



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:47 pm GMT

PDB ID : 3SEY
Title : Zn-mediated Polymer of Maltose-binding Protein A216H/K220H by Synthetic Symmetrization (Form II)
Authors : Zhao, M.; Soriaga, A.B.; Laganowsky, A.; Sawaya, M.R.; Cascio, D.; Yeates, T.O.
Deposited on : 2011-06-11
Resolution : 1.85 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

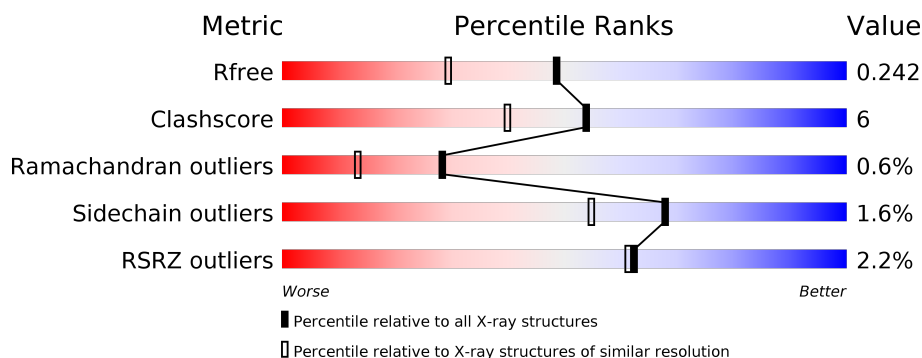
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	100719	1923 (1.86-1.86)
Clashscore	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)
RSRZ outliers	101464	1932 (1.86-1.86)

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	372	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 90% 8% • </div> </div>
1	C	372	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 87% 12% • </div> </div>
1	E	372	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 1%, green 93%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 5% 85% 14% •• </div> </div>

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	ZN	A	373	-	-	-	X
3	ZN	A	375	-	-	-	X
4	ACT	A	383	-	-	-	X
4	ACT	A	384	-	-	-	X
4	ACT	C	382	-	-	-	X
5	GOL	A	386	-	-	-	X
5	GOL	A	387	-	-	-	X
5	GOL	C	383	-	-	-	X
5	GOL	C	384	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9260 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 Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	4	0
			2879	1852	470	550	7			
1	C	371	Total	C	N	O	S	0	5	0
			2879	1856	470	546	7			
1	E	370	Total	C	N	O	S	0	1	0
			2845	1831	465	543	6			

There are 48 discrepancies between the modelled and reference sequences:

