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](#)

10 ligands 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
3	EDO	B	406	-	3,3,3	1.60	1 (33%)	2,2,2	2.51	2 (100%)
2	MPD	A	401	-	7,7,7	0.53	0	9,10,10	1.29	1 (11%)
3	EDO	A	404	-	3,3,3	0.56	0	2,2,2	1.74	1 (50%)
3	EDO	B	405	-	3,3,3	1.13	0	2,2,2	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EPE	B	401	-	15,15,15	1.18	2 (13%)	19,20,20	2.45	8 (42%)
3	EDO	A	402	-	3,3,3	0.76	0	2,2,2	0.82	0
3	EDO	A	403	-	3,3,3	0.74	0	2,2,2	0.23	0
3	EDO	B	403	-	3,3,3	0.58	0	2,2,2	0.67	0
2	MPD	B	402	-	7,7,7	0.61	0	9,10,10	0.94	0
3	EDO	B	404	-	3,3,3	0.55	0	2,2,2	0.99	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
3	EDO	B	406	-	-	1/1/1/1	-
2	MPD	A	401	-	-	0/5/5/5	-
3	EDO	A	404	-	-	1/1/1/1	-
3	EDO	B	405	-	-	0/1/1/1	-
4	EPE	B	401	-	-	2/9/19/19	0/1/1/1
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	A	403	-	-	0/1/1/1	-
3	EDO	B	403	-	-	0/1/1/1	-
2	MPD	B	402	-	-	0/5/5/5	-
3	EDO	B	404	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	EPE	C10-S	2.66	1.81	1.77
3	B	406	EDO	O2-C2	2.62	1.55	1.42
4	B	401	EPE	C6-N1	2.36	1.53	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	EPE	C5-N4-C3	5.71	121.14	108.84
4	B	401	EPE	O3S-S-C10	3.94	113.72	106.00
4	B	401	EPE	C9-N1-C2	-3.53	101.84	111.24
4	B	401	EPE	O2S-S-O1S	-3.37	102.87	113.82
4	B	401	EPE	C8-C7-N4	-2.95	103.08	113.44
4	B	401	EPE	C6-N1-C2	2.77	114.81	108.84
3	B	406	EDO	O2-C2-C1	-2.75	91.44	112.39
4	B	401	EPE	C9-N1-C6	2.55	118.04	111.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	MPD	O4-C4-C3	-2.25	102.40	111.35
3	B	406	EDO	O1-C1-C2	2.24	129.41	112.39
3	A	404	EDO	O1-C1-C2	-2.13	96.18	112.39
4	B	401	EPE	O1S-S-C10	2.11	109.92	106.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	EPE	N4-C7-C8-O8
3	B	406	EDO	O1-C1-C2-O2
3	A	404	EDO	O1-C1-C2-O2
4	B	401	EPE	C8-C7-N4-C3

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	406	EDO	8	0
3	A	404	EDO	7	0
4	B	401	EPE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	264/266 (99%)	-0.47	1 (0%) 88 91	5, 10, 21, 32	9 (3%)
1	B	263/266 (98%)	-0.42	3 (1%) 78 82	3, 10, 21, 41	11 (4%)
All	All	527/532 (99%)	-0.44	4 (0%) 82 86	3, 10, 21, 41	20 (3%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	69	GLU	2.4
1	B	54	PRO	2.3
1	A	117	ARG	2.1
1	B	316	ALA	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 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
3	EDO	B	406	4/4	0.73	0.22	17,25,30,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	404	4/4	0.84	0.14	19,20,26,40	0
4	EPE	B	401	15/15	0.90	0.11	21,24,30,32	0
3	EDO	B	404	4/4	0.92	0.10	18,21,24,28	0
3	EDO	A	403	4/4	0.92	0.11	14,19,20,22	0
2	MPD	B	402	8/8	0.92	0.09	15,19,22,23	0
2	MPD	A	401	8/8	0.94	0.08	17,20,24,25	0
3	EDO	B	405	4/4	0.97	0.07	13,16,18,23	0
3	EDO	B	403	4/4	0.97	0.05	10,12,13,13	0
3	EDO	A	402	4/4	0.97	0.06	15,16,17,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.