



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2024 – 12:04 AM EST

PDB ID : 1T3H
Title : X-ray Structure of Dephospho-CoA Kinase from E. coli Northeast Structural Genomics Consortium Target ER57
Authors : Kuzin, A.P.; Chen, Y.; Forouhar, F.; Edstrom, W.; Benach, J.; Vorobiev, S.; Acton, T.; Shastry, R.; Ma, L.-C.; Xia, R.; Montelione, G.; Tong, L.; Hunt, J.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2004-04-26
Resolution : 2.50 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

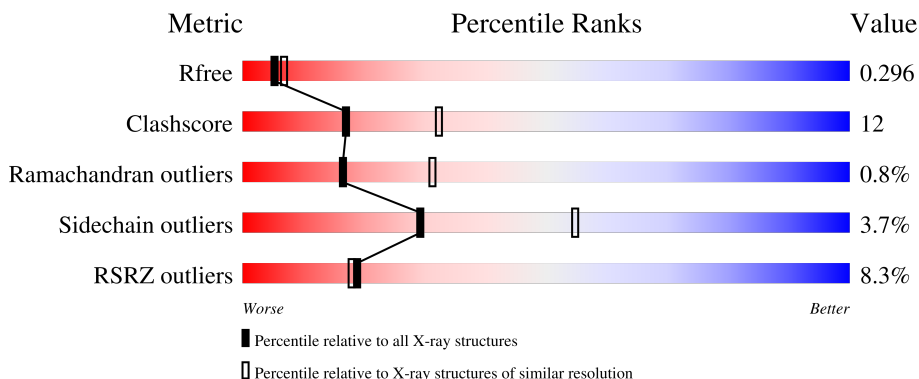
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	214	<div> <div>8%</div> <div>72%</div> <div>23%</div> <div>• •</div> </div>
1	B	214	<div> <div>5%</div> <div>75%</div> <div>19%</div> <div>• •</div> </div>
1	C	214	<div> <div>10%</div> <div>59%</div> <div>25%</div> <div>• 13%</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
2	SO4	B	302	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4803 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 Dephospho-CoA kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	Se	0	0	0
			1603	1004	293	303	3			
1	B	207	Total	C	N	O	Se	0	0	0
			1603	1004	293	303	3			
1	C	187	Total	C	N	O	Se	0	0	0
			1444	906	259	276	3			

There are 33 discrepancies between the modelled and reference sequences:

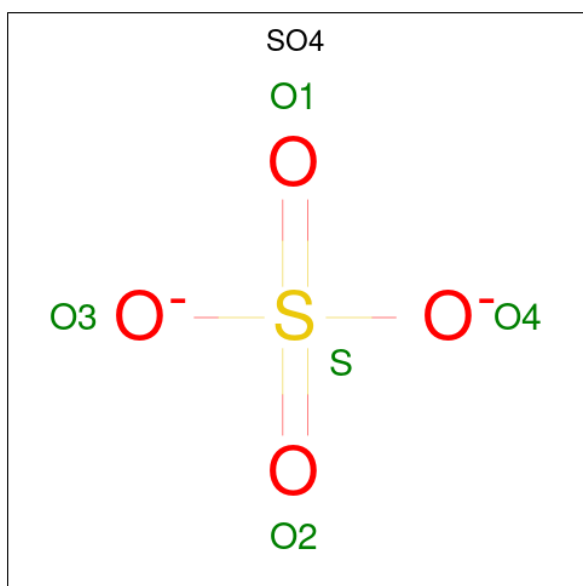
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P0A6I9
A	58	MSE	MET	modified residue	UNP P0A6I9
A	142	MSE	MET	modified residue	UNP P0A6I9
A	207	GLU	-	expression tag	UNP P0A6I9
A	208	LEU	-	expression tag	UNP P0A6I9
A	209	HIS	-	expression tag	UNP P0A6I9
A	210	HIS	-	expression tag	UNP P0A6I9
A	211	HIS	-	expression tag	UNP P0A6I9
A	212	HIS	-	expression tag	UNP P0A6I9
A	213	HIS	-	expression tag	UNP P0A6I9
A	214	HIS	-	expression tag	UNP P0A6I9
B	1	MSE	MET	modified residue	UNP P0A6I9
B	58	MSE	MET	modified residue	UNP P0A6I9
B	142	MSE	MET	modified residue	UNP P0A6I9
B	207	GLU	-	expression tag	UNP P0A6I9
B	208	LEU	-	expression tag	UNP P0A6I9
B	209	HIS	-	expression tag	UNP P0A6I9
B	210	HIS	-	expression tag	UNP P0A6I9
B	211	HIS	-	expression tag	UNP P0A6I9
B	212	HIS	-	expression tag	UNP P0A6I9
B	213	HIS	-	expression tag	UNP P0A6I9
B	214	HIS	-	expression tag	UNP P0A6I9
C	1	MSE	MET	modified residue	UNP P0A6I9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	58	MSE	MET	modified residue	UNP P0A6I9
C	142	MSE	MET	modified residue	UNP P0A6I9
C	207	GLU	-	expression tag	UNP P0A6I9
C	208	LEU	-	expression tag	UNP P0A6I9
C	209	HIS	-	expression tag	UNP P0A6I9
C	210	HIS	-	expression tag	UNP P0A6I9
C	211	HIS	-	expression tag	UNP P0A6I9
C	212	HIS	-	expression tag	UNP P0A6I9
C	213	HIS	-	expression tag	UNP P0A6I9
C	214	HIS	-	expression tag	UNP P0A6I9

