



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:39 PM UTC

PDB ID : 5K23 / pdb_00005k23
Title : Crystal structure of the complex between human phosphatase PRL-2 in the oxidized state with the Bateman domain of human magnesium transporter CNNM3
Authors : Gulerez, I.; Kozlov, G.; Gehring, K.
Deposited on : 2016-05-18
Resolution : 2.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
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

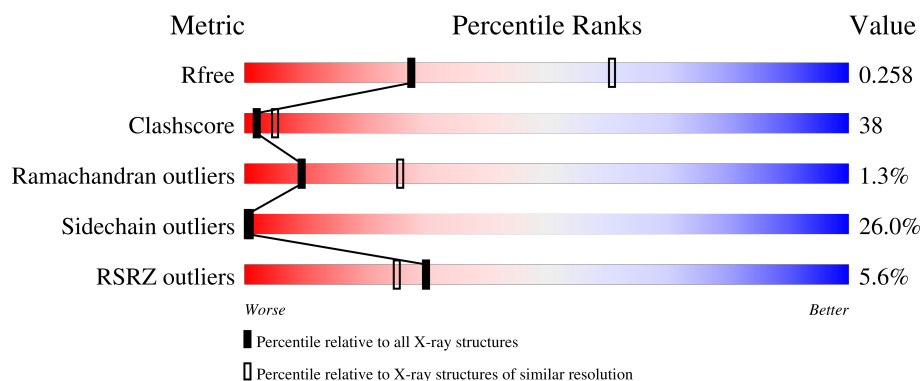
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	189	5% 35% 31% 15% • 17%
2	C	155	5% 52% 30% 11% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2401 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 Protein tyrosine phosphatase type IVA 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1226	783	215	219	9			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q12974
A	-20	SER	-	expression tag	UNP Q12974
A	-19	TYR	-	expression tag	UNP Q12974
A	-18	TYR	-	expression tag	UNP Q12974
A	-17	HIS	-	expression tag	UNP Q12974
A	-16	HIS	-	expression tag	UNP Q12974
A	-15	HIS	-	expression tag	UNP Q12974
A	-14	HIS	-	expression tag	UNP Q12974
A	-13	HIS	-	expression tag	UNP Q12974
A	-12	HIS	-	expression tag	UNP Q12974
A	-11	LEU	-	expression tag	UNP Q12974
A	-10	GLU	-	expression tag	UNP Q12974
A	-9	SER	-	expression tag	UNP Q12974
A	-8	THR	-	expression tag	UNP Q12974
A	-7	SER	-	expression tag	UNP Q12974
A	-6	LEU	-	expression tag	UNP Q12974
A	-5	TYR	-	expression tag	UNP Q12974
A	-4	LYS	-	expression tag	UNP Q12974
A	-3	LYS	-	expression tag	UNP Q12974
A	-2	ALA	-	expression tag	UNP Q12974
A	-1	GLY	-	expression tag	UNP Q12974
A	0	PHE	-	expression tag	UNP Q12974

- Molecule 2 is a protein called Metal transporter CNNM3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	149	Total	C	N	O	S	0	0	0
			1175	751	187	230	7			

