



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:54 AM UTC

PDB ID : 4MB0 / pdb_00004mb0
Title : Crystal structure of TON1374
Authors : Kim, M.-K.; An, Y.J.; Cha, S.-S.
Deposited on : 2013-08-19
Resolution : 1.96 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)
Xtrriage (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

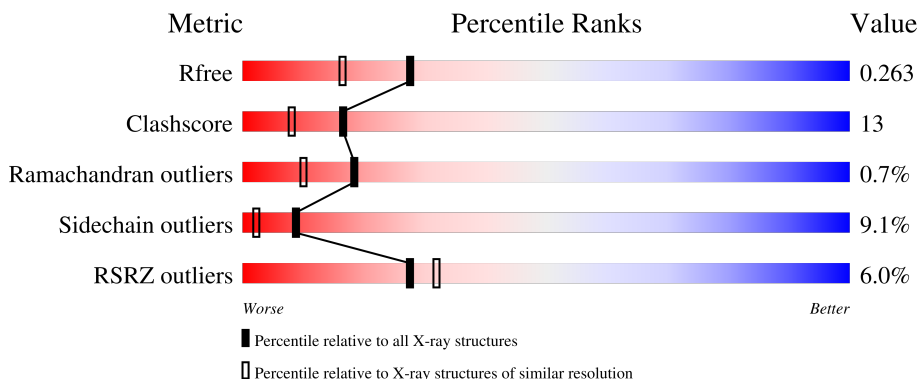
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 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	261	 5% 75% 18% . .
1	B	261	 4% 68% 23% 7% .
1	C	261	 5% 72% 20% . .
1	D	261	 9% 74% 18% . . .

2 Entry composition [i](#)

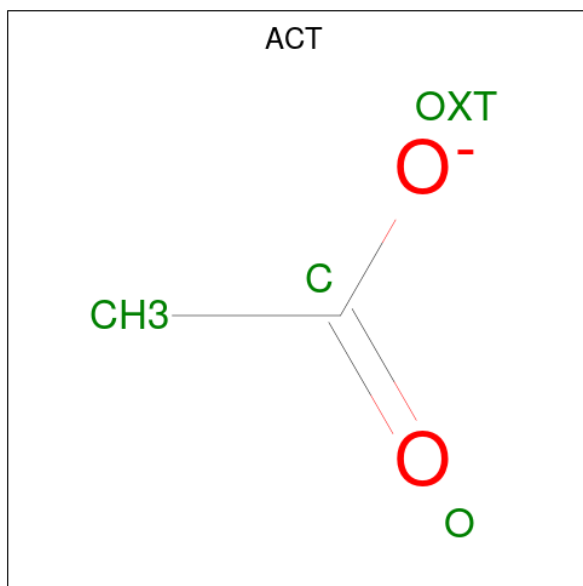
There are 3 unique types of molecules in this entry. The entry contains 8358 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 phosphopantothenate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	253	Total 2027	C 1281	N 364	O 375	S 7	0	1	0
1	B	257	Total 2038	C 1292	N 365	O 374	S 7	0	0	0
1	C	253	Total 2016	C 1275	N 360	O 374	S 7	0	0	0
1	D	252	Total 2004	C 1267	N 357	O 373	S 7	0	0	0

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

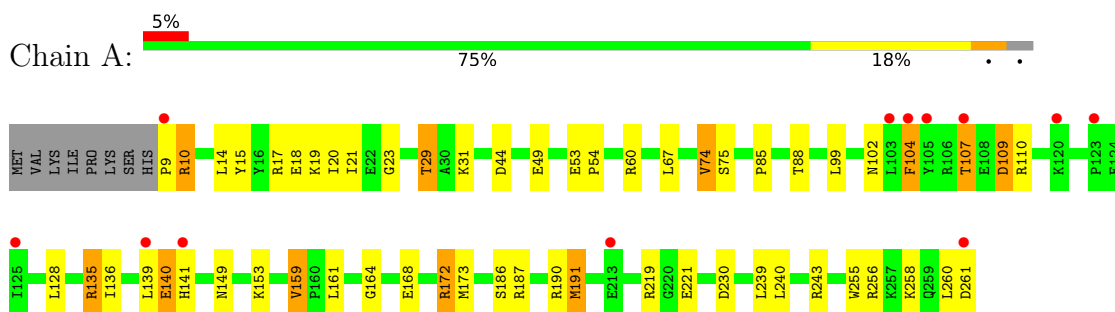
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total 52	O 52	0	0
3	B	87	Total 87	O 87	0	0
3	C	67	Total 67	O 67	0	0
3	D	63	Total 63	O 63	0	0

