



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:58 AM UTC

PDB ID : 5KTE / pdb_00005kte
Title : Crystal structure of Deinococcus radiodurans MntH, an Nramp-family transition metal transporter
Authors : Bane, L.B.; Gaudet, R.; Weihofen, W.A.; Singharoy, A.
Deposited on : 2016-07-11
Resolution : 3.94 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

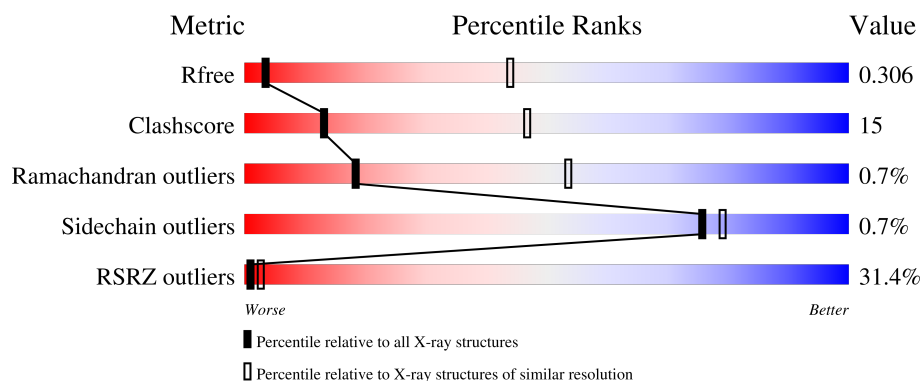
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.94 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	1022 (4.12-3.76)
Clashscore	190562	1000 (4.10-3.78)
Ramachandran outliers	187476	1009 (4.12-3.76)
Sidechain outliers	187428	1002 (4.12-3.76)
RSRZ outliers	180081	1022 (4.12-3.76)

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	420	39% 57% 23% 20%
2	H	213	13% 65% 34% .
3	L	213	23% 63% 36% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5625 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 Divalent metal cation transporter MntH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2407	1586	385	420	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP Q9RTP8
A	18	HIS	-	expression tag	UNP Q9RTP8
A	19	HIS	-	expression tag	UNP Q9RTP8
A	20	HIS	-	expression tag	UNP Q9RTP8
A	21	HIS	-	expression tag	UNP Q9RTP8
A	22	HIS	-	expression tag	UNP Q9RTP8
A	23	HIS	-	expression tag	UNP Q9RTP8
A	24	HIS	-	expression tag	UNP Q9RTP8
A	25	HIS	-	expression tag	UNP Q9RTP8
A	168	HIS	GLN	engineered mutation	UNP Q9RTP8
A	169	HIS	LYS	engineered mutation	UNP Q9RTP8
A	251	TYR	GLU	engineered mutation	UNP Q9RTP8
A	252	TYR	GLU	engineered mutation	UNP Q9RTP8
A	253	TYR	LYS	engineered mutation	UNP Q9RTP8
A	398	HIS	ARG	engineered mutation	UNP Q9RTP8
A	399	HIS	ARG	engineered mutation	UNP Q9RTP8

- Molecule 2 is a protein called Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	211	Total	C	N	O	S	0	0	0
			1567	992	251	316	8			

- Molecule 3 is a protein called Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total 1648	C 1019	N 282	O 341	S 6	0	0	0