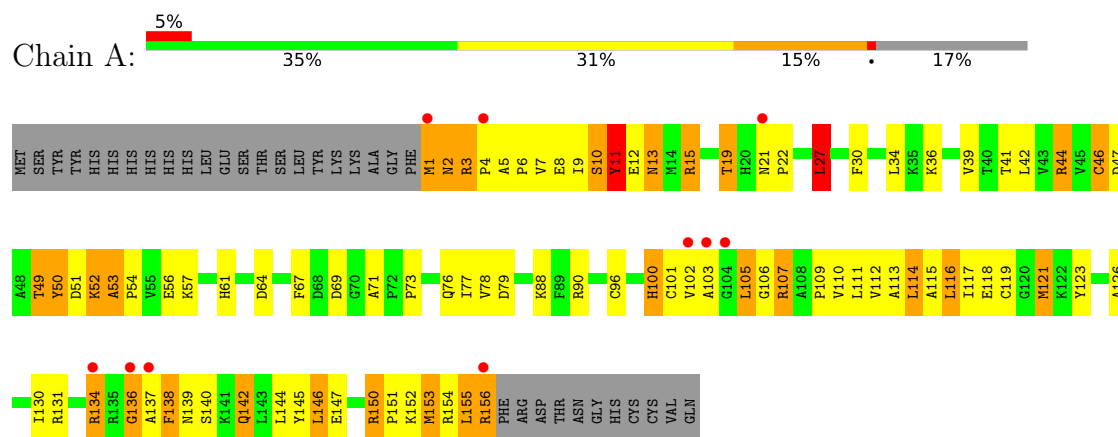
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	298	GLY	-	expression tag	UNP Q8NE01
C	299	PRO	-	expression tag	UNP Q8NE01
C	300	LEU	-	expression tag	UNP Q8NE01
C	301	ASN	-	expression tag	UNP Q8NE01
C	302	MET	-	expression tag	UNP Q8NE01
C	303	ILE	-	expression tag	UNP Q8NE01
C	304	GLN	-	expression tag	UNP Q8NE01
C	305	GLY	-	expression tag	UNP Q8NE01
C	306	VAL	-	expression tag	UNP Q8NE01
C	307	LEU	-	expression tag	UNP Q8NE01
C	308	GLU	-	expression tag	UNP Q8NE01

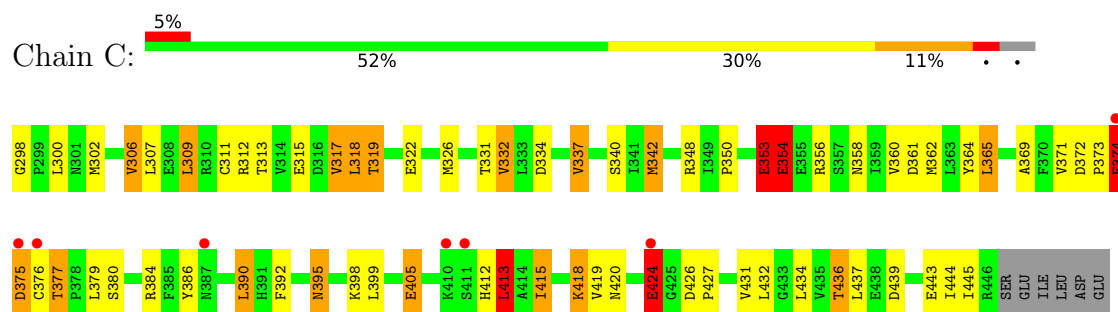
3 Residue-property plots [i](#)

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: Protein tyrosine phosphatase type IVA 2



• Molecule 2: Metal transporter CNNM3



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	51.16Å 124.49Å 159.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.02 – 2.96 49.02 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.02-2.96) 99.6 (49.02-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.205 , 0.264 0.220 , 0.258	Depositor DCC
R_{free} test set	528 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	79.8	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2401	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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	1.02	1/1255 (0.1%)	1.34	15/1708 (0.9%)
2	C	1.05	1/1197 (0.1%)	1.29	12/1628 (0.7%)
All	All	1.04	2/2452 (0.1%)	1.32	27/3336 (0.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	319	THR	C-N	5.17	1.40	1.33
1	A	54	PRO	N-CD	5.12	1.54	1.47

