



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:35 AM UTC

PDB ID : 3KZG / pdb_00003kzg
Title : Crystal structure of an arginine 3rd transport system periplasmic binding protein from *Legionella pneumophila*
Authors : Palani, K.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-12-08
Resolution : 2.06 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)
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

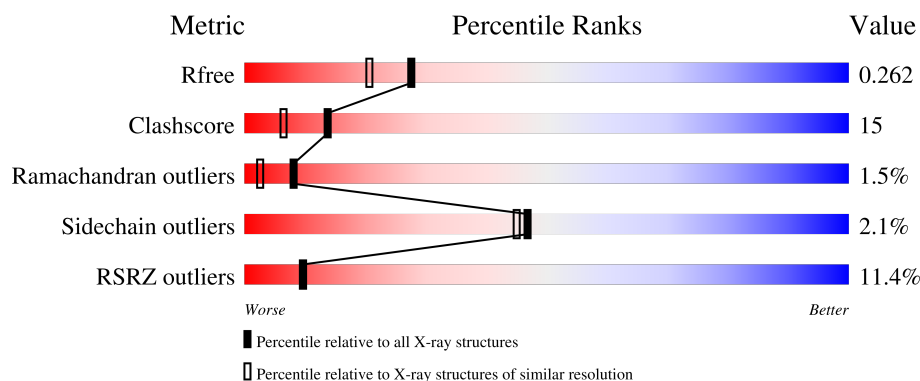
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	237	8% 66% 30% .
1	B	237	9% 73% 22% ..
1	C	237	11% 73% 19% ..
1	D	237	14% 67% 26% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7786 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 Arginine 3rd transport system periplasmic binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	Se	0	0	0
			1851	1196	298	347	2	8			
1	B	228	Total	C	N	O	S	Se	0	0	0
			1851	1196	298	347	2	8			
1	C	228	Total	C	N	O	S	Se	0	0	0
			1851	1196	298	347	2	8			
1	D	228	Total	C	N	O	S	Se	0	0	0
			1851	1196	298	347	2	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MSE	-	expression tag	UNP Q5ZV85
A	246	GLU	-	expression tag	UNP Q5ZV85
A	247	GLY	-	expression tag	UNP Q5ZV85
A	248	HIS	-	expression tag	UNP Q5ZV85
A	249	HIS	-	expression tag	UNP Q5ZV85
A	250	HIS	-	expression tag	UNP Q5ZV85
A	251	HIS	-	expression tag	UNP Q5ZV85
A	252	HIS	-	expression tag	UNP Q5ZV85
A	253	HIS	-	expression tag	UNP Q5ZV85
B	17	MSE	-	expression tag	UNP Q5ZV85
B	246	GLU	-	expression tag	UNP Q5ZV85
B	247	GLY	-	expression tag	UNP Q5ZV85
B	248	HIS	-	expression tag	UNP Q5ZV85
B	249	HIS	-	expression tag	UNP Q5ZV85
B	250	HIS	-	expression tag	UNP Q5ZV85
B	251	HIS	-	expression tag	UNP Q5ZV85
B	252	HIS	-	expression tag	UNP Q5ZV85
B	253	HIS	-	expression tag	UNP Q5ZV85
C	17	MSE	-	expression tag	UNP Q5ZV85
C	246	GLU	-	expression tag	UNP Q5ZV85
C	247	GLY	-	expression tag	UNP Q5ZV85

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Chain	Residue	Modelled	Actual	Comment	Reference
C	248	HIS	-	expression tag	UNP Q5ZV85
C	249	HIS	-	expression tag	UNP Q5ZV85
C	250	HIS	-	expression tag	UNP Q5ZV85
C	251	HIS	-	expression tag	UNP Q5ZV85
C	252	HIS	-	expression tag	UNP Q5ZV85
C	253	HIS	-	expression tag	UNP Q5ZV85
D	17	MSE	-	expression tag	UNP Q5ZV85
D	246	GLU	-	expression tag	UNP Q5ZV85
D	247	GLY	-	expression tag	UNP Q5ZV85
D	248	HIS	-	expression tag	UNP Q5ZV85
D	249	HIS	-	expression tag	UNP Q5ZV85
D	250	HIS	-	expression tag	UNP Q5ZV85
D	251	HIS	-	expression tag	UNP Q5ZV85
D	252	HIS	-	expression tag	UNP Q5ZV85
D	253	HIS	-	expression tag	UNP Q5ZV85