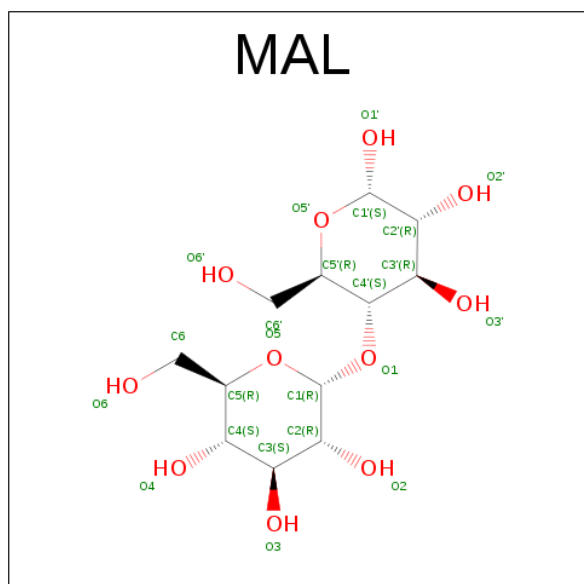
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP P0AEX9
A	216	HIS	ALA	ENGINEERED MUTATION	UNP P0AEX9
A	220	HIS	LYS	ENGINEERED MUTATION	UNP P0AEX9
A	360	ALA	-	EXPRESSION TAG	UNP P0AEX9
A	361	ALA	-	EXPRESSION TAG	UNP P0AEX9
A	362	LEU	-	EXPRESSION TAG	UNP P0AEX9
A	363	ALA	-	EXPRESSION TAG	UNP P0AEX9
A	364	ALA	-	EXPRESSION TAG	UNP P0AEX9
A	365	ALA	-	EXPRESSION TAG	UNP P0AEX9
A	366	GLN	-	EXPRESSION TAG	UNP P0AEX9
A	367	THR	-	EXPRESSION TAG	UNP P0AEX9
A	368	ASN	-	EXPRESSION TAG	UNP P0AEX9
A	369	ALA	-	EXPRESSION TAG	UNP P0AEX9
A	370	ALA	-	EXPRESSION TAG	UNP P0AEX9
A	371	ALA	-	EXPRESSION TAG	UNP P0AEX9
A	372	ALA	-	EXPRESSION TAG	UNP P0AEX9
C	1	MET	-	INITIATING METHIONINE	UNP P0AEX9
C	216	HIS	ALA	ENGINEERED MUTATION	UNP P0AEX9
C	220	HIS	LYS	ENGINEERED MUTATION	UNP P0AEX9
C	360	ALA	-	EXPRESSION TAG	UNP P0AEX9
C	361	ALA	-	EXPRESSION TAG	UNP P0AEX9
C	362	LEU	-	EXPRESSION TAG	UNP P0AEX9
C	363	ALA	-	EXPRESSION TAG	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	364	ALA	-	EXPRESSION TAG	UNP P0AEX9
C	365	ALA	-	EXPRESSION TAG	UNP P0AEX9
C	366	GLN	-	EXPRESSION TAG	UNP P0AEX9
C	367	THR	-	EXPRESSION TAG	UNP P0AEX9
C	368	ASN	-	EXPRESSION TAG	UNP P0AEX9
C	369	ALA	-	EXPRESSION TAG	UNP P0AEX9
C	370	ALA	-	EXPRESSION TAG	UNP P0AEX9
C	371	ALA	-	EXPRESSION TAG	UNP P0AEX9
C	372	ALA	-	EXPRESSION TAG	UNP P0AEX9
E	1	MET	-	INITIATING METHIONINE	UNP P0AEX9
E	216	HIS	ALA	ENGINEERED MUTATION	UNP P0AEX9
E	220	HIS	LYS	ENGINEERED MUTATION	UNP P0AEX9
E	360	ALA	-	EXPRESSION TAG	UNP P0AEX9
E	361	ALA	-	EXPRESSION TAG	UNP P0AEX9
E	362	LEU	-	EXPRESSION TAG	UNP P0AEX9
E	363	ALA	-	EXPRESSION TAG	UNP P0AEX9
E	364	ALA	-	EXPRESSION TAG	UNP P0AEX9
E	365	ALA	-	EXPRESSION TAG	UNP P0AEX9
E	366	GLN	-	EXPRESSION TAG	UNP P0AEX9
E	367	THR	-	EXPRESSION TAG	UNP P0AEX9
E	368	ASN	-	EXPRESSION TAG	UNP P0AEX9
E	369	ALA	-	EXPRESSION TAG	UNP P0AEX9
E	370	ALA	-	EXPRESSION TAG	UNP P0AEX9
E	371	ALA	-	EXPRESSION TAG	UNP P0AEX9
E	372	ALA	-	EXPRESSION TAG	UNP P0AEX9

- Molecule 2 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: C₁₂H₂₂O₁₁).

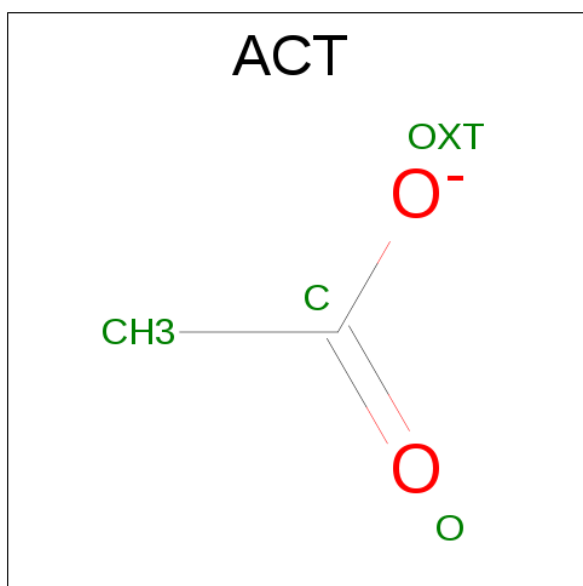


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			23	12	11		
2	C	1	Total	C	O	0	1
			23	12	11		
2	E	1	Total	C	O	0	1
			46	24	22		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	Zn	0	0
			10	10		
3	C	7	Total	Zn	0	0
			7	7		
3	E	6	Total	Zn	0	0
			6	6		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



