



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:08 AM GMT

PDB ID : 1ZVR
Title : Crystal Structure of MTMR2 in complex with phosphatidylinositol 3,5-bisphosphate
Authors : Begley, M.J.; Taylor, G.S.; Brock, M.A.; Ghosh, P.; Woods, V.L.; Dixon, J.E.
Deposited on : 2005-06-02
Resolution : 1.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

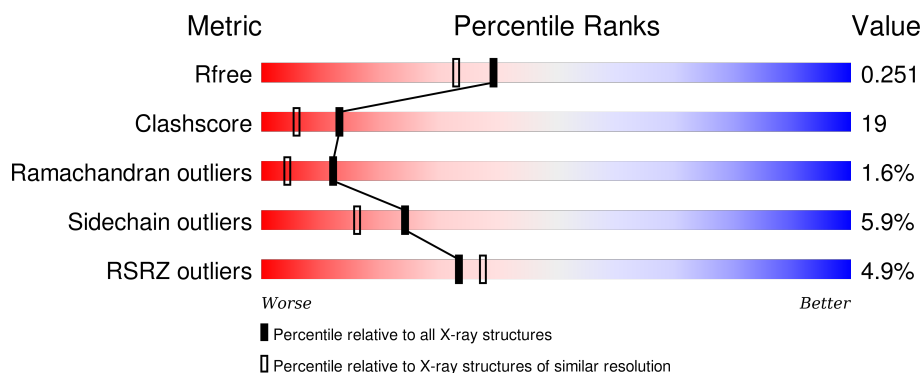
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	528	

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
2	EDO	A	1878	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	1880	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4646 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 Myotubularin-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4197	2684	730	765	18			

There are 15 discrepancies between the modelled and reference sequences:

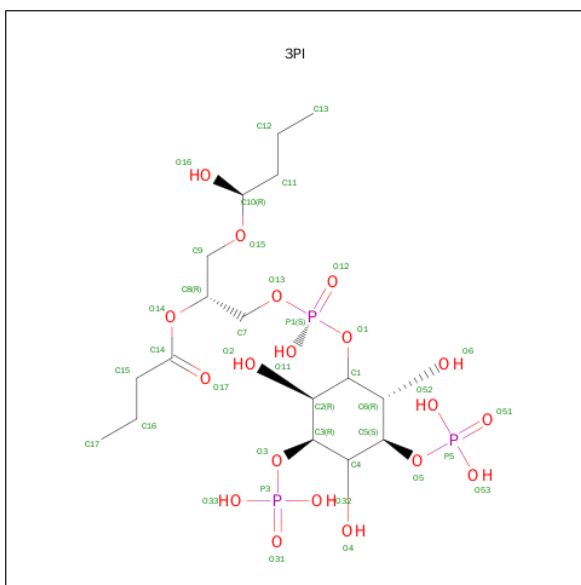
Chain	Residue	Modelled	Actual	Comment	Reference
A	70	MET	-	CLONING ARTIFACT	UNP Q13614
A	71	ALA	-	CLONING ARTIFACT	UNP Q13614
A	72	SER	-	CLONING ARTIFACT	UNP Q13614
A	417	SER	CYS	ENGINEERED	UNP Q13614
A	587	ALA	-	CLONING ARTIFACT	UNP Q13614
A	588	ALA	-	CLONING ARTIFACT	UNP Q13614
A	589	ALA	-	CLONING ARTIFACT	UNP Q13614
A	590	LEU	-	CLONING ARTIFACT	UNP Q13614
A	591	GLU	-	CLONING ARTIFACT	UNP Q13614
A	592	HIS	-	EXPRESSION TAG	UNP Q13614
A	593	HIS	-	EXPRESSION TAG	UNP Q13614
A	594	HIS	-	EXPRESSION TAG	UNP Q13614
A	595	HIS	-	EXPRESSION TAG	UNP Q13614
A	596	HIS	-	EXPRESSION TAG	UNP Q13614
A	597	HIS	-	EXPRESSION TAG	UNP Q13614