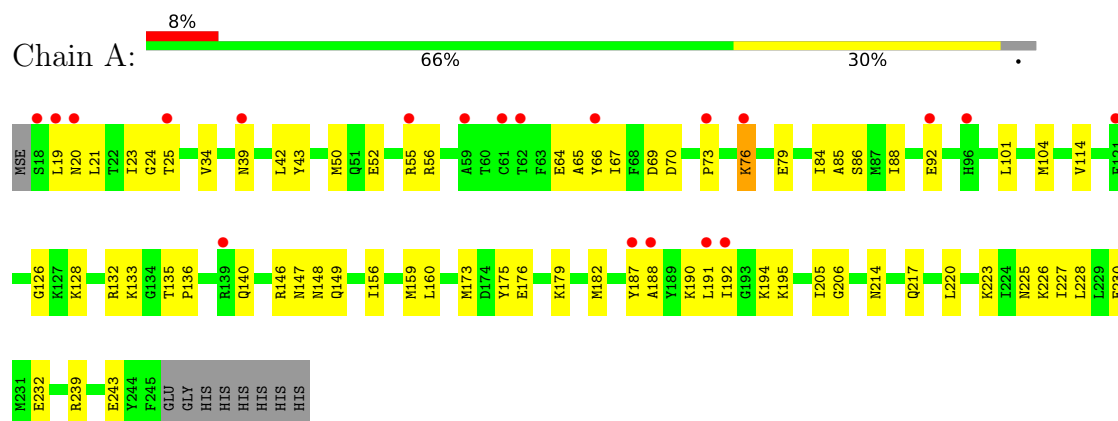
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	80	Total O 80 80	0	0
2	B	125	Total O 125 125	0	0
2	C	94	Total O 94 94	0	0
2	D	83	Total O 83 83	0	0

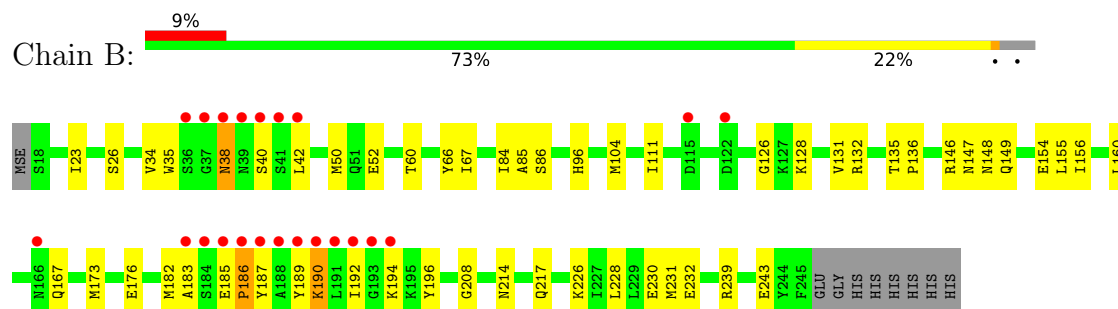
3 Residue-property plots [i](#)

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.

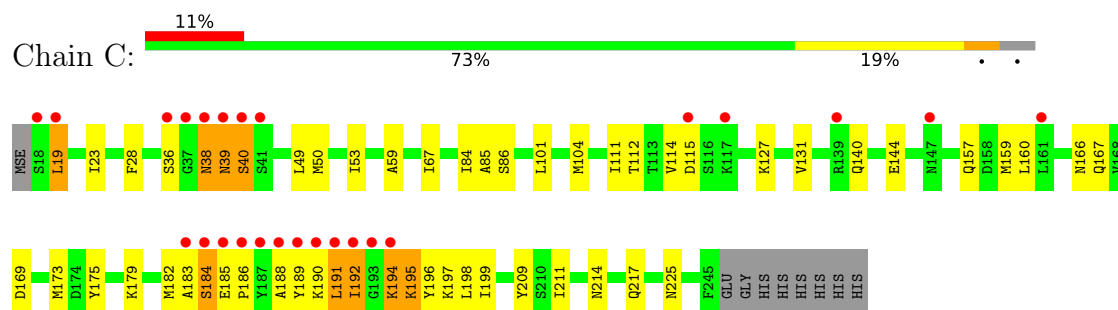
- Molecule 1: Arginine 3rd transport system periplasmic binding protein