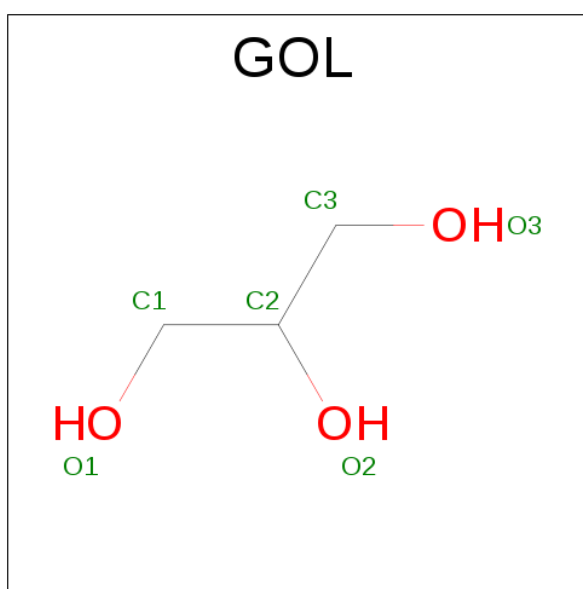
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

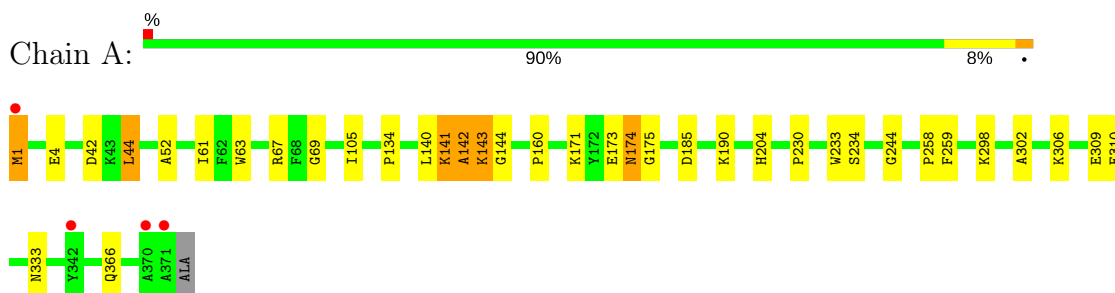
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	220	Total 220	O 220	0	0
6	C	200	Total 200	O 200	0	0
6	E	60	Total 60	O 60	0	0

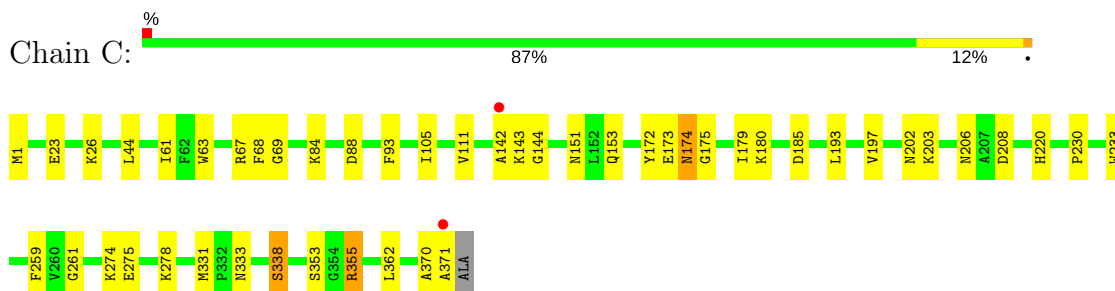
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