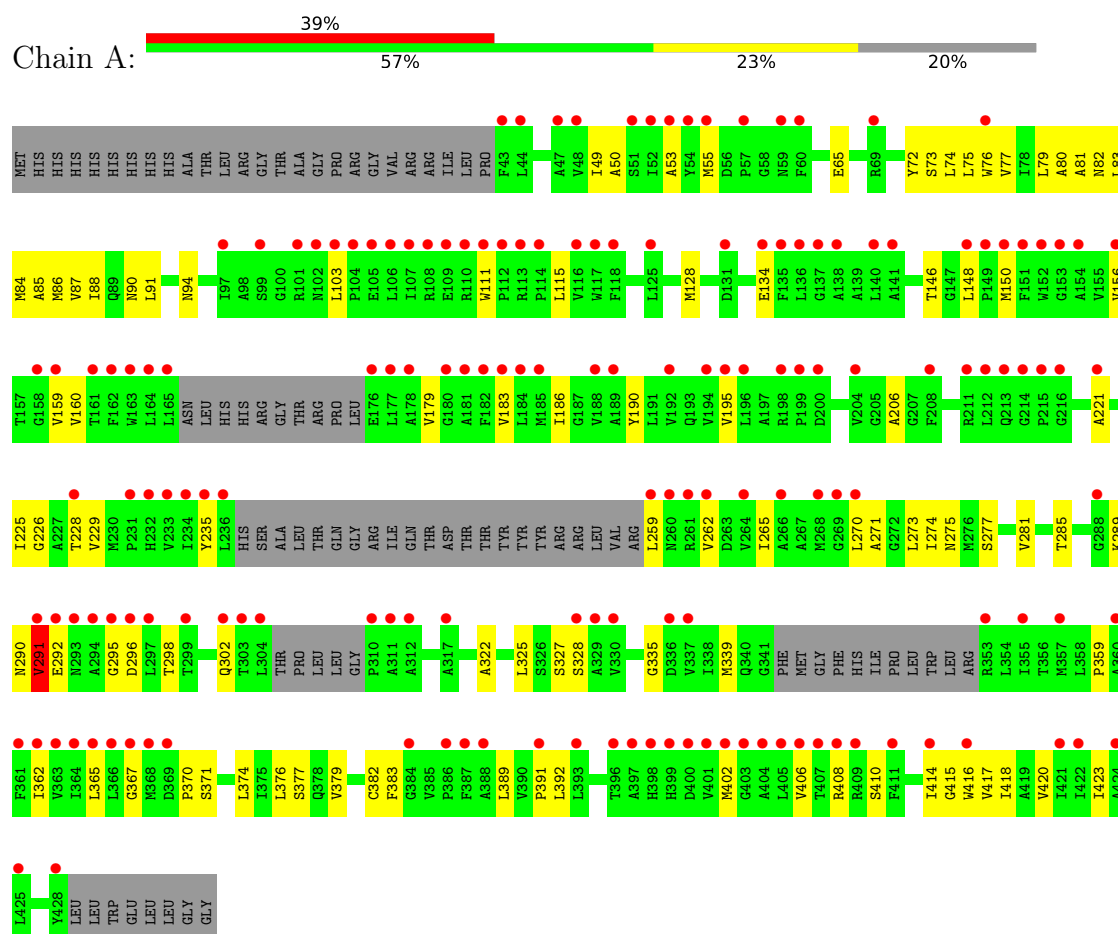
- Molecule 4 is OSMIUM ION (CCD ID: OS) (formula: Os).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Os 2	0	0
4	H	1	Total 1	Os 1	0	0