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 3 is (1S)-2-(1-HYDROXYBUTOXY)-1-[[[(HYDROXY{[(2R,3S,5R,6S)-2,4,6-TRI HYDROXY-3,5-BIS(PHOSPHONOOXY)CYCLOHEXYL]OXY}PHOSPHORYL)OXY]M ETHYL}ETHYL BUTYRATE (three-letter code: 3PI) (formula: C₁₇H₃₅O₁₉P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	3	0
			39	17	19	3		

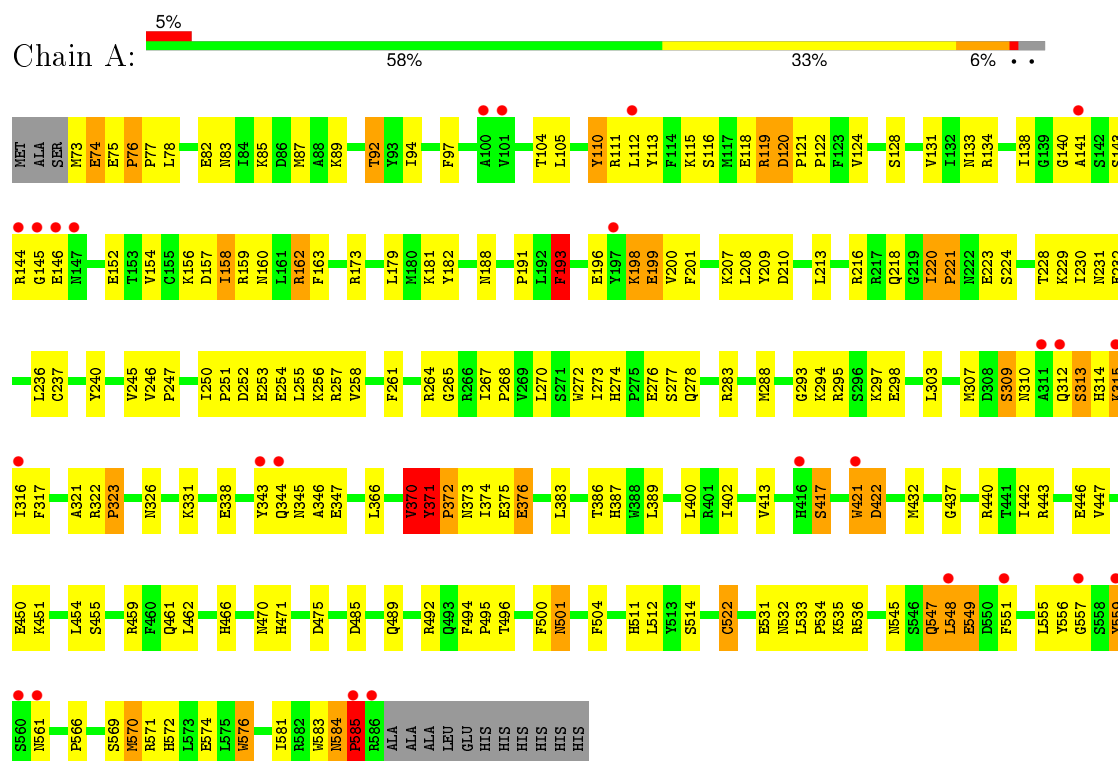
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	398	Total	O	0	0
			398	398		

3 Residue-property plots

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

• Molecule 1: Myotubularin-related protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	66.18 Å 66.18 Å 262.37 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.98 46.80 – 1.98	Depositor EDS
% Data completeness (in resolution range)	89.0 (50.00-1.98) 89.1 (46.80-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 1.98 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.252 0.228 , 0.251	Depositor DCC
R_{free} test set	3716 reflections (10.01%)	DCC
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 40313 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4646	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 3PI, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.75	8/4308 (0.2%)	1.20	40/5839 (0.7%)