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	CYS	N-CA-C	-11.82	91.53	109.14
1	A	50	TYR	N-CA-C	-10.88	92.53	109.07
1	A	52	LYS	N-CA-C	9.67	123.03	111.33
2	C	353	GLU	N-CA-C	-8.86	94.19	108.55
2	C	353	GLU	CB-CA-C	7.25	122.91	109.86
1	A	27	LEU	N-CA-C	7.07	125.85	110.80
1	A	71	ALA	CA-C-N	-6.89	113.28	120.38
1	A	71	ALA	C-N-CA	-6.89	113.28	120.38
2	C	354	GLU	N-CA-CB	6.61	121.73	110.50
2	C	413	LEU	N-CA-C	6.23	118.21	107.93
1	A	49	THR	N-CA-C	-6.07	95.15	107.41
2	C	377	THR	CA-C-N	-5.91	113.88	119.85
2	C	377	THR	C-N-CA	-5.91	113.88	119.85
1	A	49	THR	CB-CA-C	5.56	120.86	111.41
2	C	319	THR	CA-C-N	-5.50	114.04	119.92
2	C	319	THR	C-N-CA	-5.50	114.04	119.92
1	A	136	GLY	N-CA-C	-5.46	107.74	113.58
2	C	369	ALA	CA-C-N	-5.42	114.57	122.86
2	C	369	ALA	C-N-CA	-5.42	114.57	122.86
2	C	354	GLU	N-CA-C	-5.41	95.86	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ASP	CA-C-N	5.34	127.69	120.38
1	A	51	ASP	C-N-CA	5.34	127.69	120.38
1	A	53	ALA	CA-C-N	-5.32	113.43	119.28
1	A	53	ALA	C-N-CA	-5.32	113.43	119.28
1	A	5	ALA	CA-C-N	5.29	126.45	119.84
1	A	5	ALA	C-N-CA	5.29	126.45	119.84
2	C	424	GLU	N-CA-C	-5.01	105.53	111.69

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	1226	0	1205	127	1
2	C	1175	0	1148	65	1
All	All	2401	0	2353	181	1

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 38.