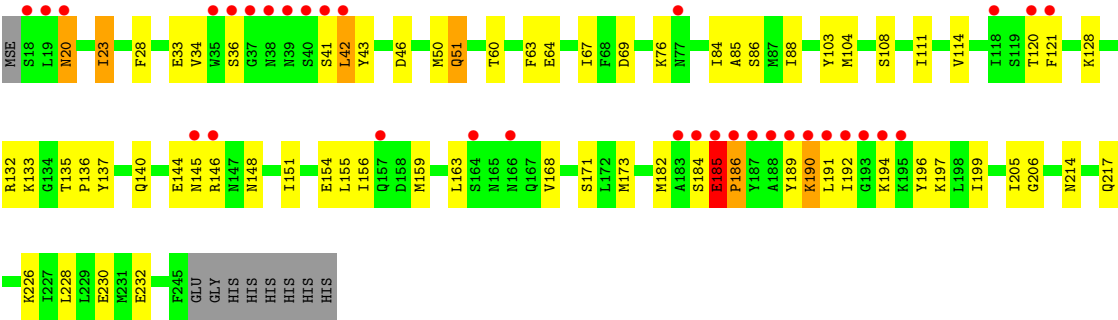
- Molecule 1: Arginine 3rd transport system periplasmic binding protein



- Molecule 1: Arginine 3rd transport system periplasmic binding protein



- Molecule 1: Arginine 3rd transport system periplasmic binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	41.97Å 148.25Å 149.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.31 – 2.06 41.31 – 2.06	Depositor EDS
% Data completeness (in resolution range)	98.7 (41.31-2.06) 98.8 (41.31-2.06)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.35 (at 2.06Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.262 0.222 , 0.262	Depositor DCC
R_{free} test set	2925 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7786	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 17.92% 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](#)