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	A	1	13

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	PRO	N-CD	12.86	1.65	1.47
1	A	372	PRO	N-CD	11.32	1.63	1.47
1	A	221	PRO	N-CD	10.46	1.62	1.47
1	A	373	ASN	C-N	-7.31	1.17	1.34
1	A	120	ASP	C-O	6.72	1.36	1.23
1	A	495	PRO	N-CD	5.73	1.55	1.47
1	A	371	TYR	C-O	5.65	1.34	1.23
1	A	75	GLU	C-N	5.17	1.44	1.34

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422	ASP	CB-CG-OD2	-13.20	106.42	118.30
1	A	121	PRO	CA-N-CD	-11.55	95.33	111.50
1	A	584	ASN	C-N-CD	11.32	152.17	128.40
1	A	75	GLU	C-N-CD	10.98	151.46	128.40
1	A	322	ARG	C-N-CD	10.83	151.14	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ASP	CA-C-N	10.76	147.23	117.10
1	A	76	PRO	C-N-CD	10.55	150.55	128.40
1	A	372	PRO	CA-N-CD	-10.12	97.33	111.50
1	A	121	PRO	C-N-CD	9.89	149.18	128.40
1	A	221	PRO	CA-N-CD	-9.43	98.30	111.50
1	A	371	TYR	CB-CA-C	9.09	128.58	110.40
1	A	157	ASP	CB-CG-OD1	8.70	126.13	118.30
1	A	120	ASP	O-C-N	-8.60	104.75	121.10
1	A	371	TYR	O-C-N	-8.53	104.89	121.10
1	A	121	PRO	N-CA-CB	8.41	113.39	103.30
1	A	585	PRO	CA-N-CD	-8.24	99.97	111.50
1	A	559	TYR	CB-CG-CD1	-8.02	116.19	121.00
1	A	494	PHE	C-N-CD	7.89	144.98	128.40
1	A	371	TYR	CA-C-N	7.37	137.73	117.10
1	A	585	PRO	O-C-N	-7.25	111.10	122.70
1	A	110	TYR	CB-CG-CD2	-7.21	116.67	121.00
1	A	323	PRO	CA-N-CD	-6.91	101.83	111.50
1	A	77	PRO	CA-N-CD	-6.85	101.91	111.50
1	A	422	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	A	76	PRO	CA-N-CD	-6.44	102.49	111.50
1	A	576	TRP	O-C-N	-6.34	112.55	122.70
1	A	370	VAL	CA-CB-CG1	6.33	120.40	110.90
1	A	220	ILE	CA-C-N	6.15	134.32	117.10
1	A	122	PRO	CA-N-CD	-6.04	103.04	111.50
1	A	495	PRO	CA-N-CD	-5.99	103.12	111.50
1	A	371	TYR	CA-CB-CG	5.93	124.67	113.40
1	A	494	PHE	CB-CG-CD2	5.92	124.94	120.80
1	A	120	ASP	CA-C-O	-5.86	107.79	120.10
1	A	372	PRO	N-CA-CB	5.40	109.78	103.30
1	A	193	PHE	CD1-CG-CD2	-5.38	111.30	118.30
1	A	120	ASP	CB-CA-C	5.35	121.10	110.40
1	A	317	PHE	CB-CG-CD1	5.29	124.50	120.80
1	A	121	PRO	O-C-N	5.12	130.83	121.10
1	A	92	THR	O-C-N	-5.07	114.58	122.70
1	A	220	ILE	O-C-N	-5.03	111.55	121.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	371	TYR	CA

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	TYR	Sidechain
1	A	193	PHE	Sidechain
1	A	220	ILE	Mainchain
1	A	314	HIS	Mainchain,Peptide
1	A	370	VAL	Mainchain
1	A	371	TYR	Mainchain,Peptide
1	A	387	HIS	Mainchain
1	A	417	SER	Mainchain
1	A	422	ASP	Sidechain
1	A	522	CYS	Mainchain
1	A	585	PRO	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	4197	0	4121	157	5
2	A	12	0	18	1	0
3	A	39	0	27	3	0
4	A	398	0	0	25	3
All	All	4646	0	4166	159	8

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 19.