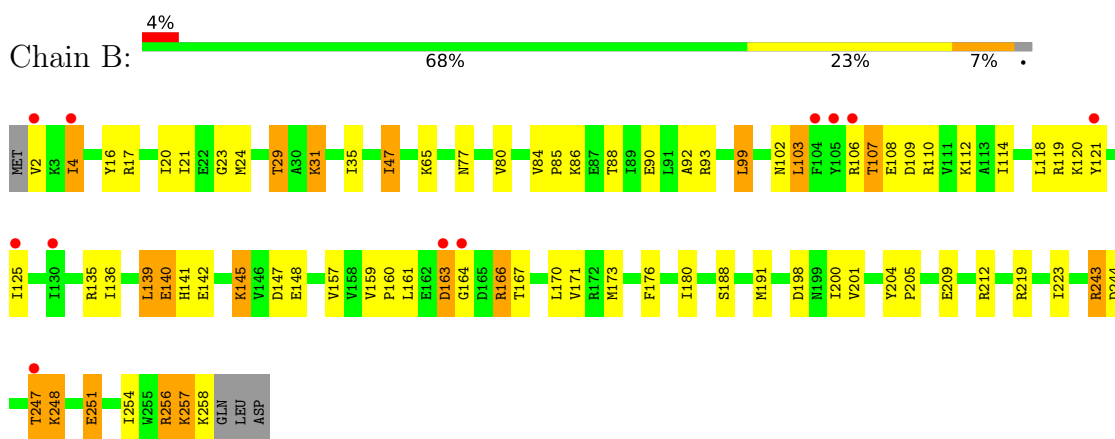
3 Residue-property plots [i](#)

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.

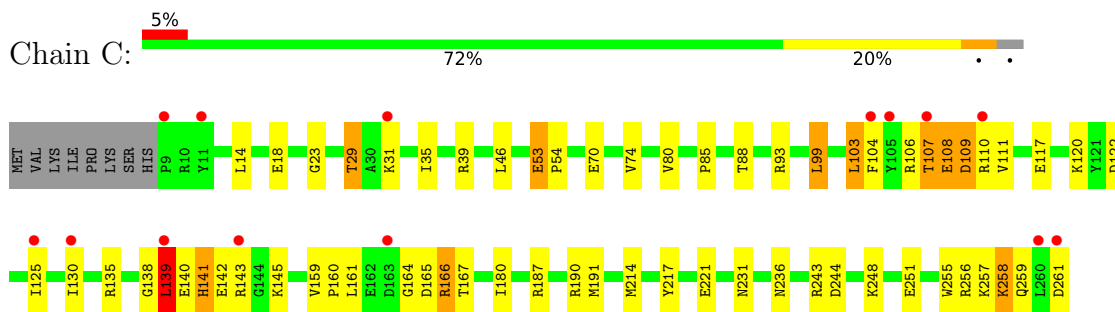
- Molecule 1: phosphopantothenate synthetase




- Molecule 1: phosphopantothenate synthetase

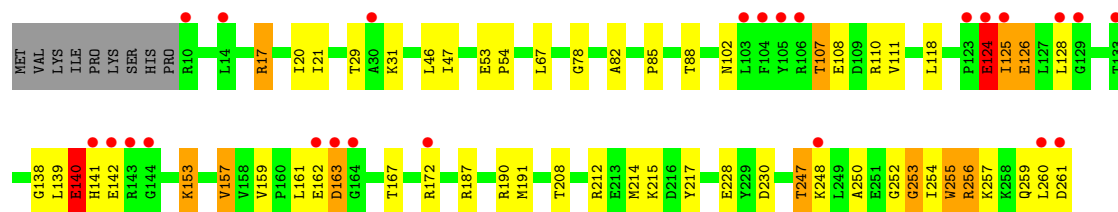


- Molecule 1: phosphopantothenate synthetase



- Molecule 1: phosphopantothenate synthetase

Chain D: 