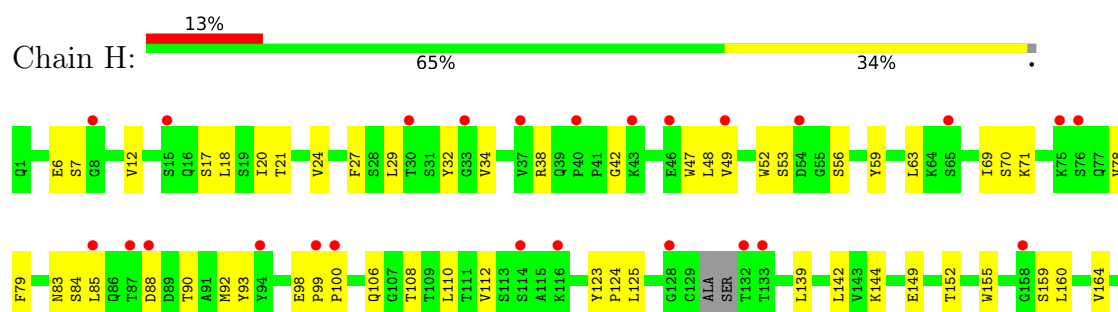
3 Residue-property plots

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

• Molecule 1: Divalent metal cation transporter MntH

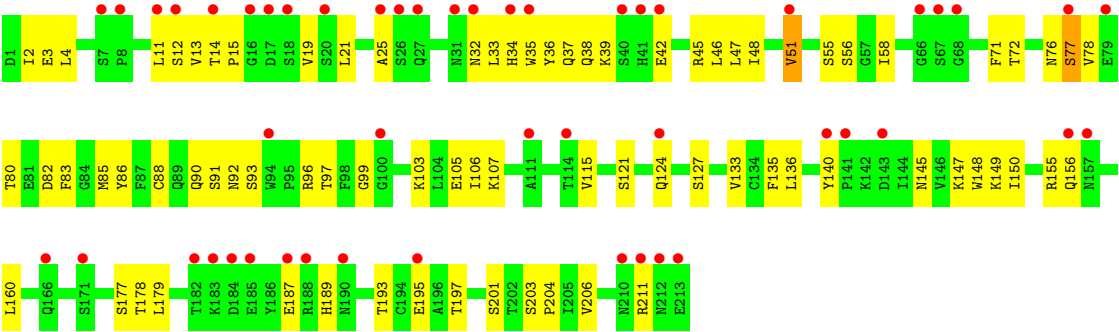


• Molecule 2: Fab Heavy Chain





● Molecule 3: Fab Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	113.13Å 132.08Å 221.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.47 – 3.94 46.47 – 3.94	Depositor EDS
% Data completeness (in resolution range)	76.0 (46.47-3.94) 75.1 (46.47-3.94)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.43 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.268 , 0.313 0.265 , 0.306	Depositor DCC
R_{free} test set	1179 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	-4.7	Xtriage
Anisotropy	5.659	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	5625	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, 0.333 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:
OS

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	0.15	0/2455	0.39	0/3363
2	H	0.19	0/1609	0.46	0/2205
3	L	0.18	0/1685	0.44	0/2286
All	All	0.17	0/5749	0.42	0/7854

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	VAL	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	2407	0	2426	66	0
2	H	1567	0	1532	53	0
3	L	1648	0	1565	54	0
4	A	2	0	0	0	0
4	H	1	0	0	0	0
All	All	5625	0	5523	166	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 15.

