



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:23 PM UTC

PDB ID : 4NNP / pdb_00004nnp
Title : Crystal Structure of Apo Manganese ABC transporter MntC from Staphylococcus aureus bound to an antagonistic fab fragment
Authors : Rouge, L.; Sudhamsu, J.
Deposited on : 2013-11-18
Resolution : 2.69 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

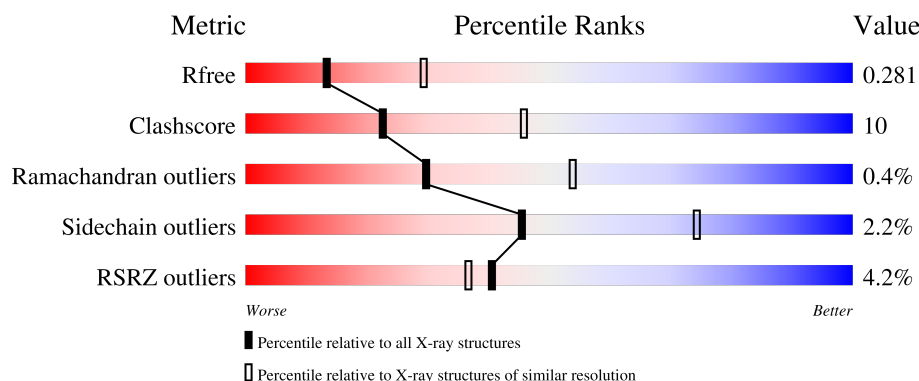
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	291	3% 71% 20% 6%
1	B	291	3% 73% 19% 6%
2	H	238	5% 79% 15% 5%
2	X	238	9% 79% 15% 5%
3	L	216	3% 76% 21% ..

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Mol	Chain	Length	Quality of chain
3	Y	216	2% 75% 23% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11297 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 Lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2189	1388	365	429	7			
1	B	274	Total	C	N	O	S	0	0	0
			2192	1388	366	431	7			

- Molecule 2 is a protein called Heavy chain of antagonistic fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	227	Total	C	N	O	S	0	0	0
			1700	1074	279	341	6			
2	X	227	Total	C	N	O	S	0	0	0
			1700	1074	279	341	6			

- Molecule 3 is a protein called Light chain of antagonistic fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1634	1023	273	333	5			
3	Y	213	Total	C	N	O	S	0	0	0
			1634	1023	273	333	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total	O	0	0
			63	63		
4	B	49	Total	O	0	0
			49	49		
4	H	27	Total	O	0	0
			27	27		
4	X	35	Total	O	0	0
			35	35		

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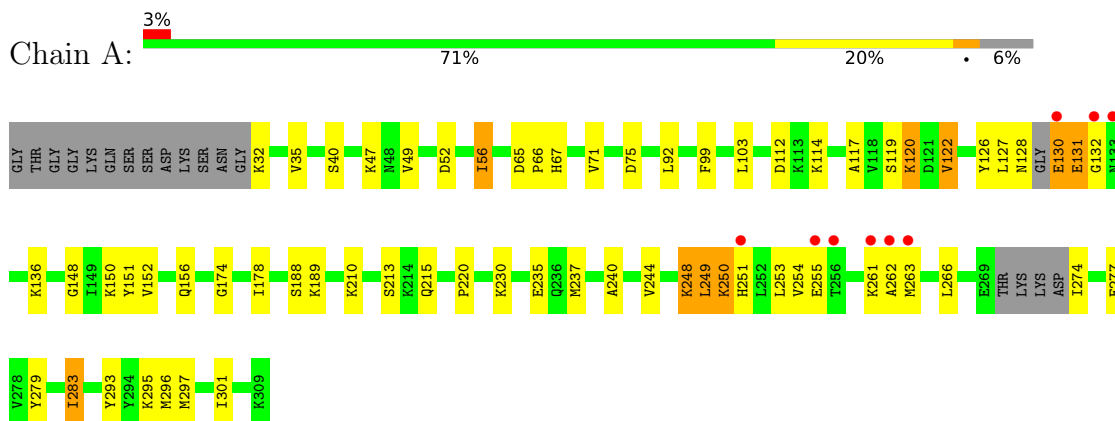
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	42	Total 42	O 42	0	0
4	Y	32	Total 32	O 32	0	0