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	41	Total O 41 41	0	0
3	B	59	Total O 59 59	0	0

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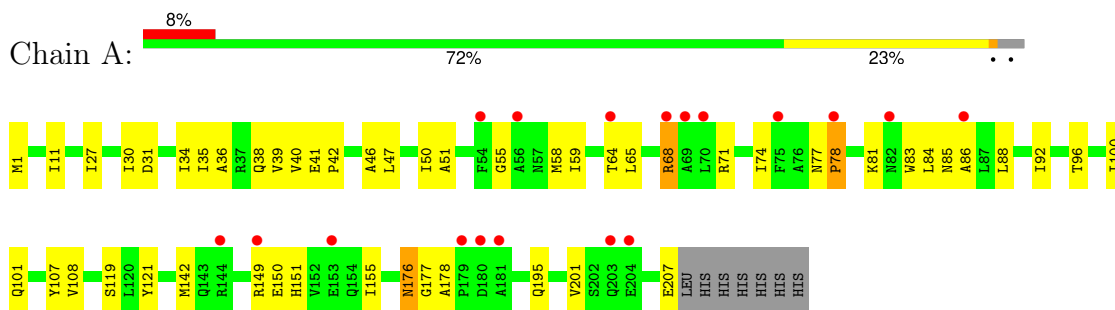
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	43	Total	O	0	0
			43	43		

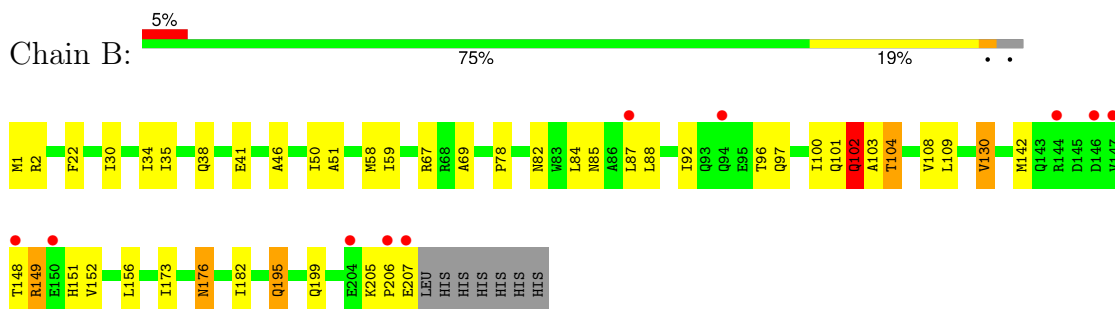
3 Residue-property plots [i](#)

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.