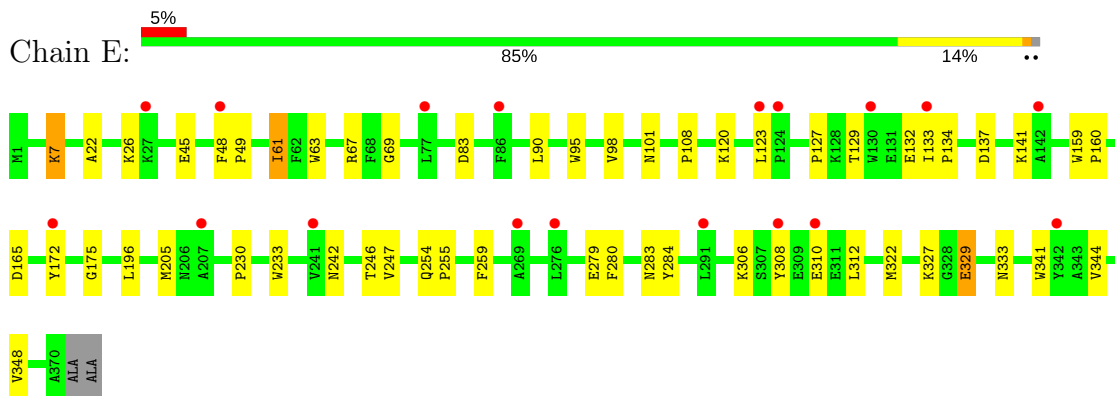
• Molecule 1: Maltose-binding periplasmic protein



• Molecule 1: Maltose-binding periplasmic protein



• Molecule 1: Maltose-binding periplasmic protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.66Å 63.65Å 221.83Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	49.09 – 1.85 73.94 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.09-1.85) 99.8 (73.94-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 1.84Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.208 , 0.247 0.205 , 0.242	Depositor DCC
R_{free} test set	5990 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9260	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, MAL, ACT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/2963	0.54	1/4030 (0.0%)
1	C	0.41	0/2966	0.54	0/4033
1	E	0.28	0/2919	0.42	0/3973
All	All	0.37	0/8848	0.50	1/12036 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	LYS	N-CA-C	5.41	125.62	111.00

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	2879	0	2821	36	0
1	C	2879	0	2827	36	0
1	E	2845	0	2774	33	0
2	A	23	0	22	0	0
2	C	23	0	22	0	0
2	E	46	0	44	1	0
3	A	10	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	7	0	0	0	1
3	E	6	0	0	0	0
4	A	12	0	9	2	0
4	C	16	0	12	0	1
4	E	4	0	3	1	0
5	A	18	0	24	4	0
5	C	12	0	16	4	0
6	A	220	0	0	5	1
6	C	200	0	0	5	0
6	E	60	0	0	2	0
All	All	9260	0	8574	105	2