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	266.14Å 60.96Å 75.35Å 90.00° 92.38° 90.00°	Depositor
Resolution (Å)	33.26 – 1.96 33.26 – 1.96	Depositor EDS
% Data completeness (in resolution range)	96.5 (33.26-1.96) 96.7 (33.26-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 1.97Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.211 , 0.264 0.214 , 0.263	Depositor DCC
R_{free} test set	4231 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtrriage
Anisotropy	0.333	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8358	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: 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	0.52	0/2057	0.74	0/2774
1	B	0.59	0/2069	0.77	0/2792
1	C	0.54	0/2046	0.76	3/2760 (0.1%)
1	D	0.54	0/2032	0.75	0/2741
All	All	0.55	0/8204	0.76	3/11067 (0.0%)

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	0	2
1	B	0	3
1	D	0	6
All	All	0	11

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	53	GLU	CA-C-N	-6.28	112.53	119.19
1	C	53	GLU	C-N-CA	-6.28	112.53	119.19
1	C	244	ASP	N-CA-C	-5.01	105.95	111.71

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	MET	Mainchain
1	A	9	PRO	Peptide
1	B	139	LEU	Peptide
1	B	198	ASP	Mainchain
1	B	251	GLU	Peptide
1	D	124	GLU	Peptide
1	D	140	GLU	Peptide
1	D	252	GLY	Peptide
1	D	253	GLY	Peptide
1	D	255	TRP	Peptide
1	D	260	LEU	Peptide

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	2027	0	2087	47	1
1	B	2038	0	2107	81	0
1	C	2016	0	2075	55	1
1	D	2004	0	2062	52	1
2	D	4	0	3	0	0
3	A	52	0	0	2	0
3	B	87	0	0	2	2
3	C	67	0	0	2	0
3	D	63	0	0	1	2
All	All	8358	0	8334	211	4

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 13.