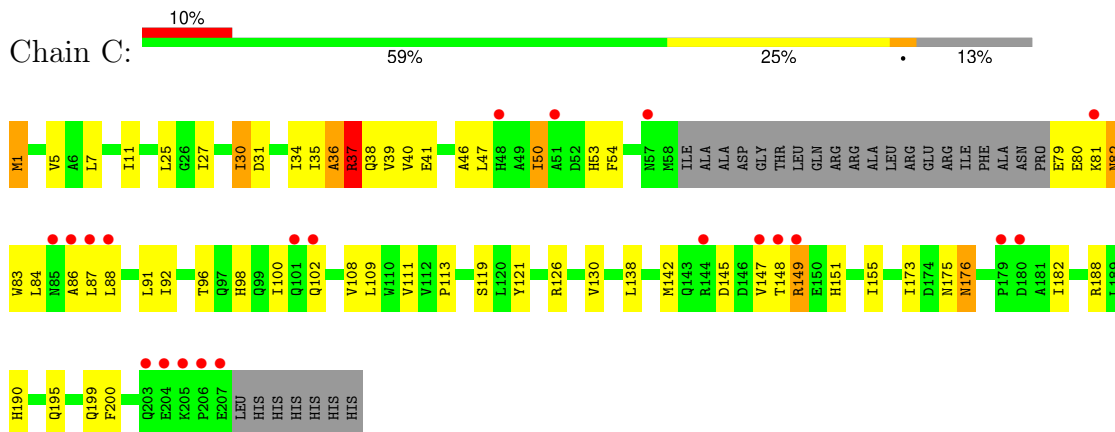
• Molecule 1: Dephospho-CoA kinase



• Molecule 1: Dephospho-CoA kinase



• Molecule 1: Dephospho-CoA kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.63Å 80.91Å 75.45Å 90.00° 93.95° 90.00°	Depositor
Resolution (Å)	19.53 – 2.50 19.53 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.2 (19.53-2.50) 96.6 (19.53-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.284 0.250 , 0.296	Depositor DCC
R_{free} test set	1154 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4803	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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: SO4

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	0/1628	0.63	0/2214
1	B	1.01	4/1628 (0.2%)	1.00	9/2214 (0.4%)
1	C	0.55	3/1466 (0.2%)	0.87	7/1994 (0.4%)
All	All	0.71	7/4722 (0.1%)	0.85	16/6422 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	2
1	C	0	1
All	All	1	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	GLN	CG-CD	-25.72	0.91	1.51
1	B	104	THR	N-CA	-20.23	1.05	1.46
1	B	102	GLN	CB-CG	-15.53	1.10	1.52
1	C	37	ARG	CA-C	-8.30	1.31	1.52
1	C	36	ALA	C-N	-8.11	1.15	1.34
1	B	102	GLN	CA-CB	-7.16	1.38	1.53
1	C	37	ARG	C-N	-6.90	1.18	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	GLN	CA-CB-CG	21.58	160.87	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	ARG	CB-CA-C	-16.30	77.81	110.40
1	B	102	GLN	CB-CA-C	15.35	141.10	110.40
1	B	104	THR	N-CA-CB	12.95	134.91	110.30
1	B	103	ALA	C-N-CA	10.99	149.18	121.70
1	C	37	ARG	N-CA-C	10.37	139.00	111.00
1	B	102	GLN	CG-CD-OE1	-9.95	101.70	121.60
1	C	36	ALA	C-N-CA	-9.81	97.18	121.70
1	C	36	ALA	O-C-N	9.19	137.41	122.70
1	B	149	ARG	NE-CZ-NH2	8.13	124.37	120.30
1	C	36	ALA	CA-C-N	-8.12	99.34	117.20
1	B	149	ARG	NE-CZ-NH1	-7.81	116.39	120.30
1	B	103	ALA	O-C-N	-6.61	112.13	122.70
1	C	37	ARG	CA-C-N	-5.89	104.24	117.20
1	C	149	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	102	GLN	CG-CD-NE2	5.15	129.05	116.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	102	GLN	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	102	GLN	Sidechain
1	B	104	THR	Mainchain
1	C	37	ARG	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	1603	0	1609	37	0
1	B	1603	0	1608	31	0
1	C	1444	0	1441	48	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	41	0	0	4	0
3	B	59	0	0	5	0
3	C	43	0	0	3	0
All	All	4803	0	4658	116	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 12.