All (181) 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:90:ARG:NH2	1:A:156:ARG:NH1	1.61	1.47
1:A:155:LEU:O	1:A:156:ARG:O	1.60	1.18
1:A:7:VAL:HG21	1:A:134:ARG:NH1	1.60	1.17
1:A:131:ARG:HE	1:A:137:ALA:CB	1.64	1.10
1:A:7:VAL:CG2	1:A:134:ARG:NH1	2.13	1.10
1:A:131:ARG:HG2	1:A:137:ALA:HB2	1.12	1.10
1:A:131:ARG:HE	1:A:137:ALA:HB3	0.98	1.08
1:A:7:VAL:HG21	1:A:134:ARG:HH11	1.11	1.05
1:A:121:MET:CE	1:A:126:ALA:HA	1.90	1.02
1:A:118:GLU:OE1	1:A:151:PRO:HA	1.61	1.01
2:C:348:ARG:HD2	2:C:412:HIS:CE1	1.96	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:NH1	1:A:64:ASP:OD2	1.94	1.00
2:C:373:PRO:O	2:C:374:GLU:HG3	1.59	1.00
1:A:131:ARG:NE	1:A:137:ALA:HB3	1.77	0.99
1:A:7:VAL:HG23	1:A:134:ARG:HH12	1.27	0.99
1:A:137:ALA:HB1	1:A:138:PHE:CD1	1.96	0.99
1:A:131:ARG:CG	1:A:137:ALA:HB2	1.91	0.99
2:C:373:PRO:O	2:C:374:GLU:O	1.83	0.95
1:A:105:LEU:O	1:A:137:ALA:O	1.86	0.94
2:C:373:PRO:C	2:C:374:GLU:HG3	1.90	0.94
1:A:3:ARG:HB3	1:A:4:PRO:HD2	1.52	0.91
2:C:311:CYS:O	2:C:398:LYS:NZ	2.04	0.89
1:A:121:MET:HE3	1:A:126:ALA:HA	1.55	0.89
1:A:106:GLY:HA3	2:C:426:ASP:OD1	1.74	0.87
1:A:7:VAL:CG2	1:A:134:ARG:HH12	1.80	0.86
1:A:121:MET:HE2	1:A:126:ALA:HA	1.57	0.86
1:A:118:GLU:OE1	1:A:151:PRO:CA	2.25	0.84
2:C:348:ARG:HG2	2:C:364:TYR:CD2	2.14	0.81
1:A:138:PHE:HB3	1:A:142:GLN:HB2	1.60	0.81
2:C:424:GLU:OE1	2:C:424:GLU:N	2.10	0.81
1:A:131:ARG:NE	1:A:137:ALA:CB	2.37	0.80
1:A:137:ALA:HB1	1:A:138:PHE:CE1	2.18	0.78
2:C:348:ARG:HD2	2:C:412:HIS:NE2	1.97	0.78
1:A:3:ARG:CB	1:A:4:PRO:HD2	2.13	0.78
2:C:326:MET:HE3	2:C:356:ARG:CZ	2.14	0.77
1:A:2:ASN:HD22	1:A:2:ASN:N	1.83	0.77
2:C:317:VAL:HG13	2:C:439:ASP:HB3	1.66	0.76
2:C:374:GLU:N	2:C:375:ASP:O	2.20	0.75
1:A:142:GLN:O	1:A:146:LEU:HD22	1.87	0.74
1:A:139:ASN:H	1:A:142:GLN:CG	2.00	0.74
1:A:10:SER:O	1:A:11:TYR:HB3	1.86	0.74
1:A:105:LEU:HD21	2:C:427:PRO:O	1.88	0.73
1:A:139:ASN:H	1:A:142:GLN:HG3	1.53	0.73
1:A:151:PRO:HB2	1:A:153:MET:HB2	1.70	0.73
1:A:3:ARG:CB	1:A:4:PRO:CD	2.66	0.73
2:C:332:VAL:O	2:C:337:VAL:HG11	1.89	0.72
1:A:7:VAL:HG23	1:A:134:ARG:NH1	1.93	0.72
1:A:106:GLY:HA3	2:C:426:ASP:HB3	1.70	0.71
1:A:3:ARG:HB3	1:A:4:PRO:CD	2.20	0.71
1:A:39:VAL:HG12	1:A:96:CYS:HB3	1.70	0.71
1:A:105:LEU:H	1:A:105:LEU:HD22	1.54	0.70
2:C:405:GLU:HA	2:C:405:GLU:OE2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:372:ASP:OD2	2:C:373:PRO:O	2.09	0.69
1:A:76:GLN:O	1:A:79:ASP:N	2.25	0.69
1:A:2:ASN:HD22	1:A:2:ASN:H	1.38	0.69
1:A:8:GLU:C	1:A:9:ILE:HD12	2.17	0.69
1:A:118:GLU:OE1	1:A:152:LYS:N	2.25	0.69
2:C:309:LEU:HD21	2:C:444:ILE:HD11	1.73	0.69
2:C:373:PRO:O	2:C:374:GLU:C	2.32	0.69
1:A:138:PHE:HB3	1:A:142:GLN:CB	2.22	0.69
1:A:61:HIS:HD2	1:A:88:LYS:CE	2.06	0.68
1:A:152:LYS:N	1:A:153:MET:HA	2.08	0.68