All (166) 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)
3:L:189:HIS:O	3:L:211:ARG:NH1	2.07	0.86
2:H:49:VAL:HG12	2:H:59:TYR:HA	1.68	0.75
3:L:147:LYS:NZ	3:L:156:GLN:HG2	2.00	0.75
2:H:53:SER:HA	2:H:71:LYS:HE3	1.67	0.74
3:L:149:LYS:HB2	3:L:193:THR:HB	1.71	0.72
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.70	0.72
1:A:83:LEU:HD23	1:A:408:ARG:HH12	1.56	0.71
2:H:172:GLN:HE21	3:L:160:LEU:HD12	1.56	0.70
3:L:38:GLN:HB3	3:L:85:MET:HB2	1.74	0.69
1:A:65:GLU:OE2	1:A:295:GLY:HA2	1.93	0.69
2:H:17:SER:OG	2:H:83:ASN:OD1	2.10	0.69
1:A:271:ALA:O	1:A:275:ASN:ND2	2.26	0.69
1:A:49:ILE:O	1:A:53:ALA:HB2	1.95	0.67
1:A:290:ASN:HB3	2:H:99:PRO:HA	1.77	0.66
1:A:73:SER:HA	1:A:206:ALA:HB1	1.78	0.66
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.79	0.65
3:L:133:VAL:HG12	3:L:178:THR:HG22	1.78	0.64
2:H:6:GLU:H	2:H:106:GLN:HE22	1.44	0.64
3:L:147:LYS:HZ2	3:L:156:GLN:HG2	1.62	0.63
3:L:115:VAL:HB	3:L:136:LEU:HD23	1.80	0.63
2:H:70:SER:HB2	2:H:79:PHE:HB2	1.80	0.63
2:H:52:TRP:HB3	2:H:56:SER:HB2	1.80	0.62
3:L:187:GLU:OE1	3:L:211:ARG:NH2	2.33	0.61
1:A:72:TYR:HA	1:A:75:LEU:HD13	1.83	0.60
2:H:20:ILE:HG21	2:H:108:THR:HG21	1.82	0.60
3:L:3:GLU:HA	3:L:97:THR:HG21	1.83	0.59
3:L:33:LEU:HB3	3:L:51:VAL:CG2	2.32	0.59
2:H:47:TRP:CG	3:L:96:ARG:HB2	2.38	0.58
3:L:13:VAL:HG11	3:L:78:VAL:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:32:TYR:CZ	2:H:99:PRO:HD3	2.38	0.57
2:H:48:LEU:HG	2:H:49:VAL:HG22	1.86	0.57
2:H:155:TRP:CZ3	2:H:196:CYS:HB2	2.39	0.57
1:A:85:ALA:HB2	1:A:229:VAL:HG22	1.87	0.56
1:A:225:ILE:HG12	1:A:416:TRP:HZ3	1.71	0.56
2:H:24:VAL:HG21	2:H:29:LEU:HB2	1.86	0.56
3:L:15:PRO:HG3	3:L:80:THR:HG22	1.88	0.56
2:H:90:THR:HG22	2:H:112:VAL:H	1.70	0.56
3:L:147:LYS:HZ1	3:L:156:GLN:HG2	1.69	0.56
1:A:417:VAL:HA	1:A:420:VAL:HG22	1.88	0.55
1:A:50:ALA:HB1	1:A:271:ALA:HB2	1.87	0.55
1:A:289:LYS:NZ	3:L:92:ASN:HA	2.22	0.55
3:L:4:LEU:HD23	3:L:25:ALA:HA	1.88	0.55
1:A:359:PRO:HA	1:A:362:ILE:HG12	1.88	0.55
1:A:325:LEU:O	1:A:328:SER:OG	2.21	0.54
3:L:4:LEU:HD11	3:L:90:GLN:HB3	1.90	0.54
1:A:81:ALA:HA	1:A:225:ILE:HG13	1.88	0.54
2:H:12:VAL:HG21	2:H:18:LEU:HD23	1.90	0.54
1:A:77:VAL:O	1:A:81:ALA:N	2.42	0.53
3:L:145:ASN:HB3	3:L:197:THR:OG1	2.08	0.53
3:L:85:MET:HE2	3:L:103:LYS:HD2	1.90	0.53
1:A:414:ILE:HA	1:A:417:VAL:HG22	1.91	0.53
1:A:289:LYS:NZ	3:L:32:ASN:CG	2.67	0.53
1:A:415:GLY:O	1:A:418:ILE:HG13	2.08	0.53
3:L:47:LEU:HA	3:L:58:ILE:HG13	1.91	0.53
1:A:190:TYR:O	1:A:277:SER:OG	2.28	0.52
3:L:88:CYS:O	3:L:99:GLY:N	2.41	0.52
3:L:150:ILE:HD12	3:L:155:ARG:HH11	1.74	0.52