All (116) 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:30:ILE:HD12	1:B:100:ILE:HD13	1.44	0.95
1:A:30:ILE:HD13	1:A:100:ILE:HD13	1.62	0.79
1:C:38:GLN:HA	1:C:41:GLU:HG3	1.63	0.78
1:A:47:LEU:HD22	1:A:59:ILE:HD12	1.69	0.74
1:C:36:ALA:HA	1:C:92:ILE:CD1	2.19	0.71
1:C:82:ASN:HD22	1:C:82:ASN:N	1.94	0.66
1:A:31:ASP:O	1:A:35:ILE:HG12	1.96	0.65
1:C:82:ASN:HD22	1:C:82:ASN:H	1.45	0.64
1:A:101:GLN:HB3	3:A:336:HOH:O	1.97	0.64
1:C:82:ASN:H	1:C:82:ASN:ND2	1.95	0.63
1:B:30:ILE:CD1	1:B:100:ILE:HD13	2.22	0.63
1:A:38:GLN:O	1:A:41:GLU:HG2	1.99	0.62
1:B:96:THR:O	1:B:100:ILE:HG12	2.01	0.60
1:A:58:MSE:HE3	1:A:58:MSE:HA	1.83	0.60
1:C:79:GLU:CD	1:C:80:GLU:H	2.05	0.60
1:B:30:ILE:HG23	1:B:35:ILE:HD11	1.84	0.59
1:C:36:ALA:HA	1:C:92:ILE:HD12	1.84	0.59
1:C:84:LEU:C	1:C:86:ALA:H	2.05	0.59
1:A:30:ILE:HD13	1:A:100:ILE:CD1	2.33	0.58
1:B:88:LEU:O	1:B:92:ILE:HG12	2.03	0.57
1:B:46:ALA:O	1:B:50:ILE:HG12	2.04	0.57
1:C:100:ILE:HD12	1:C:108:VAL:HG21	1.87	0.56
1:C:39:VAL:HG23	1:C:88:LEU:HD22	1.87	0.56
1:A:96:THR:O	1:A:100:ILE:HG12	2.05	0.56
1:C:1:MSE:HE2	1:C:200:PHE:HE1	1.71	0.56
1:B:1:MSE:HA	3:B:343:HOH:O	2.04	0.56
1:B:182:ILE:HD13	3:B:332:HOH:O	2.05	0.56
1:B:100:ILE:HD12	1:B:108:VAL:HG21	1.88	0.56
1:B:51:ALA:HB2	1:B:59:ILE:HD11	1.87	0.55
1:A:51:ALA:HA	1:A:55:GLY:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ILE:CG2	1:B:35:ILE:HD11	2.37	0.55
1:C:34:ILE:O	1:C:38:GLN:HG3	2.06	0.55
1:C:5:VAL:HG22	1:C:126:ARG:HB3	1.87	0.54
1:B:58:MSE:HE1	1:B:69:ALA:O	2.06	0.54
1:C:98:HIS:O	1:C:102:GLN:HG2	2.09	0.53
1:C:188:ARG:HD2	3:C:230:HOH:O	2.07	0.53
1:C:25:LEU:HD13	1:C:190:HIS:CD2	2.43	0.53
1:B:85:ASN:C	1:B:87:LEU:H	2.13	0.52
1:C:36:ALA:HA	1:C:92:ILE:HD11	1.90	0.51
1:C:7:LEU:HD23	1:C:111:VAL:HG22	1.92	0.51
1:C:53:HIS:HD1	1:C:54:PHE:HD1	1.57	0.51
1:A:31:ASP:HB3	1:A:34:ILE:HD13	1.92	0.51
1:C:27:ILE:HD11	1:C:190:HIS:CE1	2.46	0.51
1:A:83:TRP:C	1:A:85:ASN:H	2.13	0.51
1:A:100:ILE:HD12	1:A:108:VAL:HG21	1.92	0.51
1:C:46:ALA:HB2	1:C:91:LEU:CD1	2.41	0.50
1:C:142:MSE:HE3	1:C:149:ARG:N	2.26	0.50
1:A:42:PRO:HG3	1:A:64:THR:HA	1.93	0.50
1:A:151:HIS:O	1:A:155:ILE:HG12	2.12	0.50
1:A:36:ALA:HA	1:A:92:ILE:CD1	2.42	0.50
1:C:46:ALA:O	1:C:50:ILE:HG13	2.11	0.50
1:A:39:VAL:HG23	1:A:40:VAL:HG13	1.94	0.50
1:A:88:LEU:O	1:A:92:ILE:HG12	2.11	0.49
1:C:31:ASP:O	1:C:35:ILE:HD13	2.12	0.49
1:C:40:VAL:CG1	1:C:88:LEU:HD21	2.43	0.49
1:C:1:MSE:HE2	1:C:200:PHE:CE1	2.48	0.48
1:B:152:VAL:O	1:B:156:LEU:HG	2.13	0.48