All (211) 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:141:HIS:CB	1:B:142:GLU:HA	1.49	1.35
1:D:140:GLU:HB2	1:D:141:HIS:CA	1.76	1.15
1:B:243:ARG:HG2	1:B:243:ARG:HH11	0.97	1.10
1:D:140:GLU:HB2	1:D:141:HIS:C	1.78	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:ARG:NH1	1:D:191:MET:O	1.87	1.07
1:A:136:ILE:HG23	1:A:173:MET:SD	1.98	1.03
1:B:141:HIS:CB	1:B:142:GLU:CA	2.36	1.02
1:D:107:THR:HG22	1:D:110:ARG:H	1.25	1.01
1:B:243:ARG:HG2	1:B:243:ARG:NH1	1.76	0.94
1:B:243:ARG:HH11	1:B:243:ARG:CG	1.78	0.93
1:A:243:ARG:HD3	1:B:247:THR:HG22	1.49	0.92
1:D:140:GLU:CB	1:D:141:HIS:HA	1.99	0.92
1:D:140:GLU:CB	1:D:141:HIS:CA	2.50	0.90
1:A:260:LEU:O	1:A:261:ASP:HB2	1.72	0.90
1:D:140:GLU:HB2	1:D:141:HIS:HA	1.56	0.86
1:B:243:ARG:NH1	1:B:244:ASP:OD1	2.13	0.81
1:D:140:GLU:CG	1:D:141:HIS:HA	2.10	0.81
1:A:256:ARG:NH1	1:B:191:MET:O	2.14	0.81
1:C:74:VAL:HG23	1:C:99:LEU:CD1	2.11	0.80
1:C:85:PRO:O	1:C:88:THR:HG22	1.82	0.80
1:C:191:MET:O	1:D:256:ARG:NH1	2.14	0.79
1:D:159:VAL:HG23	1:D:159:VAL:O	1.81	0.79
1:B:256:ARG:HA	1:B:257:LYS:HB3	1.63	0.78
1:B:31:LYS:N	1:B:31:LYS:HD3	1.99	0.78
1:D:141:HIS:CB	1:D:142:GLU:HA	2.13	0.76
1:B:23:GLY:C	1:B:29:THR:HG23	2.12	0.75
1:C:138:GLY:HA2	1:C:139:LEU:CB	2.17	0.75
1:C:139:LEU:O	1:C:141:HIS:N	2.19	0.73
1:A:243:ARG:CD	1:B:247:THR:HG22	2.20	0.71
1:B:256:ARG:HA	1:B:257:LYS:CB	2.21	0.70
1:D:107:THR:HG22	1:D:110:ARG:N	2.04	0.69
1:C:74:VAL:CG2	1:C:99:LEU:HD13	2.22	0.69
1:C:74:VAL:CG2	1:C:99:LEU:CD1	2.71	0.68
1:C:138:GLY:HA2	1:C:139:LEU:HG	1.74	0.68
1:A:74:VAL:CG2	1:A:99:LEU:HD12	2.23	0.68
1:A:107:THR:HG22	1:A:110:ARG:H	1.57	0.68
1:D:17:ARG:O	1:D:20:ILE:HG22	1.94	0.68
1:D:141:HIS:CB	1:D:142:GLU:CA	2.73	0.67
1:D:85:PRO:O	1:D:88:THR:HG22	1.96	0.66
1:B:2:VAL:HG13	1:B:2:VAL:O	1.95	0.66
1:A:159:VAL:HG23	1:A:159:VAL:O	1.95	0.65
1:C:138:GLY:HA2	1:C:139:LEU:CG	2.27	0.65
1:A:74:VAL:CG2	1:A:99:LEU:CD1	2.75	0.65
1:A:159:VAL:O	1:A:159:VAL:CG2	2.45	0.65
1:B:219:ARG:HG2	1:B:223:ILE:HD12	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:VAL:HG22	1:A:99:LEU:HD12	1.80	0.64
1:C:159:VAL:O	1:C:159:VAL:HG23	1.97	0.64
1:B:140:GLU:HB2	1:B:141:HIS:O	1.98	0.64
1:C:74:VAL:HG23	1:C:99:LEU:HD12	1.80	0.63
1:A:23:GLY:C	1:A:29:THR:HG23	2.23	0.63
1:B:107:THR:O	1:B:110:ARG:N	2.32	0.63
1:C:23:GLY:C	1:C:29:THR:HG23	2.24	0.63
1:B:135:ARG:NH1	1:B:142:GLU:HG2	2.14	0.63
1:D:153:LYS:HD2	3:D:454:HOH:O	1.99	0.62
1:C:190:ARG:HH21	1:D:259:GLN:NE2	1.98	0.62
1:A:135:ARG:NH1	1:A:140:GLU:O	2.32	0.62
1:A:191:MET:HE1	1:B:257:LYS:HD3	1.82	0.62
1:A:243:ARG:HD3	1:B:247:THR:CG2	2.25	0.61
1:B:159:VAL:HG23	1:B:159:VAL:O	2.01	0.61
1:C:243:ARG:HD3	1:D:247:THR:HG22	1.81	0.61
1:B:212:ARG:HD2	3:B:448:HOH:O	2.02	0.60
1:C:93:ARG:HH21	1:C:122:ASP:CG	2.10	0.60
1:C:140:GLU:O	1:C:141:HIS:CB	2.50	0.60
1:A:260:LEU:O	1:A:261:ASP:CB	2.49	0.59
1:C:142:GLU:HA	1:C:145:LYS:HE3	1.85	0.58
1:D:139:LEU:O	1:D:140:GLU:C	2.46	0.58
1:D:250:ALA:O	1:D:253:GLY:HA2	2.03	0.57
1:A:53:GLU:HB3	1:A:54:PRO:HD3	1.86	0.57
1:B:219:ARG:NH1	3:B:424:HOH:O	2.24	0.57