All (159) 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:559:TYR:CD2	1:A:561:ASN:O	2.08	1.06
1:A:231:ASN:ND2	1:A:237:CYS:H	1.59	1.01
1:A:232:GLU:CB	4:A:1427:HOH:O	2.13	0.96
3:A:3632:3PI:H91	4:A:1250:HOH:O	1.66	0.95
1:A:559:TYR:HD2	1:A:561:ASN:O	1.51	0.93
1:A:231:ASN:HD21	1:A:237:CYS:H	1.18	0.91
1:A:216:ARG:NH1	4:A:1523:HOH:O	2.05	0.87
1:A:310:ASN:O	1:A:313:SER:OG	1.94	0.84
1:A:232:GLU:HB2	4:A:1427:HOH:O	1.71	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:HD11	1:A:112:LEU:HD11	1.59	0.84
1:A:374:ILE:HD11	1:A:581:ILE:HD13	1.64	0.79
1:A:74:GLU:HG3	1:A:104:THR:HB	1.63	0.78
1:A:274:HIS:HD2	1:A:277:SER:H	1.30	0.78
3:A:3632:3PI:H8	4:A:1465:HOH:O	1.83	0.77
1:A:559:TYR:CE2	1:A:561:ASN:O	2.39	0.76
1:A:198:LYS:HE3	4:A:1463:HOH:O	1.85	0.75
1:A:231:ASN:HD22	1:A:236:LEU:HB3	1.52	0.73
1:A:76:PRO:HB3	1:A:113:TYR:CG	2.24	0.72
1:A:232:GLU:HB3	4:A:1427:HOH:O	1.79	0.72
1:A:570:MET:HA	1:A:570:MET:HE3	1.71	0.71
1:A:216:ARG:HH11	1:A:216:ARG:HG2	1.55	0.70
1:A:496:THR:HG22	1:A:555:LEU:HB3	1.72	0.70
1:A:402:ILE:HG23	1:A:413:VAL:HG21	1.75	0.69
1:A:141:ALA:HA	4:A:1184:HOH:O	1.93	0.68
1:A:370:VAL:HG22	1:A:581:ILE:HD11	1.75	0.68
1:A:274:HIS:CD2	1:A:277:SER:H	2.12	0.68
1:A:251:PRO:HG2	1:A:254:GLU:HB2	1.77	0.67
1:A:570:MET:HA	1:A:570:MET:CE	2.25	0.67
1:A:310:ASN:HB3	4:A:1044:HOH:O	1.94	0.66
1:A:208:LEU:HD21	1:A:446:GLU:HB2	1.79	0.65
1:A:201:PHE:HB2	4:A:1466:HOH:O	1.97	0.65
1:A:74:GLU:HA	1:A:115:LYS:HE2	1.78	0.64
1:A:94:ILE:HD12	1:A:162:ARG:HD2	1.81	0.63
1:A:247:PRO:HB2	1:A:250:ILE:HG12	1.82	0.62
1:A:370:VAL:HG22	1:A:581:ILE:CD1	2.29	0.62
1:A:138:ILE:HD11	1:A:152:GLU:HB2	1.82	0.61
1:A:315:LYS:HG3	1:A:316:ILE:H	1.66	0.60
1:A:338:GLU:HB3	1:A:343:TYR:CD1	2.37	0.60
1:A:105:LEU:HD11	1:A:112:LEU:CD1	2.30	0.59
1:A:138:ILE:HD11	1:A:152:GLU:CB	2.32	0.59
1:A:389:LEU:HB3	1:A:570:MET:HE1	1.84	0.59
1:A:199:GLU:HG2	1:A:201:PHE:CE1	2.38	0.59
1:A:273:ILE:HD11	1:A:278:GLN:HG3	1.85	0.58
1:A:82:GLU:OE2	1:A:111:ARG:HG2	2.03	0.58
1:A:133:ASN:HD21	1:A:156:LYS:HE3	1.69	0.58
1:A:470:ASN:HB3	4:A:1121:HOH:O	2.03	0.57
1:A:532:ASN:OD1	1:A:535:LYS:HB2	2.03	0.57
1:A:115:LYS:HD2	1:A:124:VAL:HG22	1.86	0.57
1:A:116:SER:OG	1:A:118:GLU:HB2	2.04	0.57
1:A:218:GLN:HE22	1:A:272:TRP:HA	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ARG:HH21	1:A:443:ARG:HG3	1.70	0.57