1:B:142:MSE:HE3	1:B:149:ARG:N	2.29	0.48
1:B:207:GLU:HB2	3:B:324:HOH:O	2.13	0.47
1:C:173:ILE:HD11	1:C:182:ILE:HG23	1.96	0.47
1:A:74:ILE:HD11	1:A:81:LYS:N	2.30	0.47
1:A:207:GLU:HA	3:A:335:HOH:O	2.14	0.47
1:A:77:ASN:N	1:A:78:PRO:HD3	2.29	0.47
1:C:151:HIS:O	1:C:155:ILE:HG12	2.14	0.47
1:A:201:VAL:HG23	3:A:311:HOH:O	2.14	0.46
1:A:176:ASN:ND2	1:A:176:ASN:H	2.14	0.46
1:B:34:ILE:O	1:B:38:GLN:HG3	2.15	0.46
1:C:84:LEU:C	1:C:86:ALA:N	2.70	0.46
1:A:119:SER:HA	1:A:121:TYR:CE2	2.51	0.45
1:B:38:GLN:HA	1:B:41:GLU:HG3	1.98	0.45
1:C:31:ASP:OD2	1:C:34:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:ASN:H	1:C:176:ASN:ND2	2.15	0.45
1:A:39:VAL:O	1:A:46:ALA:HB3	2.17	0.44
1:A:55:GLY:O	1:A:58:MSE:HB2	2.17	0.44
1:B:84:LEU:O	1:B:88:LEU:HG	2.16	0.44
1:C:175:ASN:CG	1:C:175:ASN:O	2.56	0.44
1:A:83:TRP:C	1:A:85:ASN:N	2.71	0.44
1:B:22:PHE:CD2	1:B:109:LEU:HD22	2.53	0.44
1:C:46:ALA:HB2	1:C:91:LEU:HD11	1.99	0.44
1:A:142:MSE:HE3	1:A:149:ARG:N	2.32	0.43
1:C:35:ILE:HG22	1:C:92:ILE:HG23	1.99	0.43
1:B:176:ASN:C	1:B:176:ASN:HD22	2.22	0.43
1:B:195:GLN:O	1:B:199:GLN:HG2	2.18	0.43
1:B:78:PRO:O	1:B:82:ASN:ND2	2.52	0.43
1:A:176:ASN:H	1:A:176:ASN:HD22	1.66	0.43
1:B:148:THR:HG23	1:B:151:HIS:HB2	2.01	0.43
1:C:96:THR:O	1:C:100:ILE:HG12	2.19	0.43
1:A:86:ALA:HB3	3:A:309:HOH:O	2.19	0.43
1:C:84:LEU:O	1:C:87:LEU:HB3	2.18	0.43
1:A:40:VAL:HB	1:A:65:LEU:HD22	2.01	0.43
1:C:7:LEU:HD22	1:C:109:LEU:HD21	2.01	0.43
1:A:68:ARG:HD2	1:A:68:ARG:C	2.39	0.42
1:C:119:SER:HA	1:C:121:TYR:CE2	2.54	0.42
1:A:34:ILE:O	1:A:38:GLN:HG3	2.20	0.42
1:B:85:ASN:C	1:B:87:LEU:N	2.72	0.42
1:C:145:ASP:O	1:C:147:VAL:HG13	2.20	0.42
1:A:27:ILE:HG23	1:A:107:TYR:O	2.20	0.42
1:A:46:ALA:O	1:A:50:ILE:HG13	2.20	0.42
1:B:67:ARG:NH2	3:B:326:HOH:O	2.52	0.42
1:B:130:VAL:HA	1:B:173:ILE:HG23	2.02	0.42
1:B:206:PRO:O	1:B:207:GLU:HB2	2.20	0.42
1:C:30:ILE:HG13	1:C:100:ILE:HD13	2.02	0.41
1:C:35:ILE:C	1:C:37:ARG:N	2.69	0.41
1:C:81:LYS:C	1:C:83:TRP:H	2.23	0.41
1:C:40:VAL:HG12	1:C:88:LEU:HD21	2.02	0.41
1:C:138:LEU:O	1:C:142:MSE:HG3	2.20	0.41
1:B:87:LEU:HB2	3:B:307:HOH:O	2.20	0.41
1:B:205:LYS:HA	1:B:206:PRO:HD3	1.86	0.41
1:C:79:GLU:CD	1:C:80:GLU:N	2.72	0.41
1:C:113:PRO:HD2	3:C:256:HOH:O	2.20	0.41
1:C:199:GLN:HG3	3:C:249:HOH:O	2.20	0.41
1:B:97:GLN:O	1:B:101:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:HG23	1:A:11:ILE:O	2.22	0.40
1:A:71:ARG:O	1:A:74:ILE:HG22	2.21	0.40
1:A:30:ILE:HD12	1:A:108:VAL:HB	2.04	0.40
1:C:148:THR:HG23	1:C:151:HIS:H	1.86	0.40