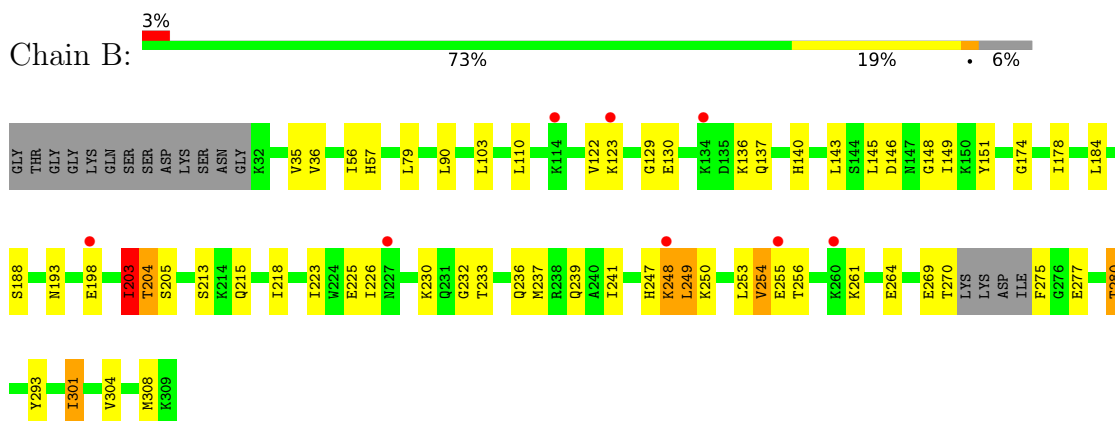
3 Residue-property plots [i](#)

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.

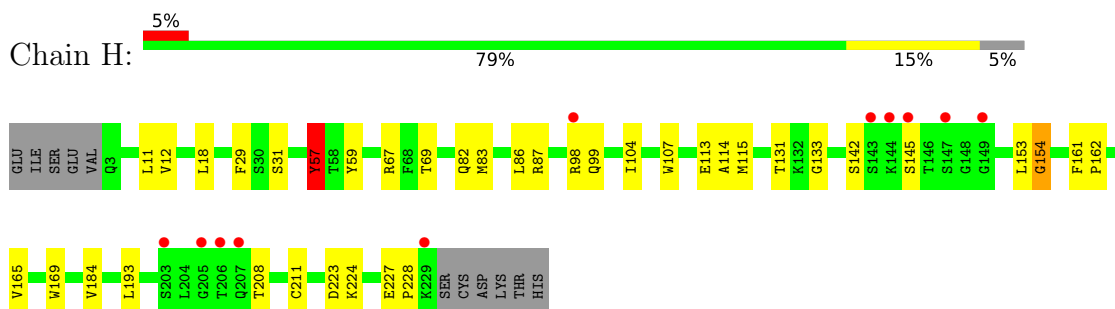
• Molecule 1: Lipoprotein



• Molecule 1: Lipoprotein

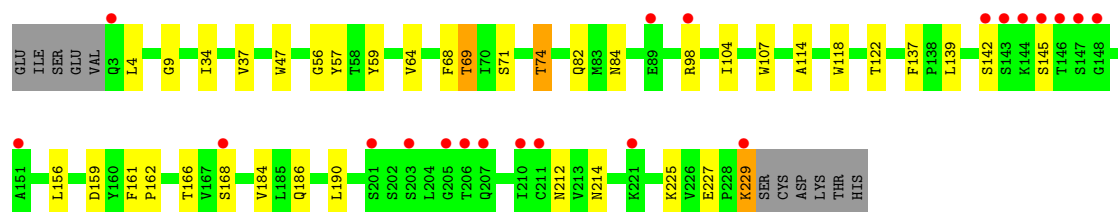


• Molecule 2: Heavy chain of antagonistic fab fragment



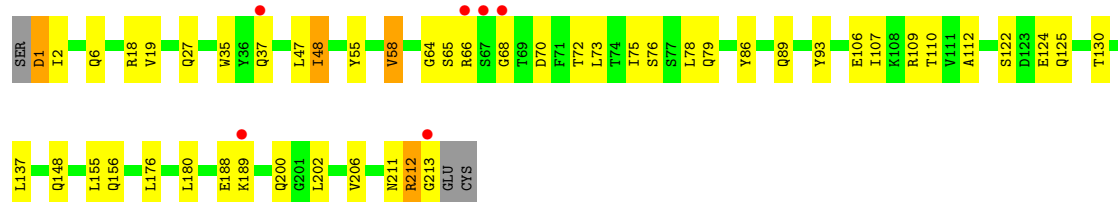
- Molecule 2: Heavy chain of antagonistic fab fragment

Chain X: 



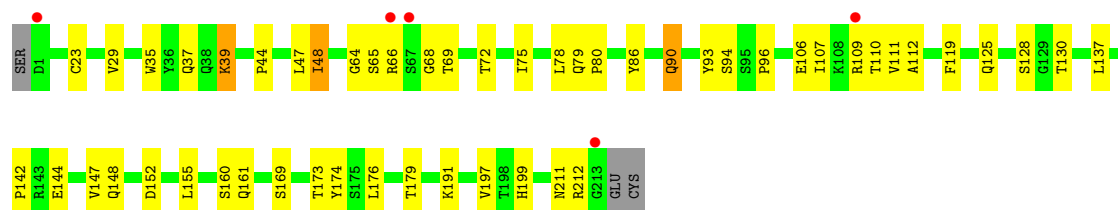
- Molecule 3: Light chain of antagonistic fab fragment