1:A:459:ARG:NH2	3:A:3632:3PI:O51	2.38	0.57
1:A:459:ARG:HD3	4:A:1071:HOH:O	2.05	0.57
1:A:216:ARG:NH1	1:A:216:ARG:HG2	2.20	0.57
1:A:119:ARG:HG2	1:A:119:ARG:HH21	1.69	0.56
1:A:216:ARG:HG2	4:A:1523:HOH:O	2.04	0.56
1:A:231:ASN:ND2	1:A:237:CYS:N	2.42	0.56
1:A:134:ARG:HG2	1:A:471:HIS:CD2	2.40	0.56
1:A:196:GLU:O	1:A:198:LYS:HD2	2.05	0.56
1:A:569:SER:HB3	1:A:572:HIS:HD2	1.71	0.56
1:A:274:HIS:CD2	1:A:276:GLU:H	2.24	0.55
1:A:173:ARG:NH2	4:A:1521:HOH:O	2.39	0.55
1:A:94:ILE:HD12	1:A:162:ARG:CD	2.37	0.55
1:A:531:GLU:O	1:A:536:ARG:HD3	2.06	0.55
1:A:344:GLN:C	1:A:346:ALA:H	2.10	0.55
1:A:569:SER:HB3	1:A:572:HIS:CD2	2.42	0.54
1:A:112:LEU:HD13	1:A:179:LEU:HD21	1.89	0.54
1:A:315:LYS:HD2	1:A:345:ASN:HA	1.90	0.54
1:A:119:ARG:NH2	1:A:119:ARG:HG2	2.23	0.53
1:A:256:LYS:NZ	4:A:1484:HOH:O	2.40	0.53
1:A:556:TYR:CG	1:A:557:GLY:N	2.77	0.53
1:A:74:GLU:HG3	1:A:104:THR:CB	2.34	0.53
1:A:437:GLY:HA2	1:A:440:ARG:NH2	2.24	0.52
1:A:210:ASP:HB3	1:A:213:LEU:HB2	1.92	0.52
1:A:231:ASN:HD21	1:A:237:CYS:N	1.99	0.52
1:A:254:GLU:OE1	4:A:1105:HOH:O	2.19	0.52
1:A:257:ARG:NE	4:A:1477:HOH:O	2.42	0.52
1:A:442:ILE:O	1:A:446:GLU:HG3	2.09	0.52
1:A:307:MET:SD	1:A:345:ASN:HB3	2.50	0.52
1:A:140:GLY:O	1:A:143:SER:HB2	2.10	0.52
1:A:73:MET:N	4:A:1333:HOH:O	2.42	0.51
1:A:446:GLU:OE2	1:A:545:ASN:ND2	2.43	0.51
1:A:443:ARG:NH2	1:A:548:LEU:HD11	2.25	0.51
1:A:119:ARG:HH21	1:A:119:ARG:CG	2.24	0.51
1:A:94:ILE:HB	1:A:162:ARG:HD2	1.93	0.51
1:A:370:VAL:CG2	1:A:581:ILE:HD11	2.40	0.50
1:A:462:LEU:HG	1:A:475:ASP:HB3	1.93	0.50
1:A:228:THR:OG1	1:A:252:ASP:OD1	2.22	0.50
1:A:199:GLU:HG3	1:A:200:VAL:N	2.26	0.50
1:A:97:PHE:CD1	1:A:585:PRO:HD3	2.46	0.50
1:A:231:ASN:ND2	1:A:236:LEU:HB3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLU:HB2	1:A:115:LYS:HB3	1.93	0.50
1:A:257:ARG:NH2	4:A:1218:HOH:O	2.45	0.50
1:A:82:GLU:HB2	1:A:193:PHE:HZ	1.76	0.49
1:A:181:LYS:HA	1:A:188:ASN:ND2	2.27	0.49
1:A:274:HIS:HD2	1:A:277:SER:N	2.05	0.49
1:A:237:CYS:HB2	1:A:265:GLY:O	2.13	0.48
1:A:512:LEU:HD21	2:A:1878:EDO:H11	1.94	0.48
1:A:245:VAL:HB	1:A:270:LEU:HB3	1.95	0.48
1:A:253:GLU:O	1:A:256:LYS:HB2	2.14	0.48
1:A:442:ILE:HG12	1:A:500:PHE:HB3	1.96	0.48
1:A:443:ARG:HH22	1:A:548:LEU:HD11	1.79	0.48
1:A:584:ASN:ND2	4:A:1487:HOH:O	2.47	0.48
1:A:209:TYR:CD1	1:A:447:VAL:HG13	2.49	0.47
1:A:82:GLU:HB2	1:A:193:PHE:CZ	2.49	0.47