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	0.38	0/1883	0.81	2/2527 (0.1%)
1	B	0.46	0/1883	0.87	5/2527 (0.2%)
1	C	0.42	0/1883	0.84	4/2527 (0.2%)
1	D	0.39	0/1883	0.84	2/2527 (0.1%)
All	All	0.41	0/7532	0.84	13/10108 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	67	ILE	N-CA-C	-8.91	98.17	109.30
1	D	67	ILE	N-CA-C	-8.32	98.90	109.30
1	B	67	ILE	N-CA-C	-8.20	97.83	109.63
1	A	67	ILE	N-CA-C	-7.10	100.42	109.30
1	B	183	ALA	N-CA-C	-7.08	103.95	112.59
1	B	208	GLY	N-CA-C	5.70	117.37	111.95
1	D	28	PHE	N-CA-C	5.53	117.11	107.49
1	C	166	ASN	N-CA-C	5.46	119.24	112.47
1	C	28	PHE	N-CA-C	5.27	116.66	107.49
1	C	167	GLN	N-CA-C	-5.20	105.79	111.82
1	B	60	THR	N-CA-C	-5.16	103.23	110.50
1	A	79	GLU	N-CA-C	-5.16	106.25	112.54
1	B	167	GLN	N-CA-C	-5.07	106.60	112.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1851	0	1847	60	0
1	B	1851	0	1847	45	0
1	C	1851	0	1847	63	0
1	D	1851	0	1847	58	0
2	A	80	0	0	1	0
2	B	125	0	0	6	0
2	C	94	0	0	1	0
2	D	83	0	0	2	0
All	All	7786	0	7388	215	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 (215) 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:146:ARG:HG3	1:A:148:ASN:ND2	1.82	0.94
1:C:50:MSE:HE2	1:C:84:ILE:HB	1.49	0.92
1:D:159:MSE:HE3	1:D:173:MSE:HE2	1.52	0.91
1:B:111:ILE:HG21	1:B:173:MSE:HE3	1.55	0.89
1:A:34:VAL:HG21	1:A:43:TYR:CZ	2.08	0.88
1:A:104:MSE:HE1	1:A:176:GLU:HG3	1.62	0.81
1:D:50:MSE:HE2	1:D:84:ILE:HB	1.62	0.80
1:C:36:SER:HB2	1:C:39:ASN:HD21	1.48	0.79
1:B:228:LEU:O	1:B:232:GLU:HG3	1.84	0.77
1:B:111:ILE:CG2	1:B:173:MSE:HE3	2.14	0.77
1:C:104:MSE:HE2	1:C:209:TYR:CE2	2.21	0.76
1:C:182:MSE:HE3	1:C:198:LEU:CD2	2.14	0.76
1:D:214:ASN:H	1:D:217:GLN:HE21	1.33	0.76
1:D:163:LEU:HD12	1:D:168:VAL:HG23	1.68	0.76
1:C:50:MSE:HE2	1:C:84:ILE:CB	2.15	0.75
1:B:160:LEU:HD21	1:B:173:MSE:HE1	1.67	0.75
1:D:186:PRO:HG2	1:D:192:ILE:HG21	1.68	0.75
1:A:188:ALA:HA	1:B:190:LYS:HG2	1.69	0.74
1:C:214:ASN:H	1:C:217:GLN:HE21	1.37	0.72
1:B:189:TYR:HA	1:B:192:ILE:HB	1.71	0.72
1:C:50:MSE:HE2	1:C:84:ILE:CG2	2.20	0.72
1:A:239:ARG:O	1:A:243:GLU:HG3	1.90	0.71
1:A:146:ARG:HG3	1:A:148:ASN:HD21	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:MSE:CE	1:A:84:ILE:HB	2.22	0.70
1:B:194:LYS:HB3	2:B:319:HOH:O	1.90	0.70
1:A:228:LEU:O	1:A:232:GLU:HG3	1.93	0.68
1:C:36:SER:O	1:D:190:LYS:HD3	1.94	0.67
1:D:214:ASN:H	1:D:217:GLN:NE2	1.92	0.67
1:D:228:LEU:O	1:D:232:GLU:HG3	1.94	0.67
1:C:39:ASN:HB3	1:D:190:LYS:HD2	1.77	0.67
1:A:226:LYS:O	1:A:230:GLU:HG3	1.95	0.67
1:C:50:MSE:CE	1:C:84:ILE:HB	2.21	0.67
1:C:111:ILE:HG13	1:C:182:MSE:HE1	1.78	0.66
1:C:36:SER:HB2	1:C:39:ASN:ND2	2.10	0.65
1:D:189:TYR:CD2	1:D:194:LYS:HE3	2.31	0.65
1:A:50:MSE:HE2	1:A:84:ILE:HB	1.77	0.65
1:A:76:LYS:HB2	1:A:76:LYS:NZ	2.12	0.64
1:D:23:ILE:N	1:D:23:ILE:HD12	2.12	0.64
1:C:175:TYR:CZ	1:C:179:LYS:HD2	2.34	0.64
1:A:188:ALA:O	1:A:192:ILE:HG22	1.99	0.63
1:A:56:ARG:HB3	1:A:227:ILE:HD12	1.81	0.62
1:C:159:MSE:HE3	1:C:173:MSE:HE2	1.81	0.62
1:A:214:ASN:H	1:A:217:GLN:HE21	1.48	0.62
1:A:52:GLU:OE1	1:A:55:ARG:HD3	2.00	0.62
1:C:182:MSE:HE3	1:C:198:LEU:HD23	1.82	0.61
1:D:189:TYR:HD2	1:D:194:LYS:HE3	1.65	0.61
1:C:214:ASN:H	1:C:217:GLN:NE2	1.99	0.60
1:C:39:ASN:HD22	1:C:40:SER:N	2.00	0.60
1:D:34:VAL:HG11	1:D:43:TYR:CZ	2.36	0.60
1:A:132:ARG:HD2	1:A:156:ILE:HD11	1.83	0.59
1:B:214:ASN:H	1:B:217:GLN:HE21	1.48	0.59
1:C:104:MSE:HE2	1:C:209:TYR:HE2	1.68	0.58
1:B:50:MSE:CE	1:B:84:ILE:HB	2.34	0.58
1:C:19:LEU:HD12	1:C:59:ALA:HB2	1.85	0.58
1:B:38:ASN:C	1:B:40:SER:H	2.11	0.58
1:C:190:LYS:HG2	1:D:36:SER:O	2.04	0.58