2:C:424:GLU:H	2:C:424:GLU:CD	1.98	0.68
1:A:61:HIS:HD2	1:A:88:LYS:HE2	1.60	0.67
2:C:312:ARG:NE	2:C:443:GLU:OE2	2.26	0.66
2:C:348:ARG:HG2	2:C:364:TYR:CE2	2.30	0.66
2:C:313:THR:HG22	2:C:398:LYS:HD3	1.77	0.66
2:C:348:ARG:CD	2:C:412:HIS:CE1	2.75	0.66
2:C:362:MET:HE2	2:C:413:LEU:HD11	1.79	0.65
2:C:415:ILE:HD11	2:C:431:VAL:HG22	1.78	0.65
1:A:138:PHE:CD1	1:A:138:PHE:N	2.65	0.65
2:C:413:LEU:HD13	2:C:413:LEU:O	1.98	0.64
1:A:21:ASN:OD1	1:A:102:VAL:HA	1.98	0.63
1:A:121:MET:HE3	1:A:126:ALA:CA	2.28	0.63
1:A:67:PHE:O	1:A:107:ARG:NH1	2.32	0.62
1:A:138:PHE:CB	1:A:142:GLN:HB2	2.29	0.62
2:C:353:GLU:O	2:C:358:ASN:HB3	2.00	0.61
1:A:105:LEU:CD2	2:C:427:PRO:O	2.47	0.61
1:A:139:ASN:OD1	1:A:142:GLN:HG2	2.00	0.60
1:A:76:GLN:O	1:A:77:ILE:C	2.44	0.60
1:A:106:GLY:HA3	2:C:426:ASP:CG	2.27	0.60
2:C:326:MET:CE	2:C:356:ARG:CZ	2.79	0.60
1:A:1:MET:HE3	2:C:405:GLU:HG2	1.84	0.60
1:A:106:GLY:HA3	2:C:426:ASP:CB	2.32	0.59
2:C:318:LEU:C	2:C:318:LEU:HD23	2.27	0.59
1:A:101:CYS:SG	1:A:102:VAL:N	2.76	0.58
2:C:354:GLU:HA	2:C:354:GLU:OE1	2.01	0.58
1:A:44:ARG:HD2	1:A:50:TYR:OH	2.03	0.58
2:C:334:ASP:OD1	2:C:337:VAL:HG12	2.03	0.57
1:A:134:ARG:HH11	1:A:134:ARG:CG	2.17	0.57
1:A:2:ASN:H	1:A:2:ASN:ND2	2.01	0.57
1:A:131:ARG:CG	1:A:137:ALA:CB	2.76	0.57
1:A:118:GLU:CD	1:A:151:PRO:HA	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:313:THR:HG22	2:C:398:LYS:CD	2.35	0.55
1:A:53:ALA:O	1:A:57:LYS:N	2.25	0.55
1:A:155:LEU:C	1:A:156:ARG:O	2.39	0.55
1:A:150:ARG:CD	1:A:150:ARG:N	2.70	0.55
1:A:53:ALA:O	1:A:56:GLU:N	2.40	0.55
1:A:106:GLY:CA	2:C:426:ASP:HB3	2.37	0.54
1:A:103:ALA:HB1	1:A:105:LEU:HD22	1.90	0.54
1:A:105:LEU:HD22	1:A:105:LEU:N	2.23	0.53
1:A:114:LEU:HD11	1:A:145:TYR:HE2	1.73	0.53
1:A:123:TYR:CZ	1:A:147:GLU:HB2	2.44	0.52
2:C:326:MET:CE	2:C:356:ARG:NH2	2.72	0.52
2:C:337:VAL:O	2:C:340:SER:HB3	2.10	0.52
2:C:331:THR:HG22	2:C:332:VAL:N	2.24	0.52
1:A:150:ARG:HH21	1:A:154:ARG:NH2	2.07	0.51
1:A:7:VAL:CG2	1:A:134:ARG:HH11	1.92	0.51
1:A:131:ARG:HA	1:A:134:ARG:O	2.10	0.51
1:A:139:ASN:H	1:A:142:GLN:HG2	1.75	0.51
2:C:374:GLU:CA	2:C:375:ASP:C	2.83	0.51
1:A:19:THR:HG21	1:A:30:PHE:CE1	2.45	0.51
1:A:105:LEU:HA	1:A:109:PRO:HG3	1.94	0.50
1:A:131:ARG:HG2	1:A:137:ALA:CB	2.08	0.50
2:C:350:PRO:HG2	2:C:434:LEU:HD11	1.94	0.50
1:A:46:CYS:SG	1:A:107:ARG:CZ	3.00	0.50
1:A:3:ARG:CG	1:A:4:PRO:HD2	2.42	0.49
1:A:6:PRO:HG3	1:A:19:THR:HG23	1.95	0.49
1:A:41:THR:HA	1:A:61:HIS:O	2.12	0.49
1:A:44:ARG:NE	1:A:50:TYR:CZ	2.79	0.48
1:A:134:ARG:NH1	1:A:134:ARG:CG	2.73	0.48
1:A:150:ARG:CD	1:A:150:ARG:H	2.25	0.48
1:A:19:THR:HG21	1:A:30:PHE:HE1	1.79	0.48
1:A:145:TYR:CD2	1:A:145:TYR:C	2.92	0.48
1:A:150:ARG:N	1:A:150:ARG:HD3	2.28	0.47
1:A:118:GLU:O	1:A:153:MET:HG2	2.14	0.47