1:A:159:ARG:HD3	1:A:583:TRP:CE2	2.49	0.47
1:A:128:SER:O	1:A:131:VAL:HG22	2.14	0.47
1:A:547:GLN:O	1:A:549:GLU:HG2	2.14	0.47
1:A:501:ASN:O	1:A:504:PHE:HB3	2.15	0.47
1:A:485:ASP:O	1:A:489:GLN:HG2	2.15	0.46
1:A:76:PRO:HB3	1:A:113:TYR:CD2	2.50	0.46
1:A:313:SER:HA	4:A:1044:HOH:O	2.16	0.46
1:A:229:LYS:HG3	4:A:1294:HOH:O	2.16	0.46
1:A:245:VAL:HG11	1:A:270:LEU:HD23	1.97	0.46
1:A:323:PRO:HD2	1:A:326:ASN:ND2	2.31	0.46
1:A:87:MET:CE	1:A:89:LYS:HE3	2.46	0.46
1:A:389:LEU:HB3	1:A:570:MET:CE	2.44	0.46
1:A:331:LYS:HE2	4:A:1187:HOH:O	2.15	0.46
1:A:94:ILE:HD12	1:A:162:ARG:NE	2.31	0.45
1:A:432:MET:HE3	1:A:451:LYS:HE3	1.98	0.45
1:A:224:SER:HB3	1:A:309:SER:OG	2.16	0.45
1:A:400:LEU:HD11	1:A:566:PRO:O	2.16	0.45
1:A:85:LYS:HE3	1:A:182:TYR:CE2	2.50	0.45
1:A:547:GLN:HB2	4:A:1445:HOH:O	2.15	0.45
1:A:191:PRO:HG2	1:A:196:GLU:OE1	2.16	0.45
1:A:92:THR:O	1:A:163:PHE:HA	2.16	0.45
1:A:258:VAL:HG12	1:A:267:ILE:HG22	1.98	0.45
1:A:489:GLN:HE22	1:A:574:GLU:H	1.63	0.45
1:A:450:GLU:HA	1:A:454:LEU:HD12	1.99	0.45
1:A:511:HIS:HA	1:A:514:SER:OG	2.18	0.44
1:A:492:ARG:HD2	1:A:492:ARG:HA	1.82	0.44
1:A:218:GLN:HE21	1:A:273:ILE:HG22	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:VAL:HA	1:A:160:ASN:OD1	2.18	0.43
1:A:198:LYS:N	1:A:198:LYS:HD2	2.34	0.43
1:A:501:ASN:HD21	1:A:551:PHE:HA	1.83	0.43
1:A:533:LEU:N	1:A:534:PRO:CD	2.82	0.42
1:A:321:ALA:HB3	1:A:417:SER:HB3	2.00	0.42
1:A:461:GLN:HA	1:A:466:HIS:CD2	2.54	0.42
1:A:138:ILE:HD11	1:A:152:GLU:HB3	2.00	0.42
1:A:569:SER:CB	1:A:572:HIS:HD2	2.32	0.42
1:A:501:ASN:ND2	1:A:504:PHE:H	2.18	0.42
1:A:261:PHE:O	1:A:288:MET:HG2	2.18	0.42
1:A:383:LEU:HD21	1:A:389:LEU:CD1	2.50	0.42
1:A:254:GLU:O	1:A:257:ARG:HB2	2.20	0.42
1:A:383:LEU:HD21	1:A:389:LEU:HD12	2.00	0.41
1:A:268:PRO:HA	1:A:283:ARG:O	2.19	0.41
1:A:274:HIS:CD2	1:A:276:GLU:HB3	2.55	0.41
1:A:303:LEU:HD22	1:A:343:TYR:CD2	2.54	0.41
1:A:501:ASN:HD22	1:A:501:ASN:C	2.24	0.41
1:A:501:ASN:H	1:A:501:ASN:ND2	2.18	0.41
1:A:255:LEU:C	1:A:257:ARG:N	2.73	0.41
1:A:87:MET:HE1	1:A:89:LYS:HE3	2.03	0.41
1:A:133:ASN:ND2	1:A:156:LYS:HE3	2.33	0.41
1:A:230:ILE:O	1:A:230:ILE:HG12	2.20	0.41
1:A:366:LEU:HA	1:A:386:THR:HG21	2.03	0.40
1:A:294:LYS:HD2	4:A:1469:HOH:O	2.21	0.40
1:A:78:LEU:HD22	1:A:82:GLU:HG2	2.02	0.40
1:A:246:VAL:HB	1:A:247:PRO:CD	2.51	0.40
1:A:264:ARG:HD3	1:A:421:TRP:CH2	2.56	0.40