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 (105) 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:142:ALA:HA	1:A:144:GLY:H	1.10	1.12
1:A:142:ALA:HA	1:A:144:GLY:N	1.66	1.10
1:A:302:ALA:HB1	5:A:386:GOL:H32	1.43	1.01
1:A:142:ALA:CA	1:A:144:GLY:H	1.80	0.94
1:E:69:GLY:HA3	1:E:333:ASN:O	1.79	0.83
1:A:44:LEU:CD1	1:A:61:ILE:HD11	2.10	0.81
1:C:274:LYS:O	1:C:278[B]:LYS:HG2	1.81	0.80
1:C:174:ASN:N	1:C:175:GLY:HA2	1.97	0.78
1:A:44:LEU:HD13	1:A:61:ILE:HD11	1.65	0.78
1:A:173:GLU:OE1	6:A:402:HOH:O	2.01	0.78
1:C:278[B]:LYS:HD3	6:C:523:HOH:O	1.84	0.76
1:C:185[B]:ASP:OD2	6:C:476:HOH:O	2.04	0.74
5:C:384:GOL:O2	6:C:559:HOH:O	2.04	0.74
1:A:244:GLY:HA2	5:A:387:GOL:H2	1.71	0.73
1:A:173:GLU:OE2	6:A:401:HOH:O	2.07	0.73
1:C:179:ILE:HG13	1:C:180:LYS:HD2	1.70	0.71
1:C:173:GLU:C	1:C:175:GLY:HA2	2.11	0.71
1:C:44:LEU:CD1	1:C:61:ILE:HD11	2.22	0.69
1:C:69:GLY:HA3	1:C:333:ASN:O	1.92	0.68
1:A:302:ALA:CB	5:A:386:GOL:H32	2.23	0.67
1:A:185:ASP:OD2	1:A:366:GLN:HG3	1.95	0.66
1:A:173:GLU:O	1:A:175:GLY:N	2.28	0.65
1:E:83:ASP:OD2	6:E:388:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:GLU:HG3	1:E:283:ASN:HD22	1.62	0.62
1:C:274:LYS:O	1:C:278[B]:LYS:CG	2.47	0.61
1:E:230:PRO:HA	1:E:233:TRP:CE2	2.35	0.61
1:A:69:GLY:HA3	1:A:333:ASN:O	2.00	0.60
1:A:140:LEU:O	1:A:142:ALA:N	2.33	0.60
1:A:185:ASP:O	1:A:190:LYS:HE2	2.02	0.60
1:E:308:TYR:CE2	1:E:312:LEU:HD11	2.37	0.58
1:A:44:LEU:HD13	1:A:61:ILE:CD1	2.35	0.57
1:E:165:ASP:OD1	1:E:254:GLN:NE2	2.38	0.56
1:A:141:LYS:O	1:A:142:ALA:HB2	2.05	0.56
1:A:142:ALA:N	1:A:144:GLY:H	2.03	0.55
1:E:322:MET:HA	1:E:322:MET:CE	2.37	0.55
1:A:185:ASP:CG	1:A:366:GLN:HG3	2.28	0.54
1:C:44:LEU:HD12	1:C:44:LEU:C	2.28	0.54
1:E:22:ALA:O	1:E:26:LYS:HG2	2.07	0.53
1:C:353:SER:OG	1:C:355:ARG:HB2	2.08	0.53
1:E:279:GLU:HG3	1:E:283:ASN:ND2	2.23	0.53
1:A:309:GLU:HG2	5:A:386:GOL:H31	1.91	0.53
1:A:141:LYS:HD3	6:A:515:HOH:O	2.09	0.52
1:C:26:LYS:CE	6:C:584:HOH:O	2.57	0.52
1:C:44:LEU:HD13	1:C:61:ILE:HD11	1.91	0.52
1:A:140:LEU:C	1:A:142:ALA:H	2.13	0.51
1:E:129:THR:OG1	1:E:132:GLU:OE2	2.17	0.51
1:A:1:MET:HG2	6:A:540:HOH:O	2.10	0.51
1:A:44:LEU:HD12	1:A:44:LEU:C	2.30	0.51
1:C:44:LEU:HD13	1:C:61:ILE:CD1	2.40	0.51
1:A:4:GLU:OE1	1:C:220[A]:HIS:NE2	2.35	0.51
1:C:63:TRP:CD1	1:C:67[A]:ARG:HG3	2.47	0.49
1:A:204:HIS:HD2	4:A:383:ACT:OXT	1.95	0.49
1:C:172:TYR:CZ	1:C:175:GLY:HA3	2.48	0.48