1:A:81:ALA:HB1	1:A:228:THR:OG1	2.09	0.52
1:A:160:VAL:HG11	1:A:325:LEU:HD13	1.92	0.52
1:A:291:VAL:HG22	1:A:292:GLU:H	1.75	0.52
2:H:164:VAL:HG22	2:H:182:VAL:HG23	1.92	0.52
1:A:296:ASP:C	1:A:298:THR:H	2.18	0.51
1:A:179:VAL:HG13	1:A:322:ALA:HB1	1.92	0.51
3:L:36:TYR:HD1	3:L:46:LEU:HA	1.75	0.51
1:A:285:THR:HG21	1:A:302:GLN:HG2	1.93	0.51
3:L:33:LEU:HB3	3:L:51:VAL:HG23	1.93	0.50
2:H:24:VAL:HB	2:H:27:PHE:CE1	2.47	0.50
3:L:2:ILE:HB	3:L:90:GLN:HE22	1.77	0.50
1:A:335:GLY:O	1:A:339:MET:HB2	2.12	0.50
2:H:38:ARG:HD2	2:H:48:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:49:VAL:HG21	2:H:69:ILE:HD11	1.93	0.50
3:L:91:SER:HA	3:L:96:ARG:HD2	1.94	0.49
2:H:124:PRO:HD3	2:H:209:LYS:NZ	2.27	0.49
2:H:155:TRP:CH2	2:H:196:CYS:HB2	2.47	0.49
2:H:98:GLU:HG3	2:H:99:PRO:HD2	1.94	0.49
1:A:55:MET:O	1:A:327:SER:HB2	2.13	0.49
1:A:290:ASN:O	1:A:291:VAL:HG12	2.11	0.49
2:H:188:THR:HB	2:H:192:GLN:HB2	1.94	0.49
1:A:226:GLY:HA3	1:A:382:CYS:HB2	1.94	0.49
1:A:134:GLU:HG3	1:A:328:SER:HB3	1.95	0.48
1:A:150:MET:SD	1:A:370:PRO:HG2	2.53	0.48
1:A:296:ASP:HA	1:A:371:SER:HB2	1.95	0.48
1:A:74:LEU:HD11	1:A:221:ALA:HB2	1.95	0.48
2:H:98:GLU:CG	2:H:99:PRO:HD2	2.43	0.48
2:H:171:LEU:HD21	2:H:174:GLY:H	1.78	0.48
1:A:262:VAL:HA	1:A:265:ILE:HG22	1.96	0.48
2:H:186:SER:HA	2:H:189:TRP:HB3	1.95	0.48
2:H:197:SER:HA	2:H:208:ASP:HA	1.96	0.48
3:L:115:VAL:HA	3:L:135:PHE:O	2.13	0.48
3:L:195:GLU:HG2	3:L:206:VAL:HG22	1.95	0.48
1:A:84:MET:O	1:A:87:VAL:HB	2.14	0.48
2:H:49:VAL:CG2	2:H:69:ILE:HD11	2.43	0.48
2:H:139:LEU:HB3	2:H:211:LEU:HD21	1.96	0.48
3:L:148:TRP:CD2	3:L:179:LEU:HD22	2.49	0.48
1:A:374:LEU:O	1:A:377:SER:HB3	2.14	0.47
1:A:420:VAL:HA	1:A:423:ILE:HG22	1.95	0.47
2:H:83:ASN:CG	2:H:84:SER:H	2.22	0.47
1:A:88:ILE:HD13	1:A:389:LEU:HD21	1.96	0.47
3:L:45:ARG:HH21	3:L:58:ILE:HD13	1.79	0.47
1:A:74:LEU:O	1:A:77:VAL:HG12	2.14	0.47
3:L:34:HIS:HA	3:L:48:ILE:O	2.15	0.47
2:H:48:LEU:HD11	2:H:63:LEU:HD22	1.97	0.46
1:A:406:VAL:HG12	1:A:410:SER:HB2	1.97	0.46
1:A:183:VAL:HA	1:A:186:ILE:HG22	1.97	0.46
1:A:80:ALA:O	1:A:84:MET:HG2	2.15	0.46
3:L:124:GLN:HA	3:L:127:SER:HB3	1.98	0.46
2:H:159:SER:HB3	2:H:185:PRO:HD2	1.98	0.46
2:H:34:VAL:HG21	2:H:78:VAL:HG21	1.98	0.46
2:H:93:TYR:HE2	2:H:110:LEU:HD23	1.81	0.46
2:H:125:LEU:HD11	2:H:142:LEU:HB2	1.97	0.46
2:H:144:LYS:NZ	2:H:172:GLN:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:VAL:O	1:A:285:THR:OG1	2.25	0.45
3:L:13:VAL:HG22	3:L:14:THR:H	1.82	0.45
1:A:376:LEU:HA	1:A:379:VAL:HG22	1.98	0.45