All (8) 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)
4:A:1018:HOH:O	4:A:1399:HOH:O[4_464]	0.35	1.85
1:A:295:ARG:N	1:A:312:GLN:NE2[6_465]	0.97	1.23
1:A:294:LYS:C	1:A:312:GLN:NE2[6_465]	1.56	0.64
4:A:1165:HOH:O	4:A:1165:HOH:O[8_775]	1.73	0.47
1:A:376:GLU:OE2	1:A:571:ARG:NH2[8_775]	2.04	0.16
1:A:294:LYS:CA	1:A:312:GLN:NE2[6_465]	2.06	0.14
4:A:1476:HOH:O	4:A:1476:HOH:O[8_775]	2.14	0.06
1:A:145:GLY:N	1:A:223:GLU:OE2[8_675]	2.16	0.04

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	512/528 (97%)	479 (94%)	25 (5%)	8 (2%)	12 4

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	GLY
1	A	313	SER
1	A	548	LEU
1	A	315	LYS
1	A	576	TRP
1	A	522	CYS
1	A	547	GLN
1	A	158	ILE

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	457/467 (98%)	430 (94%)	27 (6%)	24 16

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	GLU
1	A	83	ASN
1	A	119	ARG

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Mol	Chain	Res	Type
1	A	120	ASP
1	A	144	ARG
1	A	146	GLU
1	A	158	ILE
1	A	162	ARG
1	A	198	LYS
1	A	199	GLU
1	A	207	LYS
1	A	221	PRO
1	A	240	TYR
1	A	297	LYS
1	A	298	GLU
1	A	309	SER
1	A	347	GLU
1	A	370	VAL
1	A	371	TYR
1	A	372	PRO
1	A	375	GLU
1	A	376	GLU
1	A	421	TRP
1	A	455	SER
1	A	501	ASN
1	A	549	GLU
1	A	570	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	133	ASN
1	A	188	ASN
1	A	218	GLN
1	A	231	ASN
1	A	274	HIS
1	A	416	HIS
1	A	489	GLN
1	A	501	ASN
1	A	545	ASN
1	A	572	HIS
1	A	584	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	$\# Z > 2$
2	EDO	A	1878	-	3,3,3	0.71	0	2,2,2	0.08	0
2	EDO	A	1879	-	3,3,3	0.69	0	2,2,2	0.19	0
2	EDO	A	1880	-	3,3,3	0.62	0	2,2,2	0.21	0
3	3PI	A	3632	-	39,39,39	3.72	16 (41%)	47,57,57	1.83	10 (21%)