1:E:67[A]:ARG:NH2	6:E:419:HOH:O	2.26	0.48
1:C:202:ASN:C	1:C:203:LYS:HG2	2.33	0.48
1:E:120:LYS:HB2	1:E:242:ASN:ND2	2.28	0.48
1:E:280:PHE:O	1:E:284:TYR:HB2	2.13	0.48
1:C:142:ALA:C	1:C:144:GLY:H	2.17	0.48
1:A:63:TRP:CD1	1:A:67[B]:ARG:HG3	2.47	0.48
1:A:105:ILE:HD12	1:A:105:ILE:C	2.35	0.47
1:C:23:GLU:OE1	6:C:563:HOH:O	2.20	0.47
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.49	0.47
1:A:160:PRO:HG3	1:A:258:PRO:HA	1.96	0.47
1:E:90:LEU:HD12	1:E:95:TRP:CZ2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:GLU:N	1:E:45:GLU:OE1	2.41	0.46
1:E:255:PRO:HB3	1:E:327:LYS:HD3	1.97	0.46
1:E:172:TYR:OH	1:E:175:GLY:HA2	2.16	0.46
1:E:306:LYS:O	1:E:310:GLU:HG3	2.16	0.46
1:E:61:ILE:HD13	1:E:61:ILE:C	2.36	0.46
1:A:141:LYS:O	1:A:142:ALA:CB	2.64	0.46
1:A:52:ALA:O	6:A:553:HOH:O	2.20	0.45
1:C:370:ALA:O	1:C:371:ALA:C	2.53	0.45
1:C:153:GLN:HB2	5:C:383:GOL:H12	1.98	0.45
1:E:322:MET:HE3	1:E:322:MET:HA	1.98	0.45
1:C:151:ASN:HD21	5:C:383:GOL:H2	1.82	0.45
1:E:341:TRP:CD1	2:E:5044[A]:MAL:H4	2.52	0.45
1:C:230:PRO:HA	1:C:233:TRP:CE2	2.52	0.45
1:E:123:LEU:HD21	1:E:127:PRO:HD3	1.98	0.45
1:E:329:GLU:OE1	4:E:379:ACT:C	2.65	0.45
1:E:159:TRP:N	1:E:160:PRO:CD	2.81	0.44
1:E:63:TRP:CD1	1:E:67[B]:ARG:HG3	2.53	0.44
1:C:206[A]:ASN:OD1	1:C:208:ASP:OD2	2.36	0.44
1:E:7:LYS:HB2	1:E:7:LYS:NZ	2.33	0.44
1:C:153:GLN:CB	5:C:383:GOL:H12	2.48	0.43
1:C:173:GLU:O	1:C:174:ASN:CB	2.66	0.43
1:C:84:LYS:HE2	1:C:88:ASP:OD1	2.19	0.43
1:A:306:LYS:O	1:A:310:GLU:HG3	2.17	0.43
1:C:68:PHE:HB3	1:C:105:ILE:HD13	2.01	0.43
1:C:173:GLU:O	1:C:175:GLY:HA2	2.19	0.42
1:E:98:VAL:HG21	1:E:108:PRO:HD3	2.02	0.42
1:C:193:LEU:O	1:C:197:VAL:HG23	2.20	0.42
1:E:344:VAL:O	1:E:348:VAL:HG23	2.20	0.42
1:C:275:GLU:HA	1:C:278[B]:LYS:HG3	2.01	0.42
1:E:133:ILE:N	1:E:134:PRO:CD	2.83	0.42
1:E:48:PHE:N	1:E:49:PRO:HD2	2.35	0.42
1:E:137:ASP:OD1	1:E:141:LYS:HE3	2.19	0.42
1:C:67[A]:ARG:NH1	1:C:338:SER:HB3	2.35	0.42
1:C:93:PHE:CZ	1:C:111:VAL:HG21	2.54	0.42
1:E:196:LEU:HD12	1:E:205:MET:HE1	2.02	0.41
1:A:134:PRO:HB2	4:A:384:ACT:H2	2.02	0.41
1:C:193:LEU:HD22	1:C:362:LEU:HD21	2.03	0.41
1:C:261:GLY:CA	1:C:331:MET:HE2	2.51	0.41
1:E:246:THR:OG1	1:E:247:VAL:N	2.54	0.40
1:A:234:SER:OG	1:A:298:LYS:HD3	2.20	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:374:ZN:ZN	4:C:380:ACT:O[3_455]	1.46	0.74
3:A:375:ZN:ZN	6:A:401:HOH:O[2_555]	1.51	0.69