1:D:162:GLU:HG3	1:D:163:ASP:N	2.19	0.57
1:B:147:ASP:OD1	1:B:148:GLU:N	2.38	0.57
1:C:85:PRO:HD2	3:C:320:HOH:O	2.04	0.57
1:C:85:PRO:O	1:C:88:THR:CG2	2.52	0.56
1:B:147:ASP:OD1	1:B:147:ASP:C	2.48	0.56
1:D:140:GLU:HG3	1:D:141:HIS:HA	1.85	0.56
1:A:74:VAL:HG22	1:A:99:LEU:CD1	2.35	0.56
1:A:15:TYR:CZ	1:A:19:LYS:HE2	2.40	0.56
1:A:17:ARG:O	1:A:21:ILE:HG13	2.05	0.55
1:D:159:VAL:O	1:D:159:VAL:CG2	2.51	0.55
1:B:107:THR:O	1:B:109:ASP:N	2.40	0.55
1:C:164:GLY:HA3	1:C:187:ARG:HB3	1.89	0.55
1:B:243:ARG:NH1	1:B:243:ARG:CG	2.49	0.55
1:C:258:LYS:HG2	1:D:187:ARG:HH22	1.71	0.55
1:A:164:GLY:HA3	1:A:187:ARG:HB3	1.89	0.55
1:C:138:GLY:HA2	1:C:139:LEU:HB2	1.89	0.54
1:C:106:ARG:HB2	1:C:142:GLU:CD	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ASP:N	1:C:109:ASP:OD1	2.39	0.53
1:B:107:THR:O	1:B:108:GLU:C	2.51	0.53
1:A:10:ARG:HB3	1:A:10:ARG:CZ	2.36	0.53
1:B:17:ARG:O	1:B:21:ILE:HG12	2.09	0.53
1:B:180:ILE:HD13	1:B:204:TYR:HE1	1.74	0.53
1:A:149:ASN:HA	1:A:153:LYS:HD3	1.91	0.53
1:C:107:THR:O	1:C:110:ARG:N	2.42	0.52
1:C:46:LEU:HD11	1:D:46:LEU:HD13	1.91	0.52
1:A:255:TRP:CZ3	1:C:108:GLU:HG3	2.44	0.52
1:D:53:GLU:HB3	1:D:54:PRO:HD3	1.91	0.52
1:D:29:THR:HG22	1:D:78:GLY:O	2.10	0.51
1:D:162:GLU:CG	1:D:163:ASP:N	2.72	0.51
1:B:125:ILE:O	1:B:125:ILE:HG23	2.10	0.51
1:B:102:ASN:OD1	1:B:166:ARG:NH1	2.43	0.51
1:B:4:ILE:H	1:B:4:ILE:HD13	1.76	0.50
1:B:103:LEU:HD21	1:B:114:ILE:CD1	2.42	0.50
1:C:108:GLU:H	1:C:108:GLU:CD	2.18	0.50
1:C:166:ARG:O	1:C:167:THR:C	2.54	0.50
1:A:190:ARG:HD3	1:B:257:LYS:O	2.12	0.49
1:D:124:GLU:O	1:D:125:ILE:O	2.29	0.49
1:A:230:ASP:C	1:A:230:ASP:OD1	2.55	0.49
1:B:2:VAL:O	1:B:2:VAL:CG1	2.60	0.49
1:B:107:THR:HG22	1:B:109:ASP:H	1.77	0.48
1:C:243:ARG:HD3	1:D:247:THR:CG2	2.43	0.48
1:D:126:GLU:CD	1:D:128:LEU:HD11	2.38	0.48
1:B:77:ASN:HA	1:B:103:LEU:HD23	1.96	0.48
1:B:248:LYS:CD	1:B:248:LYS:C	2.86	0.48
1:C:190:ARG:HD3	1:D:257:LYS:O	2.13	0.48
1:B:85:PRO:O	1:B:88:THR:HG22	2.13	0.48
1:B:159:VAL:O	1:B:159:VAL:CG2	2.62	0.48
1:C:93:ARG:NH2	1:C:122:ASP:OD2	2.39	0.47
1:B:140:GLU:N	1:B:141:HIS:HA	2.29	0.47
1:B:257:LYS:O	1:B:258:LYS:C	2.57	0.47
1:C:142:GLU:HA	1:C:145:LYS:CE	2.44	0.47
1:A:240:LEU:HD23	3:A:318:HOH:O	2.14	0.47
1:A:240:LEU:HD23	1:A:240:LEU:C	2.40	0.47
1:B:136:ILE:HB	1:B:139:LEU:HD12	1.96	0.47
1:A:136:ILE:HB	1:A:139:LEU:HD12	1.97	0.47
1:B:107:THR:C	1:B:109:ASP:N	2.71	0.47
1:C:236:ASN:OD1	1:D:254:ILE:HD12	2.15	0.47
1:A:191:MET:HE1	1:B:257:LYS:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LEU:CD2	3:A:318:HOH:O	2.62	0.47
1:B:17:ARG:O	1:B:20:ILE:HG22	2.15	0.47
1:B:140:GLU:HG2	1:B:141:HIS:HA	1.96	0.47
1:C:93:ARG:HD2	3:C:353:HOH:O	2.15	0.47
1:B:24:MET:HE2	1:B:24:MET:HB3	1.72	0.46
1:B:140:GLU:CG	1:B:141:HIS:HA	2.46	0.46
1:C:141:HIS:O	1:C:143:ARG:N	2.48	0.46
1:D:139:LEU:HD23	1:D:139:LEU:HA	1.83	0.46
1:B:31:LYS:HD3	1:B:31:LYS:H	1.78	0.46
1:B:163:ASP:OD2	1:B:163:ASP:C	2.57	0.46
1:D:128:LEU:HD12	1:D:128:LEU:N	2.30	0.46
1:D:141:HIS:CB	1:D:142:GLU:HB3	2.46	0.46
1:C:165:ASP:N	1:C:165:ASP:OD1	2.48	0.46
1:D:107:THR:O	1:D:111:VAL:HG23	2.14	0.46