Chain L: 



- Molecule 3: Light chain of antagonistic fab fragment

Chain Y: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.11Å 92.51Å 127.86Å 90.00° 92.48° 90.00°	Depositor
Resolution (Å)	47.27 – 2.69 47.27 – 2.69	Depositor EDS
% Data completeness (in resolution range)	88.9 (47.27-2.69) 89.4 (47.27-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.224 , 0.283 0.225 , 0.281	Depositor DCC
R_{free} test set	2486 reflections (3.79%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11297	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.63% 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

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	0.69	0/2227	0.99	4/2987 (0.1%)
1	B	0.71	2/2231 (0.1%)	1.04	7/2994 (0.2%)
2	H	0.62	1/1744 (0.1%)	0.94	5/2377 (0.2%)
2	X	0.62	0/1744	0.91	2/2377 (0.1%)
3	L	0.57	0/1670	0.94	5/2267 (0.2%)
3	Y	0.62	0/1670	0.97	2/2267 (0.1%)
All	All	0.64	3/11286 (0.0%)	0.97	25/15269 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	ILE	C-O	-7.89	1.16	1.24
1	B	203	ILE	CA-C	-5.30	1.46	1.52
2	H	57	TYR	C-O	-5.26	1.17	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	LYS	CA-C-N	-11.08	108.40	120.14
1	B	123	LYS	C-N-CA	-11.08	108.40	120.14
3	L	65	SER	N-CA-C	8.00	121.03	108.79
1	A	262	ALA	N-CA-C	-7.36	104.30	113.20
3	Y	65	SER	N-CA-C	6.74	119.10	108.79
2	H	154	GLY	N-CA-C	6.68	120.22	110.80
1	B	256	THR	N-CA-C	-6.67	105.05	113.72
1	B	203	ILE	N-CA-C	-6.59	98.70	108.45
2	X	4	LEU	N-CA-C	6.31	119.40	110.50
1	B	249	LEU	N-CA-C	6.28	124.17	110.80
1	A	250	LYS	N-CA-C	-6.26	100.09	108.74
2	H	227	GLU	CA-C-N	6.14	126.48	119.92
2	H	227	GLU	C-N-CA	6.14	126.48	119.92
3	Y	93	TYR	N-CA-C	-6.07	102.66	110.19
1	B	122	VAL	N-CA-C	6.07	117.32	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	133	GLY	CA-C-N	5.64	126.09	119.99
2	H	133	GLY	C-N-CA	5.64	126.09	119.99
1	A	120	LYS	N-CA-C	5.49	119.08	112.38
2	X	56	GLY	N-CA-C	-5.40	107.81	115.43
1	A	249	LEU	N-CA-C	5.38	122.27	110.80
3	L	58	VAL	CA-C-N	5.29	125.29	119.90
3	L	58	VAL	C-N-CA	5.29	125.29	119.90
1	B	301	ILE	N-CA-C	5.14	115.75	110.36
3	L	65	SER	CA-C-N	5.03	131.15	121.54
3	L	65	SER	C-N-CA	5.03	131.15	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2189	0	2192	59	0
1	B	2192	0	2192	52	2
2	H	1700	0	1634	30	0
2	X	1700	0	1634	30	0
3	L	1634	0	1588	40	0
3	Y	1634	0	1588	38	0
4	A	63	0	0	2	0
4	B	49	0	0	1	0
4	H	27	0	0	2	2
4	L	42	0	0	1	0
4	X	35	0	0	1	0
4	Y	32	0	0	2	0
All	All	11297	0	10828	229	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 10.