3:L:197:THR:HG22	3:L:204:PRO:HB3	1.97	0.45
2:H:149:GLU:HG2	2:H:176:TYR:CE2	2.52	0.45
2:H:7:SER:HB2	2:H:21:THR:H	1.82	0.45
1:A:82:ASN:HB3	1:A:86:MET:HE2	1.98	0.45
2:H:85:LEU:H	2:H:85:LEU:HD12	1.82	0.45
3:L:11:LEU:HD21	3:L:19:VAL:HB	1.99	0.44
2:H:92:MET:HA	2:H:108:THR:O	2.18	0.44
2:H:98:GLU:CD	2:H:99:PRO:HD2	2.43	0.44
3:L:55:SER:OG	3:L:56:SER:N	2.51	0.44
2:H:152:THR:OG1	2:H:199:ALA:HB3	2.18	0.44
2:H:189:TRP:HA	2:H:190:PRO:HA	1.72	0.43
1:A:156:VAL:HA	1:A:159:VAL:HG22	2.00	0.43
2:H:123:TYR:HB3	3:L:121:SER:OG	2.18	0.43
3:L:12:SER:OG	3:L:105:GLU:OE2	2.36	0.43
1:A:90:ASN:O	1:A:94:ASN:N	2.45	0.43
1:A:270:LEU:O	1:A:273:LEU:HB2	2.19	0.43
3:L:51:VAL:HG11	3:L:71:PHE:CD1	2.54	0.43
1:A:271:ALA:HA	1:A:274:ILE:HG12	2.00	0.43
1:A:365:LEU:C	1:A:367:GLY:H	2.27	0.42
2:H:125:LEU:HD13	3:L:133:VAL:HG21	2.00	0.42
3:L:107:LYS:HA	3:L:140:TYR:OH	2.18	0.42
1:A:91:LEU:HB2	1:A:392:LEU:HD21	2.00	0.42
3:L:83:PHE:CE2	3:L:106:ILE:HG12	2.54	0.42
3:L:201:SER:OG	3:L:203:SER:O	2.33	0.42
3:L:21:LEU:O	3:L:72:THR:HA	2.20	0.42
2:H:7:SER:HB3	2:H:20:ILE:HG23	2.02	0.42
1:A:111:TRP:HB3	1:A:115:LEU:HD22	2.02	0.42
1:A:383:PHE:CE1	1:A:420:VAL:HB	2.54	0.42
1:A:103:LEU:HD11	1:A:391:PRO:HB2	2.01	0.42
2:H:18:LEU:HD22	2:H:110:LEU:HD21	2.02	0.42
2:H:185:PRO:C	2:H:187:SER:H	2.27	0.42
2:H:203:SER:C	2:H:205:THR:H	2.26	0.42
1:A:379:VAL:O	1:A:382:CYS:HB3	2.20	0.42
3:L:160:LEU:O	3:L:177:SER:HA	2.20	0.41
1:A:291:VAL:HG13	1:A:292:GLU:N	2.35	0.41
1:A:383:PHE:HE1	1:A:420:VAL:HB	1.86	0.41
2:H:20:ILE:HD13	2:H:108:THR:HG21	2.02	0.41
1:A:83:LEU:HD23	1:A:408:ARG:NH1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:15:PRO:HB3	3:L:83:PHE:CZ	2.55	0.41
3:L:39:LYS:HB2	3:L:42:GLU:HG3	2.03	0.41
3:L:160:LEU:HD23	3:L:160:LEU:HA	1.75	0.41
1:A:76:TRP:O	1:A:79:LEU:HB3	2.21	0.41
1:A:103:LEU:HD23	1:A:235:TYR:CE1	2.56	0.41
1:A:146:THR:HG23	1:A:148:LEU:H	1.86	0.41
1:A:335:GLY:O	1:A:339:MET:CB	2.69	0.41
1:A:128:MET:HG2	1:A:359:PRO:HG2	2.03	0.40
1:A:49:ILE:O	1:A:53:ALA:CB	2.67	0.40
2:H:99:PRO:HG2	2:H:100:PRO:HD3	2.02	0.40
3:L:92:ASN:OD1	3:L:93:SER:N	2.54	0.40
1:A:94:ASN:HD21	1:A:402:MET:HB3	1.86	0.40
2:H:88:ASP:HA	2:H:112:VAL:HB	2.02	0.40
3:L:82:ASP:HB3	3:L:86:TYR:OH	2.21	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	328/420 (78%)	301 (92%)	26 (8%)	1 (0%)	36	70
2	H	207/213 (97%)	184 (89%)	21 (10%)	2 (1%)	12	45
3	L	211/213 (99%)	191 (90%)	18 (8%)	2 (1%)	14	48
All	All	746/846 (88%)	676 (91%)	65 (9%)	5 (1%)	18	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	VAL
3	L	51	VAL
2	H	160	LEU