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	373/372 (100%)	361 (97%)	8 (2%)	4 (1%)	17	5
1	C	374/372 (100%)	364 (97%)	7 (2%)	3 (1%)	22	8
1	E	369/372 (99%)	361 (98%)	8 (2%)	0	100	100
All	All	1116/1116 (100%)	1086 (97%)	23 (2%)	7 (1%)	28	13

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	ALA
1	A	143	LYS
1	A	141	LYS
1	A	174	ASN
1	C	174	ASN
1	C	355	ARG
1	C	143	LYS

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	293/293 (100%)	287 (98%)	6 (2%)	60	45
1	C	291/293 (99%)	288 (99%)	3 (1%)	80	74
1	E	286/293 (98%)	281 (98%)	5 (2%)	66	52
All	All	870/879 (99%)	856 (98%)	14 (2%)	68	55

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	42	ASP
1	A	44	LEU
1	A	171	LYS
1	A	174	ASN
1	A	259	PHE
1	C	1	MET
1	C	259	PHE
1	C	338	SER
1	E	7	LYS
1	E	61	ILE
1	E	101	ASN
1	E	259	PHE
1	E	329	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	E	283	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 23 are monoatomic - leaving 17 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
4	ACT	A	383	3	1,3,3	0.88	0	0,3,3	0.00	-
4	ACT	A	384	3	1,3,3	2.48	1 (100%)	0,3,3	0.00	-
4	ACT	A	385	3	1,3,3	1.16	0	0,3,3	0.00	-
5	GOL	A	386	-	5,5,5	0.43	0	5,5,5	0.36	0
5	GOL	A	387	-	5,5,5	0.30	0	5,5,5	0.33	0
5	GOL	A	388	-	5,5,5	0.35	0	5,5,5	0.28	0
2	MAL	A	5044[A]	-	24,24,24	0.50	0	35,35,35	1.00	1 (2%)
4	ACT	C	380	-	1,3,3	1.21	0	0,3,3	0.00	-
4	ACT	C	381	-	1,3,3	0.53	0	0,3,3	0.00	-
4	ACT	C	382	-	1,3,3	0.73	0	0,3,3	0.00	-
5	GOL	C	383	-	5,5,5	0.35	0	5,5,5	0.54	0
5	GOL	C	384	-	5,5,5	0.36	0	5,5,5	0.20	0
4	ACT	C	385	3	1,3,3	1.30	0	0,3,3	0.00	-
2	MAL	C	5044[A]	-	24,24,24	0.51	0	35,35,35	0.85	0
4	ACT	E	379	3	1,3,3	1.68	0	0,3,3	0.00	-
2	MAL	E	5044[A]	-	24,24,24	0.54	0	35,35,35	0.71	1 (2%)
2	MAL	E	5044[B]	-	24,24,24	0.57	0	35,35,35	1.28	4 (11%)

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
4	ACT	A	383	3	-	0/0/0/0	0/0/0/0
4	ACT	A	384	3	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACT	A	385	3	-	0/0/0/0	0/0/0/0
5	GOL	A	386	-	-	0/4/4/4	0/0/0/0
5	GOL	A	387	-	-	0/4/4/4	0/0/0/0
5	GOL	A	388	-	-	0/4/4/4	0/0/0/0
2	MAL	A	5044[A]	-	-	0/8/48/48	0/2/2/2
4	ACT	C	380	-	-	0/0/0/0	0/0/0/0
4	ACT	C	381	-	-	0/0/0/0	0/0/0/0
4	ACT	C	382	-	-	0/0/0/0	0/0/0/0
5	GOL	C	383	-	-	0/4/4/4	0/0/0/0
5	GOL	C	384	-	-	0/4/4/4	0/0/0/0
4	ACT	C	385	3	-	0/0/0/0	0/0/0/0
2	MAL	C	5044[A]	-	-	0/8/48/48	0/2/2/2
4	ACT	E	379	3	-	0/0/0/0	0/0/0/0
2	MAL	E	5044[A]	-	-	0/8/48/48	0/2/2/2
2	MAL	E	5044[B]	-	-	0/8/48/48	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	384	ACT	CH3-C	2.48	1.51	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5044[A]	MAL	C4-C3-C2	-2.23	106.91	110.84
2	E	5044[B]	MAL	C4-C3-C2	-2.21	106.94	110.84
2	A	5044[A]	MAL	C1'-O5'-C5'	2.59	118.07	113.39
2	E	5044[B]	MAL	C1'-C2'-C3'	2.82	115.75	110.65
2	E	5044[B]	MAL	C1'-O5'-C5'	3.58	119.85	113.39
2	E	5044[B]	MAL	O5'-C1'-C2'	4.80	118.00	110.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	383	ACT	1	0
4	A	384	ACT	1	0
5	A	386	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	387	GOL	1	0
4	C	380	ACT	0	1
5	C	383	GOL	3	0
5	C	384	GOL	1	0
4	E	379	ACT	1	0
2	E	5044[A]	MAL	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