All (229) 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:130:GLU:HA	1:A:130:GLU:OE1	1.48	1.08
1:B:255:GLU:HG3	1:B:277:GLU:OE1	1.54	1.06
1:B:253:LEU:O	1:B:253:LEU:HD12	1.62	1.00
1:A:128:ASN:C	1:A:130:GLU:HB2	1.93	0.93
1:A:266:LEU:HD11	3:L:27:GLN:HE22	1.31	0.92
1:B:255:GLU:HG3	1:B:277:GLU:CD	1.94	0.90
3:Y:109:ARG:HG2	3:Y:110:THR:H	1.42	0.85
2:H:87:ARG:NH2	4:H:302:HOH:O	2.09	0.85
1:B:253:LEU:HD12	1:B:253:LEU:C	2.03	0.83
1:A:99:PHE:O	1:A:103:LEU:HG	1.83	0.78
2:X:225:LYS:NZ	2:X:227:GLU:HB2	1.99	0.78
3:Y:68:GLY:O	3:Y:69:THR:HG22	1.84	0.76
2:H:224:LYS:NZ	3:L:124:GLU:HG2	2.00	0.76
1:B:204:THR:O	1:B:205:SER:CB	2.30	0.74
2:H:224:LYS:HZ1	3:L:124:GLU:HG2	1.53	0.74
2:X:168:SER:OG	2:X:212:ASN:HB2	1.87	0.73
2:H:69:THR:HG22	2:H:82:GLN:HB3	1.71	0.73
3:Y:109:ARG:HG2	3:Y:110:THR:N	2.04	0.72
2:X:166:THR:HG22	2:X:214:ASN:HB3	1.72	0.72
1:A:189:LYS:HE3	1:A:215:GLN:HE21	1.54	0.71
1:A:240:ALA:CB	1:A:263:MET:HE1	2.21	0.71
1:B:204:THR:O	1:B:205:SER:HB3	1.90	0.71
3:Y:191:LYS:HA	3:Y:212:ARG:HD3	1.72	0.70
1:B:193:ASN:ND2	4:B:422:HOH:O	2.23	0.70
1:B:253:LEU:HD11	1:B:277:GLU:HG2	1.72	0.70
2:X:166:THR:CG2	2:X:214:ASN:HB3	2.21	0.70
3:L:6:GLN:NE2	3:L:86:TYR:O	2.20	0.69
1:A:240:ALA:HB3	1:A:263:MET:HE1	1.76	0.68
1:B:36:VAL:HG12	1:B:57:HIS:HB3	1.78	0.66
3:L:66:ARG:HG3	3:L:66:ARG:HH11	1.61	0.66
3:L:1:ASP:OD1	3:L:1:ASP:N	2.30	0.65
1:B:232:GLY:H	1:B:236:GLN:HE22	1.45	0.65
2:X:186:GLN:HA	3:Y:161:GLN:HE22	1.63	0.64
3:L:122:SER:OG	3:L:124:GLU:OE1	2.12	0.64
3:Y:152:ASP:HB3	4:Y:320:HOH:O	1.96	0.64
1:A:71:VAL:O	4:A:428:HOH:O	2.15	0.63
1:A:130:GLU:CG	1:A:136:LYS:CD	2.77	0.63
1:B:203:ILE:O	1:B:203:ILE:HG23	1.98	0.63
3:L:109:ARG:HG2	3:L:110:THR:H	1.64	0.62
2:H:69:THR:CG2	2:H:82:GLN:HB3	2.29	0.62
2:H:31:SER:OG	2:H:98:ARG:HD3	2.00	0.62
3:L:66:ARG:HG2	3:L:68:GLY:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:225:LYS:NZ	2:X:227:GLU:OE2	2.30	0.62
2:H:12:VAL:HG11	2:H:18:LEU:HD22	1.83	0.61
3:Y:109:ARG:CG	3:Y:110:THR:H	2.12	0.61
2:X:142:SER:H	2:X:145:SER:HB2	1.66	0.61
2:H:11:LEU:CD2	2:H:131:THR:HG23	2.31	0.61
1:B:36:VAL:HG21	1:B:79:LEU:HD23	1.83	0.60
3:L:35:TRP:HD1	3:L:48:ILE:HD11	1.67	0.60
3:Y:211:ASN:O	3:Y:212:ARG:HD2	2.02	0.59
1:B:218:ILE:HD13	1:B:308:MET:HE1	1.84	0.59
1:B:230:LYS:HG3	2:X:107:TRP:CE3	2.37	0.59
3:Y:66:ARG:HG2	3:Y:68:GLY:H	1.68	0.59
1:A:130:GLU:HG2	1:A:136:LYS:HE3	1.85	0.59
1:B:255:GLU:CG	1:B:277:GLU:CD	2.72	0.58
1:B:140:HIS:HB3	1:B:143:LEU:HD12	1.85	0.58