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Mol	Chain	Res	Type
3	L	77	SER
2	H	42	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	233/326 (72%)	231 (99%)	2 (1%)	70	76
2	H	185/187 (99%)	185 (100%)	0	100	100
3	L	192/193 (100%)	190 (99%)	2 (1%)	68	76
All	All	610/706 (86%)	606 (99%)	4 (1%)	76	79

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	LEU
1	A	291	VAL
3	L	76	ASN
3	L	77	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	399	HIS
2	H	192	GLN
3	L	31	ASN
3	L	53	GLN
3	L	90	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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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	338/420 (80%)	2.37	162 (47%) 0 1	61, 116, 169, 230	0
2	H	211/213 (99%)	0.79	28 (13%) 7 10	17, 56, 98, 157	0
3	L	213/213 (100%)	1.41	49 (23%) 2 4	44, 73, 116, 175	0
All	All	762/846 (90%)	1.66	239 (31%) 1 3	17, 86, 154, 230	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	ARG	16.1
1	A	109	GLU	15.0
1	A	199	PRO	11.7
3	L	17	ASP	11.2
1	A	232	HIS	9.6
1	A	233	VAL	9.2
1	A	165	LEU	8.6
1	A	236	LEU	8.3
1	A	235	TYR	8.0
1	A	407	THR	8.0
1	A	105	GLU	7.9
1	A	181	ALA	7.7
1	A	110	ARG	7.5
1	A	107	ILE	7.0
1	A	364	ILE	6.8
3	L	16	GLY	6.2
1	A	293	ASN	6.2
1	A	215	PRO	6.1
1	A	295	GLY	6.0
1	A	162	PHE	5.7
1	A	111	TRP	5.7
1	A	112	PRO	5.6
1	A	178	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
3	L	184	ASP	5.6
1	A	54	TYR	5.5
3	L	188	ARG	5.5
1	A	151	PHE	5.4
3	L	187	GLU	5.4
1	A	101	ARG	5.4
1	A	260	ASN	5.3
3	L	210	ASN	5.2
1	A	234	ILE	5.1
1	A	299	THR	5.0
1	A	304	LEU	5.0
1	A	292	GLU	4.9
1	A	402	MET	4.9
1	A	136	LEU	4.9
1	A	102	ASN	4.9
1	A	398	HIS	4.9
1	A	261	ARG	4.8
1	A	397	ALA	4.8
1	A	296	ASP	4.7
1	A	204	VAL	4.7
1	A	388	ALA	4.7
1	A	137	GLY	4.6
3	L	77	SER	4.6
3	L	14	THR	4.4
1	A	416	TRP	4.3
1	A	189	ALA	4.3
1	A	399	HIS	4.2
2	H	99	PRO	4.2
3	L	183	LYS	4.1
1	A	405	LEU	4.1
1	A	106	LEU	4.1
1	A	140	LEU	4.1
3	L	32	ASN	4.0
1	A	361	PHE	4.0
1	A	116	VAL	3.9
1	A	135	PHE	3.9
3	L	185	GLU	3.8
1	A	363	VAL	3.8
1	A	262	VAL	3.8
1	A	367	GLY	3.8
1	A	211	ARG	3.7
1	A	117	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
3	L	114	THR	3.7
1	A	192	VAL	3.7
3	L	212	ASN	3.7
1	A	103	LEU	3.7
1	A	291	VAL	3.7
1	A	302	GLN	3.7
2	H	40	PRO	3.7
1	A	329	ALA	3.7
3	L	94	TRP	3.7
1	A	231	PRO	3.7
3	L	40	SER	3.6
1	A	365	LEU	3.6
2	H	174	GLY	3.6
3	L	68	GLY	3.6
1	A	195	VAL	3.6
2	H	133	THR	3.6
2	H	75	LYS	3.5
2	H	100	PRO	3.5
1	A	270	LEU	3.5
3	L	143	ASP	3.5
1	A	118	PHE	3.5
1	A	411	PHE	3.5
1	A	183	VAL	3.5
1	A	149	PRO	3.5
1	A	152	TRP	3.4
3	L	213	GLU	3.4
1	A	400	ASP	3.3
1	A	194	VAL	3.3
1	A	198	ARG	3.3
1	A	60	PHE	3.3
1	A	182	PHE	3.3
1	A	114	PRO	3.3
2	H	30	THR	3.3
3	L	140	TYR	3.3
1	A	185	MET	3.2