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	371/372 (99%)	0.01	4 (1%) 80 81	11, 23, 43, 73	0
1	C	371/372 (99%)	0.06	2 (0%) 90 91	10, 23, 45, 65	0
1	E	370/372 (99%)	0.61	18 (4%) 30 29	26, 43, 64, 88	0
All	All	1112/1116 (99%)	0.23	24 (2%) 62 61	10, 30, 58, 88	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	269	ALA	3.9
1	A	1	MET	3.8
1	C	371	ALA	3.8
1	E	291	LEU	3.5
1	A	371	ALA	3.4
1	E	123	LEU	3.4
1	E	133	ILE	3.2
1	E	241	VAL	2.9
1	E	124	PRO	2.9
1	E	276	LEU	2.7
1	E	77	LEU	2.7
1	E	130	TRP	2.6
1	C	142	ALA	2.6
1	A	370	ALA	2.5
1	E	172	TYR	2.4
1	E	48	PHE	2.3
1	A	342	TYR	2.2
1	E	308	TYR	2.2
1	E	342	TYR	2.2
1	E	310	GLU	2.1
1	E	142	ALA	2.1
1	E	86	PHE	2.0
1	E	207	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	27	LYS	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(Å ²)	Q<0.9
5	GOL	A	386	6/6	0.85	0.23	11.49	35,41,41,43	0
4	ACT	C	382	4/4	0.96	0.15	9.19	22,22,27,34	0
3	ZN	A	373	1/1	0.99	0.13	8.09	18,18,18,18	0
5	GOL	C	383	6/6	0.93	0.15	6.58	23,40,40,42	0
5	GOL	A	387	6/6	0.91	0.16	6.29	26,46,48,51	0
4	ACT	A	383	4/4	0.87	0.18	4.33	23,25,32,35	0
5	GOL	C	384	6/6	0.83	0.19	3.81	44,52,53,53	0
4	ACT	A	384	4/4	0.92	0.14	2.87	19,21,24,26	0
3	ZN	A	375	1/1	0.96	0.19	2.69	21,21,21,21	1
4	ACT	C	381	4/4	0.92	0.16	1.77	20,21,32,42	0
4	ACT	C	380	4/4	0.96	0.14	1.52	9,17,22,29	0
3	ZN	A	381	1/1	0.92	0.12	0.89	45,45,45,45	1
4	ACT	A	385	4/4	0.94	0.16	0.66	19,25,28,38	0
5	GOL	A	388	6/6	0.93	0.12	0.52	54,61,63,65	0
2	MAL	A	5044[A]	23/23	0.97	0.11	-0.18	7,17,20,23	0
3	ZN	C	373	1/1	0.99	0.11	-0.27	17,17,17,17	0
2	MAL	E	5044[A]	23/23	0.96	0.11	-0.27	24,29,31,34	23
2	MAL	C	5044[A]	23/23	0.98	0.10	-0.34	10,17,22,22	0
3	ZN	C	378	1/1	0.98	0.11	-0.43	39,39,39,39	1
2	MAL	E	5044[B]	23/23	0.96	0.11	-0.47	25,29,32,33	23

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	A	377	1/1	0.99	0.08	-0.88	30,30,30,30	1
3	ZN	A	376	1/1	0.99	0.07	-1.38	30,30,30,30	1
3	ZN	E	373	1/1	0.97	0.09	-1.51	34,34,34,34	0
3	ZN	C	375	1/1	0.92	0.12	-1.79	44,44,44,44	0
3	ZN	E	374	1/1	1.00	0.08	-2.65	39,39,39,39	0
3	ZN	E	375	1/1	0.99	0.04	-3.34	54,54,54,54	0
3	ZN	C	377	1/1	0.97	0.09	-	33,33,33,33	1
3	ZN	E	376	1/1	0.98	0.05	-	60,60,60,60	0
3	ZN	E	377	1/1	0.98	0.11	-	50,50,50,50	1
4	ACT	E	379	4/4	0.68	0.18	-	52,52,55,55	0
3	ZN	A	379	1/1	0.91	0.11	-	51,51,51,51	0
4	ACT	C	385	4/4	0.85	0.12	-	40,49,50,56	0
3	ZN	C	376	1/1	0.96	0.10	-	45,45,45,45	0
3	ZN	C	379	1/1	0.91	0.08	-	53,53,53,53	1
3	ZN	E	378	1/1	0.88	0.39	-	46,46,46,46	1
3	ZN	A	378	1/1	0.98	0.05	-	43,43,43,43	0
3	ZN	A	380	1/1	0.90	0.11	-	85,85,85,85	0
3	ZN	A	374	1/1	0.97	0.14	-	25,25,25,25	0
3	ZN	A	382	1/1	0.98	0.05	-	38,38,38,38	1
3	ZN	C	374	1/1	0.99	0.10	-	24,24,24,24	0

6.5 Other polymers

There are no such residues in this entry.