1:A:130:GLU:HG3	1:A:136:LYS:HD2	1.85	0.57
3:L:19:VAL:HG21	3:L:78:LEU:HD22	1.87	0.57
1:B:203:ILE:O	1:B:203:ILE:CG2	2.54	0.56
3:L:66:ARG:HG3	3:L:66:ARG:NH1	2.21	0.56
3:L:37:GLN:CD	3:L:47:LEU:HD21	2.31	0.55
2:H:104:ILE:HD12	2:H:114:ALA:HB3	1.88	0.55
2:X:142:SER:N	2:X:145:SER:HB2	2.21	0.55
1:B:233:THR:H	1:B:236:GLN:NE2	2.04	0.55
3:Y:109:ARG:CG	3:Y:110:THR:N	2.70	0.54
1:B:188:SER:HB3	1:B:301:ILE:HD13	1.89	0.54
3:Y:137:LEU:HD13	3:Y:176:LEU:HD22	1.88	0.54
1:A:240:ALA:HB1	1:A:263:MET:HE1	1.90	0.54
1:B:253:LEU:C	1:B:253:LEU:CD1	2.77	0.54
3:Y:106:GLU:HG3	3:Y:174:TYR:OH	2.08	0.54
2:H:142:SER:H	2:H:145:SER:HB2	1.72	0.54
2:X:159:ASP:HB3	2:X:190:LEU:HD13	1.88	0.54
2:H:11:LEU:HD22	2:H:131:THR:CG2	2.38	0.54
2:X:64:VAL:HB	2:X:68:PHE:CG	2.42	0.54
1:B:148:GLY:O	1:B:151:TYR:HB2	2.08	0.54
2:X:104:ILE:HD12	2:X:114:ALA:HB3	1.90	0.54
3:Y:66:ARG:CG	3:Y:68:GLY:H	2.21	0.54
3:Y:109:ARG:HH21	3:Y:173:THR:HG22	1.73	0.54
3:L:109:ARG:HG2	3:L:110:THR:N	2.22	0.54
3:Y:125:GLN:O	3:Y:128:SER:OG	2.25	0.53
1:B:35:VAL:HG12	1:B:56:ILE:HG23	1.91	0.53
1:A:148:GLY:O	1:A:151:TYR:HB2	2.07	0.53
1:A:130:GLU:HG3	1:A:136:LYS:CD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:225:LYS:HZ2	2:X:227:GLU:HB2	1.74	0.53
1:A:295:LYS:NZ	4:A:462:HOH:O	2.42	0.52
1:B:236:GLN:O	1:B:239:GLN:HG3	2.10	0.52
3:L:66:ARG:CG	3:L:68:GLY:H	2.22	0.52
3:L:106:GLU:HG2	3:L:107:ILE:N	2.25	0.51
1:B:232:GLY:H	1:B:236:GLN:NE2	2.07	0.51
3:Y:68:GLY:C	3:Y:69:THR:HG22	2.36	0.51
2:H:228:PRO:HD3	4:H:313:HOH:O	2.09	0.51
1:B:223:ILE:HG21	1:B:237:MET:HE2	1.93	0.51
2:H:99:GLN:HE22	2:H:113:GLU:HB3	1.75	0.51
2:X:57:TYR:CD2	2:X:59:TYR:CZ	2.99	0.51
1:A:251:HIS:HB2	1:A:274:ILE:HA	1.91	0.50
3:Y:68:GLY:O	3:Y:69:THR:CG2	2.55	0.50
3:Y:78:LEU:HD12	3:Y:79:GLN:H	1.77	0.50
1:A:67:HIS:HA	1:A:92:LEU:O	2.12	0.50
1:A:130:GLU:CG	1:A:136:LYS:HD3	2.41	0.50
2:X:225:LYS:HZ3	2:X:227:GLU:HB2	1.72	0.49
3:Y:125:GLN:HG2	3:Y:130:THR:O	2.12	0.49
1:A:119:SER:O	1:A:122:VAL:HG13	2.13	0.49
3:L:148:GLN:HG2	3:L:155:LEU:HD11	1.95	0.49
2:H:131:THR:HG22	2:H:162:PRO:HD3	1.94	0.49
1:B:264:GLU:HG2	1:B:269:GLU:O	2.12	0.49
3:L:2:ILE:HG12	3:L:27:GLN:HG2	1.94	0.49
3:Y:94:SER:N	4:Y:319:HOH:O	2.27	0.49
2:H:211:CYS:O	2:H:223:ASP:HA	2.13	0.48
1:A:132:GLY:HA3	2:X:71:SER:HB2	1.95	0.48
3:L:35:TRP:HB2	3:L:48:ILE:HG13	1.94	0.48
1:B:248:LYS:O	1:B:249:LEU:HD23	2.14	0.48
3:L:109:ARG:NH1	3:L:112:ALA:HB2	2.29	0.48
3:L:37:GLN:NE2	4:L:321:HOH:O	2.46	0.48
1:A:255:GLU:HB2	1:A:277:GLU:HB3	1.96	0.48