1:D:108:SER:HB3	1:D:137:TYR:CE1	2.39	0.57
1:A:34:VAL:HG21	1:A:43:TYR:CE2	2.40	0.57
1:D:50:MSE:CE	1:D:84:ILE:HB	2.32	0.57
1:D:189:TYR:HD1	1:D:189:TYR:H	1.52	0.57
1:D:140:GLN:O	1:D:144:GLU:HG3	2.04	0.56
1:A:23:ILE:N	1:A:23:ILE:HD12	2.20	0.56
1:A:159:MSE:HE3	1:A:173:MSE:HE2	1.86	0.56
1:A:92:GLU:HG3	2:A:302:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ASN:CB	1:D:190:LYS:HD2	2.36	0.56
1:D:50:MSE:HE2	1:D:84:ILE:CB	2.33	0.56
1:C:50:MSE:HE1	1:C:211:ILE:HG23	1.88	0.55
1:D:226:LYS:O	1:D:230:GLU:HG3	2.05	0.55
1:C:185:GLU:HG3	1:C:195:LYS:HG3	1.89	0.55
1:A:25:THR:O	1:A:65:ALA:HA	2.07	0.55
1:D:128:LYS:HB3	1:D:151:ILE:HD12	1.88	0.55
1:A:128:LYS:NZ	1:A:149:GLN:NE2	2.55	0.55
1:B:146:ARG:HB2	1:B:148:ASN:HD21	1.72	0.55
1:C:111:ILE:HD11	1:C:196:TYR:HB3	1.88	0.55
1:D:69:ASP:OD1	1:D:133:LYS:HE2	2.08	0.54
1:B:214:ASN:H	1:B:217:GLN:NE2	2.06	0.53
1:B:35:TRP:HD1	1:B:42:LEU:HG	1.73	0.53
1:B:154:GLU:C	1:B:155:LEU:HD12	2.34	0.53
1:C:39:ASN:HD22	1:C:39:ASN:N	2.05	0.53
1:D:85:ALA:O	1:D:86:SER:C	2.52	0.53
1:A:192:ILE:HG12	1:A:192:ILE:O	2.09	0.53
1:C:160:LEU:HD21	1:C:173:MSE:HE1	1.91	0.53
1:D:120:THR:HG22	1:D:121:PHE:N	2.24	0.53
1:D:190:LYS:HG3	1:D:191:LEU:N	2.24	0.52
1:A:190:LYS:HB3	1:A:191:LEU:HD12	1.90	0.52
1:D:154:GLU:C	1:D:155:LEU:HD12	2.35	0.52
1:A:84:ILE:HG23	1:A:84:ILE:O	2.09	0.52
1:B:85:ALA:O	1:B:86:SER:C	2.52	0.52
1:A:190:LYS:HB2	1:B:190:LYS:NZ	2.24	0.52
1:B:52:GLU:HG2	1:B:231:MSE:HE3	1.92	0.52
1:B:190:LYS:NZ	1:B:190:LYS:HB2	2.25	0.52
1:D:41:SER:HA	2:D:334:HOH:O	2.10	0.52
1:D:197:LYS:HE3	1:D:199:ILE:HD11	1.91	0.52
1:A:191:LEU:HD12	1:A:191:LEU:N	2.25	0.51
1:D:189:TYR:HB2	1:D:194:LYS:HG2	1.92	0.51
1:A:214:ASN:H	1:A:217:GLN:NE2	2.08	0.51
1:B:186:PRO:HD2	1:B:189:TYR:HB3	1.91	0.51
1:B:96:HIS:HD2	2:B:348:HOH:O	1.94	0.51
1:B:104:MSE:HE1	1:B:176:GLU:HG3	1.93	0.51
1:A:85:ALA:O	1:A:86:SER:C	2.54	0.50
1:A:52:GLU:O	1:A:55:ARG:HG2	2.10	0.50
1:C:114:VAL:HG11	1:C:194:LYS:N	2.26	0.50
1:C:140:GLN:O	1:C:144:GLU:HG3	2.11	0.50
1:A:20:ASN:HD22	1:A:21:LEU:N	2.09	0.50
1:A:126:GLY:HA2	1:A:147:ASN:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:TRP:HB2	1:B:42:LEU:HD21	1.93	0.50
1:B:182:MSE:HG2	2:B:319:HOH:O	2.11	0.50
1:A:34:VAL:HG21	1:A:43:TYR:CE1	2.45	0.49
1:C:194:LYS:O	1:C:195:LYS:HB2	2.11	0.49
1:C:39:ASN:HD22	1:C:40:SER:H	1.58	0.49
1:C:104:MSE:HE2	1:C:209:TYR:CD2	2.48	0.49
1:C:185:GLU:HG2	1:C:196:TYR:CE2	2.47	0.49
1:C:85:ALA:O	1:C:86:SER:C	2.55	0.49
1:D:185:GLU:HG2	2:D:329:HOH:O	2.10	0.49
1:A:146:ARG:CG	1:A:148:ASN:HD21	2.23	0.49
1:A:160:LEU:HD21	1:A:173:MSE:HE1	1.95	0.48
1:A:50:MSE:HE2	1:A:84:ILE:CB	2.42	0.48
1:B:23:ILE:N	1:B:23:ILE:HD12	2.28	0.48
1:C:114:VAL:HG21	1:C:194:LYS:HB3	1.94	0.48
1:D:132:ARG:HD2	1:D:156:ILE:HD11	1.96	0.48
1:D:163:LEU:HD12	1:D:168:VAL:CG2	2.41	0.48
1:A:188:ALA:HB1	1:A:191:LEU:HD13	1.94	0.48
1:A:34:VAL:HG23	1:A:34:VAL:O	2.14	0.48
1:A:220:LEU:HA	1:A:223:LYS:CE	2.44	0.48
1:A:135:THR:HB	1:A:136:PRO:HD2	1.95	0.48
1:A:146:ARG:HG3	1:A:148:ASN:HD22	1.74	0.48
1:D:182:MSE:SE	1:D:182:MSE:C	3.06	0.48
1:C:197:LYS:HE3	1:C:199:ILE:HD11	1.95	0.48
1:A:88:ILE:CG2	1:A:206:GLY:HA3	2.44	0.47
1:A:114:VAL:HG13	1:A:195:LYS:C	2.39	0.47
1:C:182:MSE:HE3	1:C:198:LEU:CG	2.44	0.47
1:C:191:LEU:O	1:C:192:ILE:HB	2.13	0.47
1:D:121:PHE:O	1:D:146:ARG:NH2	2.43	0.47
1:D:163:LEU:HD11	1:D:171:SER:OG	2.14	0.47
1:A:175:TYR:OH	1:A:179:LYS:HD2	2.15	0.47
1:C:39:ASN:H	1:D:190:LYS:HD2	1.79	0.47
1:C:182:MSE:HE3	1:C:198:LEU:HG	1.96	0.47
1:C:111:ILE:HG21	1:C:173:MSE:HE3	1.97	0.47
1:C:127:LYS:HD2	1:C:169:ASP:CG	2.40	0.47