1	A	312	ALA	3.2
1	A	196	LEU	3.2
1	A	303	THR	3.1
1	A	55	MET	3.1
2	H	49	VAL	3.1
3	L	157	ASN	3.1
1	A	404	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	59	ASN	3.1
1	A	104	PRO	3.1
3	L	12	SER	3.1
1	A	177	LEU	3.1
1	A	396	THR	3.1
1	A	176	GLU	3.0
1	A	266	ALA	3.0
2	H	94	TYR	3.0
1	A	310	PRO	3.0
1	A	406	VAL	3.0
1	A	47	ALA	3.0
1	A	401	VAL	3.0
1	A	362	ILE	2.9
1	A	97	ILE	2.9
3	L	34	HIS	2.9
1	A	163	TRP	2.9
3	L	156	GLN	2.9
1	A	311	ALA	2.9
1	A	330	VAL	2.9
1	A	393	LEU	2.9
1	A	408	ARG	2.9
1	A	384	GLY	2.9
3	L	42	GLU	2.8
2	H	33	GLY	2.8
1	A	53	ALA	2.8
1	A	188	VAL	2.8
1	A	134	GLU	2.8
1	A	360	ALA	2.8
1	A	369	ASP	2.8
1	A	391	PRO	2.8
1	A	164	LEU	2.8
2	H	85	LEU	2.8
3	L	171	SER	2.7
1	A	131	ASP	2.7
1	A	368	MET	2.7
1	A	184	LEU	2.7
1	A	259	LEU	2.7
3	L	166	GLN	2.7
1	A	221	ALA	2.7
3	L	67	SER	2.7
1	A	264	VAL	2.6
2	H	132	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	154	ALA	2.6
1	A	180	GLY	2.6
1	A	228	THR	2.6
3	L	182	THR	2.6
1	A	51	SER	2.6
3	L	7	SER	2.6
3	L	27	GLN	2.6
2	H	87	THR	2.6
1	A	44	LEU	2.6
1	A	294	ALA	2.6
1	A	69	ARG	2.6
1	A	353	ARG	2.6
1	A	150	MET	2.6
2	H	169	ALA	2.6
2	H	46	GLU	2.5
1	A	212	LEU	2.5
1	A	153	GLY	2.5
2	H	76	SER	2.5
3	L	25	ALA	2.5
1	A	414	ILE	2.5
2	H	88	ASP	2.5
1	A	328	SER	2.5
1	A	216	GLY	2.5
3	L	26	SER	2.5
3	L	51	VAL	2.5
3	L	195	GLU	2.5
3	L	141	PRO	2.5
1	A	200	ASP	2.5
3	L	18	SER	2.5
3	L	190	ASN	2.4
1	A	288	GLY	2.4
3	L	20	SER	2.4
1	A	156	VAL	2.4
1	A	337	VAL	2.4
1	A	148	LEU	2.4
1	A	403	GLY	2.4
1	A	57	PRO	2.4
1	A	214	GLY	2.4
1	A	387	PHE	2.4
1	A	421	ILE	2.4
1	A	357	MET	2.4
3	L	66	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	159	VAL	2.4
1	A	43	PHE	2.3
2	H	8	GLY	2.3
1	A	161	THR	2.3
1	A	425	LEU	2.3
2	H	128	GLY	2.3
2	H	54	ASP	2.3
2	H	213	PRO	2.3
3	L	41	HIS	2.3
1	A	268	MET	2.3
3	L	79	GLU	2.3
1	A	297	LEU	2.3
1	A	366	LEU	2.3
2	H	65	SER	2.3
2	H	158	GLY	2.3
3	L	31	ASN	2.2
3	L	35	TRP	2.2
1	A	208	PHE	2.2
1	A	422	ILE	2.2
1	A	141	ALA	2.2
1	A	424	ALA	2.2
3	L	124	GLN	2.2
1	A	113	ARG	2.2
1	A	355	ILE	2.2
1	A	99	SER	2.2
2	H	15	SER	2.2
2	H	114	SER	2.2
1	A	52	ILE	2.2
1	A	317	ALA	2.2
1	A	213	GLN	2.2
3	L	8	PRO	2.2
1	A	158	GLY	2.2
1	A	386	PRO	2.2
2	H	43	LYS	2.2
2	H	116	LYS	2.1
3	L	100	GLY	2.1
1	A	138	ALA	2.1
1	A	409	ARG	2.1
1	A	269	GLY	2.1
1	A	48	VAL	2.1
1	A	125	LEU	2.1
1	A	428	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	37	VAL	2.1
1	A	336	ASP	2.0
3	L	211	ARG	2.0
3	L	111	ALA	2.0
1	A	76	TRP	2.0
3	L	11	LEU	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($\text{\AA}^2$)	Q<0.9
4	OS	H	301	1/1	0.89	0.16	173,173,173,173	0
4	OS	A	502	1/1	0.90	0.14	192,192,192,192	0
4	OS	A	501	1/1	0.94	0.16	205,205,205,205	0

6.5 Other polymers [i](#)

There are no such residues in this entry.