3:L:188:GLU:O	3:L:212:ARG:NH1	2.47	0.48
3:Y:144:GLU:O	3:Y:199:HIS:HD2	1.96	0.48
1:B:188:SER:CB	1:B:301:ILE:HD13	2.43	0.48
2:H:57:TYR:CD2	2:H:59:TYR:CZ	3.02	0.48
1:B:205:SER:HB3	1:B:254:VAL:HG23	1.96	0.47
1:B:253:LEU:O	1:B:253:LEU:CD1	2.48	0.47
1:B:145:LEU:HD11	1:B:184:LEU:HD23	1.96	0.47
2:H:115:MET:HE2	3:L:89:GLN:HE22	1.79	0.47
3:L:156:GLN:HG3	3:L:180:LEU:HD11	1.95	0.47
1:A:150:LYS:HE2	1:B:129:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:O	1:B:149:ILE:HG13	2.14	0.47
1:A:131:GLU:HG3	2:X:74:THR:HG23	1.96	0.47
1:A:213:SER:OG	1:A:220:PRO:HB3	2.14	0.47
1:A:296:MET:HG2	1:A:297:MET:HE2	1.96	0.47
1:B:146:ASP:OD2	1:B:215:GLN:HG3	2.15	0.46
2:H:99:GLN:NE2	2:H:113:GLU:HB3	2.31	0.46
3:L:211:ASN:O	3:L:213:GLY:N	2.46	0.46
3:Y:47:LEU:O	3:Y:48:ILE:HD12	2.15	0.46
3:Y:80:PRO:HB2	3:Y:169:SER:O	2.15	0.46
1:B:270:THR:O	1:B:275:PHE:N	2.48	0.46
3:L:64:GLY:HA2	3:L:72:THR:O	2.16	0.46
1:A:249:LEU:HB3	1:A:250:LYS:H	1.48	0.46
1:B:225:GLU:OE2	1:B:226:ILE:HG12	2.15	0.46
3:Y:106:GLU:HG2	3:Y:107:ILE:N	2.31	0.46
3:L:202:LEU:HD13	3:L:206:VAL:HG23	1.98	0.45
3:Y:37:GLN:HB2	3:Y:86:TYR:CE2	2.52	0.45
2:H:83:MET:HE2	2:H:86:LEU:HD21	1.97	0.45
1:B:174:GLY:O	1:B:178:ILE:HG13	2.17	0.45
1:B:148:GLY:HA3	1:B:293:TYR:OH	2.16	0.45
2:H:12:VAL:CG1	2:H:18:LEU:HD13	2.47	0.45
1:B:247:HIS:O	1:B:248:LYS:HB3	2.16	0.45
1:A:127:LEU:O	1:A:128:ASN:C	2.59	0.45
2:X:69:THR:HG22	4:X:310:HOH:O	2.17	0.45
3:L:18:ARG:HG3	3:L:76:SER:HA	1.99	0.45
2:H:224:LYS:HZ3	3:L:124:GLU:HG2	1.78	0.45
1:B:130:GLU:OE1	1:B:136:LYS:HG3	2.16	0.45
3:L:200:GLN:O	3:L:200:GLN:HG2	2.17	0.45
1:A:127:LEU:CD2	1:A:210:LYS:NZ	2.80	0.44
1:B:255:GLU:O	1:B:255:GLU:CD	2.60	0.44
1:B:304:VAL:CG1	1:B:308:MET:HE3	2.47	0.44
3:Y:39:LYS:HB2	3:Y:39:LYS:HE3	1.71	0.44
3:Y:64:GLY:HA2	3:Y:72:THR:O	2.17	0.44
1:A:99:PHE:CE2	1:A:103:LEU:HD11	2.51	0.44
1:A:230:LYS:HG3	2:H:107:TRP:CZ3	2.52	0.44
1:B:241:ILE:HD13	3:Y:94:SER:HA	1.99	0.44
3:Y:148:GLN:HG2	3:Y:155:LEU:HD11	1.99	0.44
1:A:127:LEU:CD2	1:A:210:LYS:HZ1	2.31	0.44
1:A:112:ASP:HB3	1:A:114:LYS:NZ	2.32	0.44
1:A:261:LYS:C	1:A:263:MET:H	2.24	0.44
1:A:130:GLU:HG2	1:A:136:LYS:CE	2.48	0.43
1:A:266:LEU:HD11	3:L:27:GLN:NE2	2.14	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LYS:HD2	1:A:47:LYS:HA	1.80	0.43
1:A:174:GLY:O	1:A:178:ILE:HG13	2.18	0.43
1:B:253:LEU:CD1	1:B:255:GLU:HB2	2.48	0.43
3:Y:109:ARG:HH22	3:Y:112:ALA:HB2	1.84	0.43
1:A:65:ASP:HA	1:A:66:PRO:HD3	1.92	0.43
1:A:248:LYS:O	1:A:249:LEU:HD23	2.18	0.43