1:D:76:LYS:HA	1:D:214:ASN:HD21	1.80	0.47
1:C:19:LEU:HD12	1:C:59:ALA:CB	2.45	0.47
1:D:50:MSE:HE2	1:D:84:ILE:CG2	2.45	0.47
1:A:140:GLN:OE1	1:A:205:ILE:HD12	2.15	0.47
1:C:190:LYS:N	1:C:190:LYS:HD2	2.30	0.47
1:B:50:MSE:HE2	1:B:84:ILE:HB	1.97	0.46
1:B:226:LYS:HE3	2:B:344:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:VAL:HG11	1:C:194:LYS:H	1.80	0.46
1:B:146:ARG:HB2	1:B:148:ASN:ND2	2.30	0.46
1:C:191:LEU:HD13	1:C:191:LEU:N	2.31	0.46
1:A:42:LEU:N	1:A:42:LEU:HD12	2.30	0.46
1:B:131:VAL:HG11	2:B:350:HOH:O	2.15	0.46
1:D:103:TYR:O	1:D:104:MSE:HB3	2.15	0.46
1:D:20:ASN:HA	1:D:60:THR:OG1	2.15	0.46
1:A:64:GLU:HG2	1:A:66:TYR:CE2	2.51	0.46
1:A:179:LYS:HE2	1:A:179:LYS:HB3	1.85	0.45
1:C:182:MSE:SE	1:C:197:LYS:HA	2.66	0.45
1:C:157:GLN:HG3	2:C:264:HOH:O	2.17	0.45
1:B:189:TYR:O	1:B:190:LYS:C	2.58	0.45
1:B:190:LYS:HB2	1:B:190:LYS:HZ3	1.81	0.45
1:C:38:ASN:CG	1:D:190:LYS:HE3	2.42	0.45
1:A:104:MSE:CE	1:A:176:GLU:HG3	2.42	0.45
1:B:185:GLU:HA	1:B:186:PRO:HA	1.83	0.44
1:C:39:ASN:N	1:D:190:LYS:HD2	2.32	0.44
1:C:188:ALA:C	1:C:190:LYS:H	2.25	0.44
1:C:183:ALA:O	1:C:184:SER:HB3	2.18	0.44
1:D:23:ILE:N	1:D:23:ILE:CD1	2.81	0.44
1:D:111:ILE:HD11	1:D:196:TYR:HB3	1.98	0.44
1:C:127:LYS:HD2	1:C:169:ASP:CB	2.48	0.43
1:A:24:GLY:HA2	1:A:64:GLU:O	2.18	0.43
1:A:101:LEU:HG	1:A:225:ASN:CG	2.43	0.43
1:B:239:ARG:O	1:B:243:GLU:HG2	2.17	0.43
1:D:111:ILE:CG2	1:D:173:MSE:HE3	2.49	0.43
1:D:51:GLN:OE1	1:D:63:PHE:HE2	2.01	0.43
1:C:39:ASN:ND2	1:C:40:SER:N	2.66	0.43
1:A:76:LYS:HB2	1:A:76:LYS:HZ3	1.83	0.43
1:D:135:THR:HB	1:D:136:PRO:HD2	2.01	0.43
1:B:128:LYS:HE2	1:B:149:GLN:NE2	2.33	0.43
1:C:111:ILE:HG12	1:C:112:THR:N	2.34	0.43
1:A:220:LEU:HA	1:A:223:LYS:HE3	2.00	0.42
1:D:111:ILE:HG21	1:D:173:MSE:HE3	2.01	0.42
1:D:184:SER:O	1:D:185:GLU:O	2.37	0.42
1:C:50:MSE:HE2	1:C:84:ILE:HG21	1.99	0.42
1:D:33:GLU:OE1	1:D:46:ASP:OD2	2.38	0.42
1:B:126:GLY:HA2	1:B:147:ASN:O	2.19	0.42
1:D:114:VAL:HA	1:D:197:LYS:HD3	2.02	0.42
1:D:146:ARG:HB2	1:D:148:ASN:ND2	2.33	0.42
1:A:69:ASP:OD1	1:A:133:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LYS:HB2	1:A:76:LYS:HZ2	1.85	0.42
1:B:192:ILE:HG22	1:B:192:ILE:O	2.20	0.42
1:A:190:LYS:HB2	1:B:190:LYS:HZ1	1.84	0.42
1:B:34:VAL:O	1:B:42:LEU:HD23	2.19	0.42
1:A:70:ASP:O	1:A:73:PRO:HG2	2.20	0.42
1:B:111:ILE:HG21	1:B:173:MSE:CE	2.39	0.42
1:C:39:ASN:ND2	1:C:39:ASN:N	2.68	0.42
1:C:101:LEU:HG	1:C:225:ASN:CG	2.44	0.41
1:C:185:GLU:HG3	1:C:195:LYS:HE3	2.01	0.41
1:B:185:GLU:HG2	1:B:196:TYR:CE2	2.56	0.41
1:B:132:ARG:HD2	1:B:156:ILE:HD11	2.02	0.41
1:C:84:ILE:HG23	1:C:84:ILE:O	2.21	0.41
1:D:159:MSE:O	1:D:163:LEU:HD13	2.20	0.41
1:B:26:SER:HA	1:B:66:TYR:O	2.20	0.41
1:B:38:ASN:C	1:B:40:SER:N	2.77	0.41
1:A:182:MSE:HE3	1:A:194:LYS:NZ	2.36	0.41
1:D:88:ILE:CG2	1:D:206:GLY:HA3	2.50	0.41
1:A:128:LYS:HZ2	1:A:149:GLN:NE2	2.18	0.41
1:D:84:ILE:O	1:D:84:ILE:HG23	2.20	0.41
1:B:148:ASN:ND2	2:B:359:HOH:O	2.54	0.41
1:C:49:LEU:O	1:C:53:ILE:HG13	2.21	0.41
1:C:114:VAL:HG13	1:C:115:ASP:N	2.36	0.41
1:D:42:LEU:H	1:D:42:LEU:HD12	1.85	0.41
1:B:226:LYS:O	1:B:230:GLU:HG3	2.21	0.40
1:C:23:ILE:HD12	1:C:23:ILE:N	2.35	0.40
1:A:34:VAL:CG2	1:A:43:TYR:CE2	3.04	0.40
1:C:39:ASN:HB3	1:D:190:LYS:HB3	2.03	0.40
1:B:135:THR:HB	1:B:136:PRO:HD2	2.04	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	226/237 (95%)	216 (96%)	10 (4%)	0	100	100
1	B	226/237 (95%)	213 (94%)	11 (5%)	2 (1%)	14	7
1	C	226/237 (95%)	204 (90%)	14 (6%)	8 (4%)	3	0
1	D	226/237 (95%)	206 (91%)	16 (7%)	4 (2%)	6	2
All	All	904/948 (95%)	839 (93%)	51 (6%)	14 (2%)	8	2