1:A:69:ASP:OD1	2:C:426:ASP:OD2	2.32	0.47
2:C:426:ASP:OD2	2:C:426:ASP:N	2.47	0.47
1:A:39:VAL:HA	1:A:96:CYS:O	2.15	0.47
1:A:118:GLU:HA	1:A:151:PRO:HB3	1.96	0.47
1:A:44:ARG:NE	1:A:50:TYR:OH	2.48	0.46
1:A:121:MET:HE3	1:A:126:ALA:N	2.31	0.46
1:A:139:ASN:CG	1:A:142:GLN:HG2	2.41	0.46
2:C:326:MET:HE2	2:C:356:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:H	1:A:107:ARG:HG2	1.56	0.46
1:A:136:GLY:O	1:A:137:ALA:C	2.59	0.46
2:C:373:PRO:O	2:C:374:GLU:CG	2.49	0.46
1:A:2:ASN:N	1:A:2:ASN:ND2	2.51	0.45
1:A:113:ALA:HA	1:A:116:LEU:HD12	1.99	0.45
1:A:13:ASN:OD1	1:A:13:ASN:N	2.44	0.45
1:A:44:ARG:CD	1:A:50:TYR:OH	2.63	0.45
1:A:1:MET:HE2	1:A:1:MET:HB3	1.89	0.45
1:A:3:ARG:HG3	2:C:390:LEU:HD23	1.98	0.45
1:A:41:THR:OG1	1:A:88:LYS:HG2	2.17	0.45
1:A:118:GLU:O	1:A:118:GLU:HG3	2.17	0.45
2:C:298:GLY:O	2:C:302:MET:HG3	2.17	0.45
1:A:44:ARG:HG3	1:A:100:HIS:NE2	2.32	0.44
1:A:107:ARG:N	2:C:426:ASP:OD1	2.50	0.44
1:A:73:PRO:HD3	1:A:110:VAL:HG11	1.98	0.44
1:A:112:VAL:O	1:A:115:ALA:HB3	2.17	0.44
2:C:306:VAL:O	2:C:309:LEU:HB2	2.18	0.44
2:C:365:LEU:HD23	2:C:365:LEU:HA	1.72	0.44
2:C:380:SER:O	2:C:384:ARG:HB2	2.18	0.44
1:A:11:TYR:CD1	1:A:11:TYR:O	2.70	0.43
1:A:118:GLU:OE1	1:A:151:PRO:C	2.61	0.43
1:A:137:ALA:HB1	1:A:138:PHE:HD1	1.72	0.43
2:C:331:THR:CG2	2:C:332:VAL:N	2.82	0.43
1:A:22:PRO:HD2	1:A:50:TYR:CE1	2.53	0.43
2:C:334:ASP:CG	2:C:337:VAL:HG12	2.44	0.43
2:C:415:ILE:CD1	2:C:431:VAL:HG22	2.46	0.42
1:A:117:ILE:C	1:A:119:CYS:H	2.28	0.42
2:C:392:PHE:CE1	2:C:415:ILE:HG12	2.54	0.42
2:C:315:GLU:HG3	2:C:395:ASN:HB2	2.01	0.42
2:C:342:MET:HB3	2:C:342:MET:HE2	1.78	0.42
1:A:151:PRO:HB2	1:A:153:MET:CB	2.46	0.42
1:A:47:ASP:OD1	1:A:47:ASP:N	2.53	0.41
2:C:418:LYS:HG2	2:C:432:LEU:HD21	2.02	0.41
2:C:353:GLU:HA	2:C:354:GLU:HA	1.85	0.41
1:A:34:LEU:HD22	1:A:39:VAL:HG21	2.02	0.41
1:A:150:ARG:H	1:A:150:ARG:NE	2.19	0.41
2:C:420:ASN:OD1	2:C:420:ASN:C	2.64	0.41
1:A:61:HIS:CD2	1:A:88:LYS:CE	2.95	0.41
1:A:3:ARG:HG2	1:A:4:PRO:HD2	2.03	0.41
1:A:134:ARG:NH1	1:A:134:ARG:HG3	2.36	0.41
2:C:326:MET:HG2	2:C:350:PRO:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ARG:H	1:A:150:ARG:HD3	1.84	0.40
2:C:436:THR:HG23	2:C:439:ASP:CG	2.47	0.40
1:A:34:LEU:HB3	1:A:39:VAL:HG22	2.03	0.40
1:A:114:LEU:HD11	1:A:145:TYR:CE2	2.56	0.40
2:C:362:MET:CE	2:C:413:LEU:HD11	2.50	0.40
1:A:15:ARG:HH11	1:A:15:ARG:HG2	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:NH2	2:C:372:ASP:CG[8_455]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	154/189 (82%)	138 (90%)	14 (9%)	2 (1%)	9	26
2	C	147/155 (95%)	141 (96%)	4 (3%)	2 (1%)	9	24
All	All	301/344 (88%)	279 (93%)	18 (6%)	4 (1%)	9	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	TYR
2	C	374	GLU
1	A	27	LEU
2	C	445	ILE