1:A:14:LEU:O	1:A:18:GLU:HG2	2.16	0.46
1:B:65:LYS:HG2	1:B:176:PHE:CE2	2.51	0.46
1:B:135:ARG:HH11	1:B:142:GLU:HG2	1.80	0.46
1:B:170:LEU:O	1:B:173:MET:HB2	2.16	0.46
1:D:230:ASP:OD1	1:D:230:ASP:C	2.59	0.45
1:A:239:LEU:HD12	1:B:254:ILE:HD11	1.97	0.45
1:A:135:ARG:HD2	1:A:141:HIS:CD2	2.51	0.45
1:C:255:TRP:O	1:C:256:ARG:HB2	2.17	0.45
1:B:107:THR:HG22	1:B:109:ASP:HB2	1.99	0.45
1:C:190:ARG:NH2	1:D:259:GLN:NE2	2.62	0.45
1:B:80:VAL:HG22	1:B:200:ILE:CD1	2.46	0.45
1:A:44:ASP:OD1	1:A:49:GLU:HA	2.17	0.45
1:B:80:VAL:HG21	1:B:160:PRO:HG3	1.99	0.45
1:D:162:GLU:OE2	1:D:163:ASP:N	2.48	0.45
1:C:214:MET:O	1:C:217:TYR:HB2	2.17	0.44
1:D:126:GLU:HG2	1:D:128:LEU:HD12	2.00	0.44
1:D:162:GLU:HG2	1:D:167:THR:OG1	2.17	0.44
1:C:231:ASN:HD22	1:D:255:TRP:CD1	2.36	0.44
1:B:167:THR:O	1:B:171:VAL:HG23	2.18	0.44
1:B:84:VAL:N	1:B:85:PRO:CD	2.81	0.44
1:A:191:MET:HE2	1:B:257:LYS:HB2	1.99	0.44
1:B:140:GLU:HG2	1:B:140:GLU:H	1.63	0.44
1:C:103:LEU:HD13	1:C:110:ARG:HG2	2.00	0.44
1:C:180:ILE:HD12	1:C:180:ILE:N	2.33	0.44
1:A:75:SER:OG	1:A:102:ASN:HB3	2.18	0.43
1:D:138:GLY:HA3	1:D:172:ARG:HH22	1.82	0.43
1:C:14:LEU:O	1:C:18:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLU:OE2	1:A:172:ARG:NH1	2.47	0.43
1:B:219:ARG:HG2	1:B:223:ILE:CD1	2.46	0.43
1:C:111:VAL:CG1	1:C:130:ILE:HG13	2.49	0.43
1:D:162:GLU:CD	1:D:163:ASP:H	2.25	0.43
1:B:164:GLY:HA2	1:B:188:SER:HB2	2.01	0.43
1:B:108:GLU:O	1:B:112:LYS:HB2	2.19	0.43
1:D:157:VAL:HG23	1:D:159:VAL:HG13	2.00	0.43
1:C:117:GLU:O	1:C:120:LYS:HB3	2.19	0.43
1:B:106:ARG:O	1:B:107:THR:OG1	2.29	0.43
1:B:205:PRO:O	1:B:209:GLU:HG3	2.18	0.43
1:D:85:PRO:O	1:D:88:THR:CG2	2.67	0.42
1:B:139:LEU:O	1:B:140:GLU:C	2.62	0.42
1:B:157:VAL:O	1:B:157:VAL:HG23	2.19	0.42
1:A:109:ASP:OD1	1:A:109:ASP:N	2.51	0.42
1:A:17:ARG:HG2	1:B:35:ILE:HD13	2.01	0.42
1:A:53:GLU:N	1:A:54:PRO:CD	2.83	0.42
1:B:119:ARG:C	1:B:121:TYR:N	2.75	0.42
1:C:53:GLU:HB3	1:C:54:PRO:HD3	2.01	0.42
1:A:186:SER:O	1:A:190:ARG:HG3	2.20	0.42
1:B:142:GLU:HB3	1:B:145:LYS:HG3	2.02	0.42
1:B:16:TYR:CE2	1:B:201:VAL:HG11	2.55	0.42
1:C:139:LEU:HD23	1:C:139:LEU:HA	1.82	0.41
1:C:35:ILE:HG22	1:C:39:ARG:NH1	2.35	0.41
1:D:250:ALA:O	1:D:253:GLY:CA	2.67	0.41
1:C:80:VAL:HG21	1:C:160:PRO:HG2	2.02	0.41
1:C:139:LEU:HB3	1:C:140:GLU:H	1.56	0.41
1:A:191:MET:CE	1:B:257:LYS:HB2	2.51	0.41
1:A:243:ARG:NE	1:B:247:THR:HG22	2.36	0.41
1:D:29:THR:CG2	1:D:82:ALA:HB2	2.51	0.41
1:C:85:PRO:C	1:C:88:THR:HG22	2.44	0.41
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.92	0.41
1:B:23:GLY:HA3	1:B:29:THR:CG2	2.51	0.41
1:B:92:ALA:HB2	1:B:99:LEU:HD13	2.02	0.41
1:D:208:THR:O	1:D:212:ARG:HG3	2.21	0.41
1:C:122:ASP:OD1	1:C:125:ILE:N	2.54	0.41
1:D:67:LEU:HD23	1:D:67:LEU:HA	1.92	0.41
1:D:214:MET:O	1:D:217:TYR:HB2	2.21	0.41
1:B:159:VAL:HA	1:B:160:PRO:HD2	1.93	0.40
1:A:104:PHE:CD1	1:A:104:PHE:N	2.89	0.40
1:B:47:ILE:HD13	1:B:47:ILE:HA	1.72	0.40
1:B:86:LYS:HE2	1:B:90:GLU:OE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PRO:O	1:A:88:THR:HG22	2.21	0.40
1:C:139:LEU:C	1:C:141:HIS:N	2.79	0.40