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	1878	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1879	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1880	-	-	0/1/1/1	0/0/0/0
3	3PI	A	3632	-	-	0/35/60/60	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3632	3PI	O16-C10	-15.67	1.04	1.39
3	A	3632	3PI	O6-C6	-3.97	1.33	1.43
3	A	3632	3PI	C11-C10	-2.64	1.45	1.50
3	A	3632	3PI	O4-C4	-2.45	1.37	1.43
3	A	3632	3PI	P3-O31	2.06	1.57	1.51
3	A	3632	3PI	O3-C3	2.07	1.50	1.44
3	A	3632	3PI	C6-C5	2.42	1.59	1.52
3	A	3632	3PI	C4-C3	2.54	1.59	1.52
3	A	3632	3PI	O14-C14	2.81	1.42	1.34
3	A	3632	3PI	O2-C2	3.26	1.50	1.43
3	A	3632	3PI	C4-C5	3.46	1.62	1.52
3	A	3632	3PI	C2-C1	3.67	1.62	1.52
3	A	3632	3PI	C6-C1	4.23	1.64	1.52
3	A	3632	3PI	C2-C3	4.94	1.66	1.52
3	A	3632	3PI	O14-C8	5.17	1.59	1.46
3	A	3632	3PI	O15-C10	10.06	1.58	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3632	3PI	C9-C8-C7	-2.51	106.20	112.07
3	A	3632	3PI	C13-C12-C11	-2.31	101.34	113.58
3	A	3632	3PI	O14-C8-C9	2.03	115.53	108.36
3	A	3632	3PI	P3-O3-C3	2.29	127.06	121.56
3	A	3632	3PI	C6-C5-C4	2.47	114.14	110.89
3	A	3632	3PI	O14-C14-O17	2.53	130.46	123.67
3	A	3632	3PI	O14-C8-C7	3.08	119.21	108.36
3	A	3632	3PI	C8-O14-C14	3.56	126.42	117.89
3	A	3632	3PI	O16-C10-C11	4.99	118.06	109.05
3	A	3632	3PI	O15-C9-C8	6.59	126.66	110.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1878	EDO	1	0
3	A	3632	3PI	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	514/528 (97%)	0.49	25 (4%)	33 37	24, 44, 72, 96	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	ALA	11.0
1	A	141	ALA	5.1
1	A	559	TYR	4.6
1	A	312	GLN	4.2
1	A	560	SER	4.1
1	A	557	GLY	3.4
1	A	548	LEU	3.4
1	A	561	ASN	3.4
1	A	585	PRO	3.4
1	A	315	LYS	2.8
1	A	421	TRP	2.5
1	A	145	GLY	2.5
1	A	551	PHE	2.4
1	A	146	GLU	2.4
1	A	147	ASN	2.2
1	A	586	ARG	2.2
1	A	100	ALA	2.1
1	A	144	ARG	2.1
1	A	101	VAL	2.1
1	A	112	LEU	2.1
1	A	197	TYR	2.1
1	A	344	GLN	2.1
1	A	316	ILE	2.0
1	A	343	TYR	2.0
1	A	416	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	EDO	A	1880	4/4	0.77	0.19	5.66	51,51,52,52	0
2	EDO	A	1878	4/4	0.95	0.14	2.58	25,33,35,37	0
3	3PI	A	3632	39/39	0.92	0.18	1.35	30,64,94,96	3
2	EDO	A	1879	4/4	0.87	0.18	-	51,54,54,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.