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	129/166 (78%)	95 (74%)	34 (26%)	0	1
2	C	133/142 (94%)	99 (74%)	34 (26%)	0	1
All	All	262/308 (85%)	194 (74%)	68 (26%)	0	1

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ASN
1	A	3	ARG
1	A	10	SER
1	A	11	TYR
1	A	12	GLU
1	A	13	ASN
1	A	15	ARG
1	A	19	THR
1	A	27	LEU
1	A	36	LYS
1	A	42	LEU
1	A	44	ARG
1	A	49	THR
1	A	52	LYS
1	A	78	VAL
1	A	100	HIS
1	A	105	LEU
1	A	107	ARG
1	A	111	LEU
1	A	114	LEU
1	A	116	LEU
1	A	121	MET
1	A	130	ILE
1	A	134	ARG
1	A	138	PHE
1	A	140	SER

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Mol	Chain	Res	Type
1	A	142	GLN
1	A	144	LEU
1	A	146	LEU
1	A	150	ARG
1	A	153	MET
1	A	155	LEU
1	A	156	ARG
2	C	300	LEU
2	C	306	VAL
2	C	307	LEU
2	C	309	LEU
2	C	317	VAL
2	C	318	LEU
2	C	319	THR
2	C	322	GLU
2	C	332	VAL
2	C	337	VAL
2	C	342	MET
2	C	353	GLU
2	C	354	GLU
2	C	360	VAL
2	C	361	ASP
2	C	365	LEU
2	C	371	VAL
2	C	374	GLU
2	C	375	ASP
2	C	376	CYS
2	C	377	THR
2	C	379	LEU
2	C	386	TYR
2	C	390	LEU
2	C	395	ASN
2	C	399	LEU
2	C	405	GLU
2	C	413	LEU
2	C	415	ILE
2	C	418	LYS
2	C	419	VAL
2	C	424	GLU
2	C	436	THR
2	C	437	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	20	HIS
1	A	61	HIS
1	A	142	GLN
2	C	343	GLN
2	C	346	HIS
2	C	395	ASN
2	C	412	HIS

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	156/189 (82%)	0.37	10 (6%) 25 21	43, 75, 111, 127	0
2	C	149/155 (96%)	0.15	7 (4%) 36 30	25, 62, 93, 121	0
All	All	305/344 (88%)	0.27	17 (5%) 30 25	25, 67, 107, 127	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	375	ASP	6.1
2	C	376	CYS	5.6
1	A	156	ARG	4.9
1	A	103	ALA	3.9
2	C	374	GLU	3.7
2	C	424	GLU	3.4
2	C	410	LYS	3.3
1	A	1	MET	2.9
1	A	102	VAL	2.9
1	A	4	PRO	2.5
1	A	21	ASN	2.4
1	A	136	GLY	2.3
2	C	411	SER	2.2
1	A	104	GLY	2.1
1	A	137	ALA	2.1
2	C	387	ASN	2.1
1	A	134	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.