All (4) 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:139:LEU:O	1:A:139:LEU:O[2_554]	1.40	0.80
3:B:468:HOH:O	3:D:451:HOH:O[1_554]	1.79	0.41
3:B:431:HOH:O	3:D:430:HOH:O[1_554]	2.02	0.18
1:C:217:TYR:OH	1:D:261:ASP:OD1[4_555]	2.12	0.08

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	252/261 (97%)	244 (97%)	8 (3%)	0	100	100
1	B	255/261 (98%)	242 (95%)	10 (4%)	3 (1%)	10	4
1	C	251/261 (96%)	239 (95%)	10 (4%)	2 (1%)	16	8
1	D	250/261 (96%)	236 (94%)	12 (5%)	2 (1%)	16	8
All	All	1008/1044 (97%)	961 (95%)	40 (4%)	7 (1%)	18	10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	139	LEU
1	D	125	ILE
1	D	140	GLU
1	B	256	ARG
1	B	257	LYS

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Mol	Chain	Res	Type
1	C	141	HIS
1	B	107	THR

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	212/220 (96%)	194 (92%)	18 (8%)	10 3
1	B	213/220 (97%)	195 (92%)	18 (8%)	10 3
1	C	211/220 (96%)	191 (90%)	20 (10%)	8 2
1	D	209/220 (95%)	188 (90%)	21 (10%)	7 1
All	All	845/880 (96%)	768 (91%)	77 (9%)	9 2

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	20	ILE
1	A	29	THR
1	A	31	LYS
1	A	60	ARG
1	A	74	VAL
1	A	104	PHE
1	A	107	THR
1	A	109	ASP
1	A	128	LEU
1	A	135	ARG
1	A	140	GLU
1	A	159	VAL
1	A	161	LEU
1	A	172	ARG
1	A	219	ARG
1	A	221	GLU
1	A	258	LYS
1	B	4	ILE