1:A:279:TYR:HB2	1:A:296:MET:HG3	2.01	0.43
3:Y:147:VAL:HG22	3:Y:197:VAL:HG22	2.00	0.43
2:X:82:GLN:NE2	2:X:84:ASN:OD1	2.46	0.43
2:H:29:PHE:CZ	2:H:98:ARG:HD2	2.53	0.43
2:X:37:VAL:HG22	2:X:47:TRP:HA	2.01	0.43
3:L:66:ARG:HB3	3:L:70:ASP:O	2.19	0.43
1:A:131:GLU:HB2	2:X:74:THR:N	2.34	0.42
1:B:230:LYS:HG3	2:X:107:TRP:CZ3	2.54	0.42
1:B:249:LEU:HB3	1:B:250:LYS:H	1.48	0.42
2:H:67:ARG:HH11	2:H:67:ARG:HD2	1.72	0.42
1:A:99:PHE:O	1:A:103:LEU:CG	2.62	0.42
1:A:130:GLU:HG2	1:A:136:LYS:CD	2.48	0.42
1:A:71:VAL:HG13	1:A:75:ASP:HB2	2.00	0.42
1:B:103:LEU:HD23	1:B:103:LEU:HA	1.91	0.42
2:H:165:VAL:CG1	2:H:193:LEU:HD21	2.49	0.42
1:A:32:LYS:HE3	1:A:52:ASP:O	2.20	0.42
1:A:117:ALA:O	1:A:120:LYS:HB3	2.19	0.42
1:B:213:SER:HB3	1:B:218:ILE:O	2.20	0.42
2:X:137:PHE:HB2	2:X:156:LEU:HB3	2.02	0.42
3:L:78:LEU:HD12	3:L:79:GLN:H	1.84	0.42
3:Y:111:VAL:HG22	3:Y:142:PRO:HD3	2.01	0.42
2:H:12:VAL:CG1	2:H:18:LEU:HD22	2.48	0.42
1:A:148:GLY:HA3	1:A:293:TYR:OH	2.19	0.42
2:X:139:LEU:HB3	3:Y:119:PHE:CD1	2.55	0.42
1:B:143:LEU:HD21	1:B:280:THR:HA	2.02	0.42
3:L:55:TYR:O	3:L:58:VAL:HB	2.20	0.42
1:A:130:GLU:CB	1:A:136:LYS:HD3	2.50	0.41
2:X:34:ILE:HG12	2:X:98:ARG:HG2	2.01	0.41
2:H:161:PHE:HA	2:H:162:PRO:HA	1.74	0.41
3:L:19:VAL:CG2	3:L:78:LEU:HD22	2.49	0.41
2:X:161:PHE:HA	2:X:162:PRO:HA	1.85	0.41
3:L:137:LEU:HD13	3:L:176:LEU:HD22	2.02	0.41
1:A:49:VAL:HG11	1:A:156:GLN:HA	2.03	0.41
1:A:230:LYS:HG3	2:H:107:TRP:CE3	2.56	0.41
1:A:253:LEU:CD1	1:A:277:GLU:HG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:160:SER:HA	3:Y:179:THR:O	2.20	0.41
1:B:90:LEU:HA	1:B:137:GLN:NE2	2.35	0.41
3:Y:29:VAL:HG11	3:Y:90:GLN:HG3	2.03	0.41
1:A:188:SER:HB3	1:A:301:ILE:HD13	2.03	0.41
1:B:204:THR:O	1:B:254:VAL:CG2	2.69	0.41
3:L:37:GLN:HB3	3:L:86:TYR:CE2	2.56	0.41
1:A:237:MET:HB3	3:L:93:TYR:CD1	2.55	0.41
2:H:154:GLY:HA2	2:H:169:TRP:CH2	2.56	0.41
2:X:118:TRP:CE3	3:Y:44:PRO:HD2	2.55	0.41
1:A:49:VAL:CG2	1:A:152:VAL:HG13	2.51	0.41
1:B:110:LEU:HD12	1:B:110:LEU:HA	1.89	0.41
2:H:11:LEU:CD2	2:H:131:THR:CG2	2.95	0.41
1:A:237:MET:HB3	1:A:237:MET:HE3	1.98	0.40
2:X:47:TRP:CZ3	3:Y:96:PRO:HB3	2.56	0.40
2:X:229:LYS:HD3	2:X:229:LYS:HA	1.81	0.40
3:L:35:TRP:CD2	3:L:73:LEU:HB2	2.56	0.40
3:Y:23:CYS:HB2	3:Y:35:TRP:CH2	2.56	0.40
1:A:40:SER:HB2	1:A:283:ILE:HD13	2.02	0.40
1:A:35:VAL:HG12	1:A:56:ILE:HG23	2.04	0.40
1:A:99:PHE:CZ	1:A:103:LEU:HD21	2.56	0.40
1:A:126:TYR:CG	1:A:131:GLU:HA	2.56	0.40
2:X:9:GLY:HA3	2:X:122:THR:OG1	2.21	0.40
3:L:125:GLN:HG2	3:L:130:THR:O	2.21	0.40