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	38	ASN
1	C	194	LYS
1	D	186	PRO
1	D	185	GLU
1	B	38	ASN
1	C	195	LYS
1	C	184	SER
1	C	40	SER
1	C	189	TYR
1	C	192	ILE
1	D	20	ASN
1	D	190	LYS
1	B	186	PRO
1	C	186	PRO

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	204/203 (100%)	200 (98%)	4 (2%)	48	47
1	B	204/203 (100%)	202 (99%)	2 (1%)	68	71
1	C	204/203 (100%)	200 (98%)	4 (2%)	48	47
1	D	204/203 (100%)	197 (97%)	7 (3%)	32	27
All	All	816/812 (100%)	799 (98%)	17 (2%)	47	45

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	39	ASN
1	A	76	LYS
1	A	187	TYR
1	B	187	TYR
1	B	190	LYS
1	C	19	LEU
1	C	39	ASN
1	C	131	VAL
1	C	191	LEU
1	D	23	ILE
1	D	42	LEU
1	D	51	GLN
1	D	64	GLU
1	D	145	ASN
1	D	185	GLU
1	D	205	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	39	ASN
1	A	107	ASN
1	A	109	GLN
1	A	148	ASN
1	A	149	GLN
1	A	165	ASN
1	A	214	ASN
1	A	217	GLN
1	B	39	ASN
1	B	96	HIS
1	B	107	ASN
1	B	125	HIS
1	B	148	ASN
1	B	149	GLN
1	B	165	ASN
1	B	214	ASN
1	B	217	GLN
1	C	39	ASN
1	C	125	HIS