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Mol	Chain	Res	Type
1	B	29	THR
1	B	31	LYS
1	B	47	ILE
1	B	93	ARG
1	B	99	LEU
1	B	103	LEU
1	B	118	LEU
1	B	120	LYS
1	B	140	GLU
1	B	145	LYS
1	B	161	LEU
1	B	163	ASP
1	B	166	ARG
1	B	243	ARG
1	B	247	THR
1	B	248	LYS
1	B	251	GLU
1	C	29	THR
1	C	31	LYS
1	C	70	GLU
1	C	99	LEU
1	C	103	LEU
1	C	104	PHE
1	C	107	THR
1	C	108	GLU
1	C	109	ASP
1	C	135	ARG
1	C	139	LEU
1	C	161	LEU
1	C	166	ARG
1	C	221	GLU
1	C	248	LYS
1	C	251	GLU
1	C	257	LYS
1	C	258	LYS
1	C	259	GLN
1	C	261	ASP
1	D	17	ARG
1	D	21	ILE
1	D	31	LYS
1	D	47	ILE
1	D	102	ASN

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Mol	Chain	Res	Type
1	D	107	THR
1	D	108	GLU
1	D	118	LEU
1	D	124	GLU
1	D	126	GLU
1	D	140	GLU
1	D	153	LYS
1	D	157	VAL
1	D	161	LEU
1	D	163	ASP
1	D	190	ARG
1	D	215	LYS
1	D	228	GLU
1	D	247	THR
1	D	248	LYS
1	D	256	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	102	ASN
1	A	141	HIS
1	C	141	HIS
1	D	259	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	ACT	D	301	-	3,3,3	0.64	0	3,3,3	1.17	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 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	253/261 (96%)	0.44	12 (4%) 36 42	23, 40, 73, 110	1 (0%)
1	B	257/261 (98%)	0.39	11 (4%) 40 46	19, 38, 87, 123	0
1	C	253/261 (96%)	0.56	14 (5%) 30 36	24, 42, 84, 140	0
1	D	252/261 (96%)	0.54	24 (9%) 14 15	25, 42, 88, 146	0
All	All	1015/1044 (97%)	0.48	61 (6%) 27 32	19, 41, 84, 146	1 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	104	PHE	6.8
1	D	261	ASP	5.7
1	A	104	PHE	5.7
1	B	105	TYR	4.6
1	B	2	VAL	4.5
1	A	105	TYR	4.4
1	C	139	LEU	4.3
1	A	9	PRO	4.3
1	C	105	TYR	4.2
1	B	104	PHE	4.0
1	D	105	TYR	4.0
1	C	9	PRO	4.0
1	D	106	ARG	3.7
1	B	163	ASP	3.6
1	A	139	LEU	3.5
1	C	143	ARG	3.4
1	B	4	ILE	3.0
1	C	260	LEU	3.0
1	D	104	PHE	3.0
1	D	141	HIS	2.9
1	D	248	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	123	PRO	2.8
1	C	163	ASP	2.8
1	D	128	LEU	2.8
1	D	142	GLU	2.8
1	C	130	ILE	2.8
1	D	144	GLY	2.7
1	A	125	ILE	2.7
1	C	31	LYS	2.5
1	C	125	ILE	2.5
1	A	141	HIS	2.5
1	D	129	GLY	2.5
1	D	14	LEU	2.4
1	D	125	ILE	2.4
1	A	107	THR	2.4
1	D	30	ALA	2.4
1	A	123	PRO	2.4
1	D	103	LEU	2.4
1	D	163	ASP	2.3
1	C	11	TYR	2.3
1	B	247	THR	2.3
1	D	164	GLY	2.3
1	B	125	ILE	2.3
1	B	164	GLY	2.3
1	A	261	ASP	2.3
1	B	106	ARG	2.2
1	D	162	GLU	2.2
1	C	107	THR	2.2
1	D	260	LEU	2.2
1	B	121	TYR	2.2
1	A	103	LEU	2.2
1	D	172	ARG	2.2
1	D	124	GLU	2.1
1	A	120	LYS	2.1
1	A	213	GLU	2.1
1	D	143	ARG	2.1
1	B	130	ILE	2.0
1	C	110	ARG	2.0
1	C	261	ASP	2.0
1	D	133	THR	2.0
1	D	10	ARG	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
2	ACT	D	301	4/4	0.72	0.22	49,49,61,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.