All (2) 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:B:198:GLU:OE1	4:H:302:HOH:O[2_545]	1.21	0.99
1:B:198:GLU:CD	4:H:302:HOH:O[2_545]	2.03	0.17

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	267/291 (92%)	247 (92%)	17 (6%)	3 (1%)	11	29
1	B	270/291 (93%)	251 (93%)	18 (7%)	1 (0%)	30	54
2	H	225/238 (94%)	215 (96%)	10 (4%)	0	100	100
2	X	225/238 (94%)	214 (95%)	11 (5%)	0	100	100
3	L	211/216 (98%)	197 (93%)	13 (6%)	1 (0%)	24	48
3	Y	211/216 (98%)	193 (92%)	18 (8%)	0	100	100
All	All	1409/1490 (95%)	1317 (94%)	87 (6%)	5 (0%)	30	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	GLU
1	A	235	GLU
1	A	248	LYS
1	B	248	LYS
3	L	212	ARG

5.3.2 Protein sidechains ⓘ

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	242/255 (95%)	236 (98%)	6 (2%)	42	71
1	B	242/255 (95%)	237 (98%)	5 (2%)	47	75
2	H	188/199 (94%)	184 (98%)	4 (2%)	47	75
2	X	188/199 (94%)	184 (98%)	4 (2%)	47	75
3	L	188/191 (98%)	184 (98%)	4 (2%)	47	75
3	Y	188/191 (98%)	184 (98%)	4 (2%)	47	75
All	All	1236/1290 (96%)	1209 (98%)	27 (2%)	45	74

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

Mol	Chain	Res	Type
1	A	56	ILE
1	A	122	VAL
1	A	130	GLU
1	A	244	VAL
1	A	254	VAL
1	A	283	ILE
1	B	203	ILE
1	B	204	THR
1	B	254	VAL
1	B	261	LYS
1	B	280	THR
2	H	57	TYR
2	H	153	LEU
2	H	184	VAL
2	H	208	THR
2	X	69	THR
2	X	74	THR
2	X	184	VAL
2	X	229	LYS
3	L	1	ASP
3	L	48	ILE
3	L	75	ILE
3	L	189	LYS
3	Y	39	LYS
3	Y	48	ILE
3	Y	75	ILE
3	Y	90	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	173	GLN
1	A	215	GLN
1	A	231	GLN
1	A	251	HIS
1	B	48	ASN
1	B	53	ASN
1	B	64	GLN
1	B	231	GLN
1	B	236	GLN
2	H	39	GLN
2	H	99	GLN

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Mol	Chain	Res	Type
2	X	39	GLN
2	X	77	ASN
3	L	27	GLN
3	L	38	GLN
3	L	89	GLN
3	L	138	ASN
3	L	148	GLN
3	Y	27	GLN
3	Y	38	GLN
3	Y	79	GLN
3	Y	153	ASN
3	Y	161	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](#)

There are no ligands in this entry.

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	273/291 (93%)	-0.05	9 (3%)	49	45	3, 14, 48, 96	0
1	B	274/291 (94%)	-0.11	8 (2%)	53	50	4, 15, 49, 69	0
2	H	227/238 (95%)	0.11	11 (4%)	35	32	3, 20, 78, 110	0
2	X	227/238 (95%)	0.30	21 (9%)	14	12	2, 19, 77, 118	0
3	L	213/216 (98%)	0.07	6 (2%)	55	51	5, 20, 53, 64	0
3	Y	213/216 (98%)	0.07	5 (2%)	61	58	3, 23, 55, 67	0
All	All	1427/1490 (95%)	0.06	60 (4%)	40	37	2, 18, 57, 118	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	X	145	SER	6.1
2	H	229	LYS	5.5
3	L	37	GLN	5.5
2	X	144	LYS	4.8
2	X	143	SER	4.8
3	Y	67	SER	4.8
2	H	144	LYS	4.7
3	L	67	SER	4.6
2	X	148	GLY	4.2
3	L	68	GLY	4.0
2	X	207	GLN	3.9
1	B	123	LYS	3.9
3	L	213	GLY	3.7
3	Y	109	ARG	3.5
2	H	145	SER	3.4
2	H	205	GLY	3.2
2	X	146	THR	3.2
2	X	142	SER	3.2
2	H	203	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	263	MET	3.1
2	X	205	GLY	3.1
1	B	227	ASN	3.1
1	B	260	LYS	3.0
1	B	255	GLU	3.0
1	B	114	LYS	3.0
1	B	134	LYS	3.0
1	A	130	GLU	2.9
2	H	98	ARG	2.8
2	X	229	LYS	2.8
2	X	211	CYS	2.7
2	H	147	SER	2.7
3	Y	213	GLY	2.6
2	X	147	SER	2.6
3	Y	66	ARG	2.5
1	A	251	HIS	2.5
2	X	168	SER	2.5
2	H	207	GLN	2.5
1	A	133	ASN	2.4
3	Y	1	ASP	2.4
1	A	261	LYS	2.4
3	L	189	LYS	2.4
1	A	132	GLY	2.4
2	X	98	ARG	2.4
1	A	255	GLU	2.4
2	H	149	GLY	2.4
1	B	248	LYS	2.3
2	H	143	SER	2.3
2	X	206	THR	2.3
2	X	3	GLN	2.3
2	X	221	LYS	2.2
2	X	151	ALA	2.2
2	X	89	GLU	2.2
2	X	210	ILE	2.2
1	B	198	GLU	2.1
2	X	203	SER	2.1
1	A	262	ALA	2.1
2	X	201	SER	2.1
3	L	66	ARG	2.1
2	H	206	THR	2.1
1	A	256	THR	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.