There are no symmetry-related clashes.

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	205/214 (96%)	189 (92%)	12 (6%)	4 (2%)	6	11
1	B	205/214 (96%)	192 (94%)	13 (6%)	0	100	100
1	C	183/214 (86%)	166 (91%)	16 (9%)	1 (0%)	25	44
All	All	593/642 (92%)	547 (92%)	41 (7%)	5 (1%)	16	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	LEU
1	A	178	ALA
1	C	50	ILE
1	A	78	PRO
1	A	177	GLY

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	168/172 (98%)	163 (97%)	5 (3%)	36	63
1	B	168/172 (98%)	163 (97%)	5 (3%)	36	63
1	C	153/172 (89%)	145 (95%)	8 (5%)	19	39
All	All	489/516 (95%)	471 (96%)	18 (4%)	29	55

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	68	ARG
1	A	150	GLU
1	A	176	ASN
1	A	195	GLN
1	B	2	ARG
1	B	102	GLN
1	B	130	VAL
1	B	176	ASN
1	B	195	GLN
1	C	1	MSE
1	C	11	ILE
1	C	30	ILE
1	C	47	LEU
1	C	82	ASN
1	C	130	VAL
1	C	176	ASN
1	C	195	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	93	GLN
1	A	94	GLN
1	A	176	ASN
1	A	199	GLN
1	B	82	ASN
1	B	94	GLN
1	B	98	HIS
1	B	151	HIS

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Mol	Chain	Res	Type
1	B	176	ASN
1	B	199	GLN
1	B	203	GLN
1	C	82	ASN
1	C	93	GLN
1	C	94	GLN
1	C	97	GLN
1	C	176	ASN
1	C	199	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](#)

2 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	SO4	B	302	-	4,4,4	0.40	0	6,6,6	0.20	0
2	SO4	A	301	-	4,4,4	0.32	0	6,6,6	0.13	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	37:ARG	C	38:GLN	N	1.18
1	C	36:ALA	C	37:ARG	N	1.15

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	204/214 (95%)	0.42	18 (8%)	17 16	13, 33, 67, 78	1 (0%)
1	B	204/214 (95%)	0.07	10 (4%)	36 33	6, 24, 56, 73	2 (0%)
1	C	184/214 (85%)	0.41	21 (11%)	11 10	7, 28, 65, 80	1 (0%)
All	All	592/642 (92%)	0.30	49 (8%)	19 18	6, 27, 66, 80	4 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	ASP	4.5
1	C	86	ALA	4.0
1	C	206	PRO	3.6
1	C	85	ASN	3.6
1	C	88	LEU	3.4
1	A	181	ALA	3.4
1	C	81	LYS	3.4
1	B	207	GLU	3.2
1	B	144	ARG	3.2
1	B	150	GLU	3.1
1	B	146	ASP	3.0
1	A	179	PRO	3.0
1	A	149	ARG	2.8
1	A	86	ALA	2.8
1	C	149	ARG	2.7
1	C	205	LYS	2.7
1	B	147	VAL	2.7
1	A	203	GLN	2.6
1	C	204	GLU	2.5
1	A	54	PHE	2.5
1	A	68	ARG	2.5
1	C	87	LEU	2.4
1	C	57	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	203	GLN	2.4
1	B	148	THR	2.4
1	A	75	PHE	2.4
1	C	48	HIS	2.4
1	A	153	GLU	2.3
1	C	144	ARG	2.3
1	A	144	ARG	2.3
1	A	69	ALA	2.3
1	B	87	LEU	2.2
1	C	102	GLN	2.2
1	C	179	PRO	2.2
1	C	147	VAL	2.2
1	A	56	ALA	2.2
1	A	82	ASN	2.2
1	C	51	ALA	2.2
1	A	64	THR	2.1
1	C	148	THR	2.1
1	A	70	LEU	2.1
1	A	204	GLU	2.1
1	B	204	GLU	2.1
1	C	101	GLN	2.1
1	C	207	GLU	2.1
1	C	180	ASP	2.1
1	A	78	PRO	2.0
1	B	206	PRO	2.0
1	B	94	GLN	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 monosaccharides 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(\AA^2)	Q<0.9
2	SO4	B	302	5/5	0.69	0.51	114,114,115,115	0
2	SO4	A	301	5/5	0.95	0.08	42,42,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.