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Mol	Chain	Res	Type
1	C	145	ASN
1	C	167	GLN
1	C	214	ASN
1	C	217	GLN
1	D	39	ASN
1	D	96	HIS
1	D	107	ASN
1	D	166	ASN
1	D	167	GLN
1	D	214	ASN
1	D	217	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	220/237 (92%)	0.68	20 (9%)	15 15	12, 24, 41, 52	0
1	B	220/237 (92%)	0.28	22 (10%)	12 13	4, 14, 55, 72	0
1	C	220/237 (92%)	0.60	25 (11%)	10 10	7, 17, 61, 75	0
1	D	220/237 (92%)	0.84	33 (15%)	5 5	7, 21, 60, 72	0
All	All	880/948 (92%)	0.60	100 (11%)	10 10	4, 20, 53, 75	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	187	TYR	10.4
1	D	186	PRO	10.2
1	D	188	ALA	9.9
1	D	189	TYR	8.7
1	B	188	ALA	8.6
1	D	191	LEU	8.5
1	D	194	LYS	7.9
1	C	189	TYR	7.5
1	B	191	LEU	7.5
1	D	187	TYR	7.1
1	D	192	ILE	7.0
1	C	192	ILE	6.9
1	B	187	TYR	6.8
1	D	193	GLY	6.8
1	A	187	TYR	6.6
1	C	188	ALA	6.6
1	C	40	SER	6.1
1	C	191	LEU	6.0
1	B	186	PRO	5.9
1	B	190	LYS	5.9
1	B	39	ASN	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	189	TYR	5.8
1	B	185	GLU	5.7
1	D	40	SER	5.6
1	C	39	ASN	5.3
1	C	193	GLY	5.3
1	D	37	GLY	5.1
1	C	186	PRO	4.9
1	C	37	GLY	4.9
1	C	184	SER	4.8
1	C	194	LYS	4.7
1	B	38	ASN	4.7
1	B	193	GLY	4.7
1	B	192	ILE	4.7
1	C	18	SER	4.6
1	D	41	SER	4.6
1	D	195	LYS	4.6
1	D	185	GLU	4.6
1	D	19	LEU	4.4
1	C	185	GLU	4.3
1	B	41	SER	4.2
1	C	19	LEU	4.1
1	A	121	PHE	4.1
1	B	37	GLY	4.1
1	C	190	LYS	4.1
1	D	190	LYS	4.1
1	C	41	SER	3.9
1	A	20	ASN	3.6
1	B	183	ALA	3.4
1	A	19	LEU	3.4
1	D	39	ASN	3.4
1	D	38	ASN	3.3
1	B	40	SER	3.2
1	D	18	SER	3.2
1	A	96	HIS	3.2
1	A	92	GLU	3.1
1	B	184	SER	3.1
1	C	183	ALA	3.0
1	A	55	ARG	2.9
1	C	38	ASN	2.9
1	D	184	SER	2.9
1	D	20	ASN	2.9
1	A	62	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	145	ASN	2.9
1	A	18	SER	2.8
1	C	147	ASN	2.8
1	D	42	LEU	2.8
1	D	146	ARG	2.8
1	A	66	TYR	2.8
1	D	35	TRP	2.7
1	D	157	GLN	2.7
1	D	166	ASN	2.6
1	D	36	SER	2.6
1	D	120	THR	2.4
1	A	59	ALA	2.4
1	C	161	LEU	2.4
1	A	61	CYS	2.4
1	A	191	LEU	2.4
1	B	36	SER	2.4
1	B	194	LYS	2.4
1	C	139	ARG	2.3
1	D	121	PHE	2.3
1	D	164	SER	2.3
1	D	77	ASN	2.3
1	B	115	ASP	2.3
1	B	42	LEU	2.2
1	D	118	ILE	2.1
1	A	39	ASN	2.1
1	A	25	THR	2.1
1	D	183	ALA	2.1
1	A	73	PRO	2.1
1	A	76	LYS	2.1
1	A	188	ALA	2.1
1	B	122	ASP	2.1
1	C	115	ASP	2.1
1	A	139	ARG	2.1
1	C	36	SER	2.1
1	B	166	ASN	2.0
1	C	117	LYS	2.0
1	A	192	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.