



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:33 PM UTC

PDB ID : 4EXM / pdb_00004exm
Title : The crystal structure of an engineered phage lysin containing the binding domain of pesticin and the killing domain of T4-lysozyme
Authors : Seddiki, N.; Noinaj, N.; Fairman, J.W.; Lukacik, P.; Barnard, T.J.; Buchanan, S.K.
Deposited on : 2012-04-30
Resolution : 2.60 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

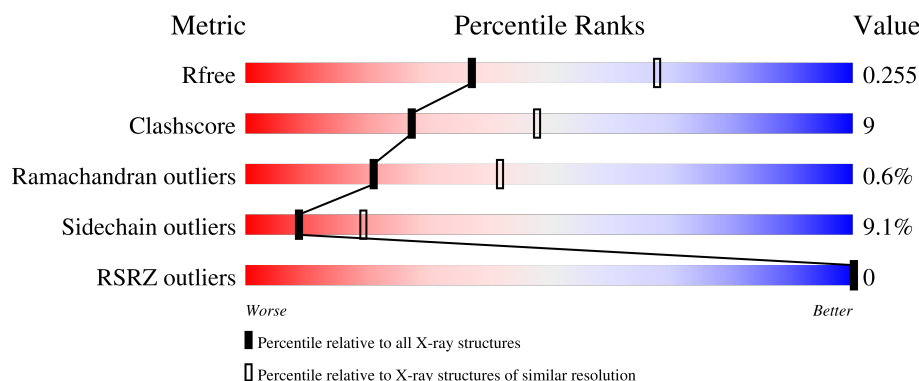
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	347	
1	B	347	
1	C	347	
1	D	347	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9875 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 Pesticin, Lysozyme Chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2269	1429	401	431	8			
1	B	291	Total	C	N	O	S	0	0	0
			2292	1444	401	439	8			
1	C	331	Total	C	N	O	S	0	0	0
			2633	1657	461	505	10			
1	D	331	Total	C	N	O	S	0	0	0
			2606	1640	456	500	10			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	expression tag	UNP Q57159
A	-11	HIS	-	expression tag	UNP Q57159
A	-10	HIS	-	expression tag	UNP Q57159
A	-9	HIS	-	expression tag	UNP Q57159
A	-8	HIS	-	expression tag	UNP Q57159
A	-7	HIS	-	expression tag	UNP Q57159
A	-6	HIS	-	expression tag	UNP Q57159
A	-5	HIS	-	expression tag	UNP Q57159
A	-4	HIS	-	expression tag	UNP Q57159
A	-3	HIS	-	expression tag	UNP Q57159
A	-2	HIS	-	expression tag	UNP Q57159
A	-1	GLU	-	expression tag	UNP Q57159
A	0	ASN	-	expression tag	UNP Q57159
A	1	LEU	-	expression tag	UNP Q57159
A	2	TYR	-	expression tag	UNP Q57159
A	3	PHE	-	expression tag	UNP Q57159
A	4	GLN	-	expression tag	UNP Q57159
A	5	SER	-	expression tag	UNP Q57159
A	182	ARG	GLY	engineered mutation	UNP P00720
A	224	THR	CYS	engineered mutation	UNP P00720
A	267	ALA	CYS	engineered mutation	UNP P00720

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Chain	Residue	Modelled	Actual	Comment	Reference
A	307	ILE	ARG	engineered mutation	UNP P00720
B	-12	MET	-	expression tag	UNP Q57159
B	-11	HIS	-	expression tag	UNP Q57159
B	-10	HIS	-	expression tag	UNP Q57159
B	-9	HIS	-	expression tag	UNP Q57159
B	-8	HIS	-	expression tag	UNP Q57159
B	-7	HIS	-	expression tag	UNP Q57159
B	-6	HIS	-	expression tag	UNP Q57159
B	-5	HIS	-	expression tag	UNP Q57159
B	-4	HIS	-	expression tag	UNP Q57159
B	-3	HIS	-	expression tag	UNP Q57159
B	-2	HIS	-	expression tag	UNP Q57159
B	-1	GLU	-	expression tag	UNP Q57159
B	0	ASN	-	expression tag	UNP Q57159
B	1	LEU	-	expression tag	UNP Q57159
B	2	TYR	-	expression tag	UNP Q57159
B	3	PHE	-	expression tag	UNP Q57159
B	4	GLN	-	expression tag	UNP Q57159
B	5	SER	-	expression tag	UNP Q57159
B	182	ARG	GLY	engineered mutation	UNP P00720
B	224	THR	CYS	engineered mutation	UNP P00720
B	267	ALA	CYS	engineered mutation	UNP P00720
B	307	ILE	ARG	engineered mutation	UNP P00720
C	-12	MET	-	expression tag	UNP Q57159
C	-11	HIS	-	expression tag	UNP Q57159
C	-10	HIS	-	expression tag	UNP Q57159
C	-9	HIS	-	expression tag	UNP Q57159
C	-8	HIS	-	expression tag	UNP Q57159
C	-7	HIS	-	expression tag	UNP Q57159
C	-6	HIS	-	expression tag	UNP Q57159
C	-5	HIS	-	expression tag	UNP Q57159
C	-4	HIS	-	expression tag	UNP Q57159
C	-3	HIS	-	expression tag	UNP Q57159
C	-2	HIS	-	expression tag	UNP Q57159
C	-1	GLU	-	expression tag	UNP Q57159
C	0	ASN	-	expression tag	UNP Q57159
C	1	LEU	-	expression tag	UNP Q57159
C	2	TYR	-	expression tag	UNP Q57159
C	3	PHE	-	expression tag	UNP Q57159
C	4	GLN	-	expression tag	UNP Q57159
C	5	SER	-	expression tag	UNP Q57159
C	182	ARG	GLY	engineered mutation	UNP P00720

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Chain	Residue	Modelled	Actual	Comment	Reference
C	224	THR	CYS	engineered mutation	UNP P00720
C	267	ALA	CYS	engineered mutation	UNP P00720
C	307	ILE	ARG	engineered mutation	UNP P00720
D	-12	MET	-	expression tag	UNP Q57159
D	-11	HIS	-	expression tag	UNP Q57159
D	-10	HIS	-	expression tag	UNP Q57159
D	-9	HIS	-	expression tag	UNP Q57159
D	-8	HIS	-	expression tag	UNP Q57159
D	-7	HIS	-	expression tag	UNP Q57159
D	-6	HIS	-	expression tag	UNP Q57159
D	-5	HIS	-	expression tag	UNP Q57159
D	-4	HIS	-	expression tag	UNP Q57159
D	-3	HIS	-	expression tag	UNP Q57159
D	-2	HIS	-	expression tag	UNP Q57159
D	-1	GLU	-	expression tag	UNP Q57159
D	0	ASN	-	expression tag	UNP Q57159
D	1	LEU	-	expression tag	UNP Q57159
D	2	TYR	-	expression tag	UNP Q57159
D	3	PHE	-	expression tag	UNP Q57159
D	4	GLN	-	expression tag	UNP Q57159
D	5	SER	-	expression tag	UNP Q57159
D	182	ARG	GLY	engineered mutation	UNP P00720
D	224	THR	CYS	engineered mutation	UNP P00720
D	267	ALA	CYS	engineered mutation	UNP P00720
D	307	ILE	ARG	engineered mutation	UNP P00720

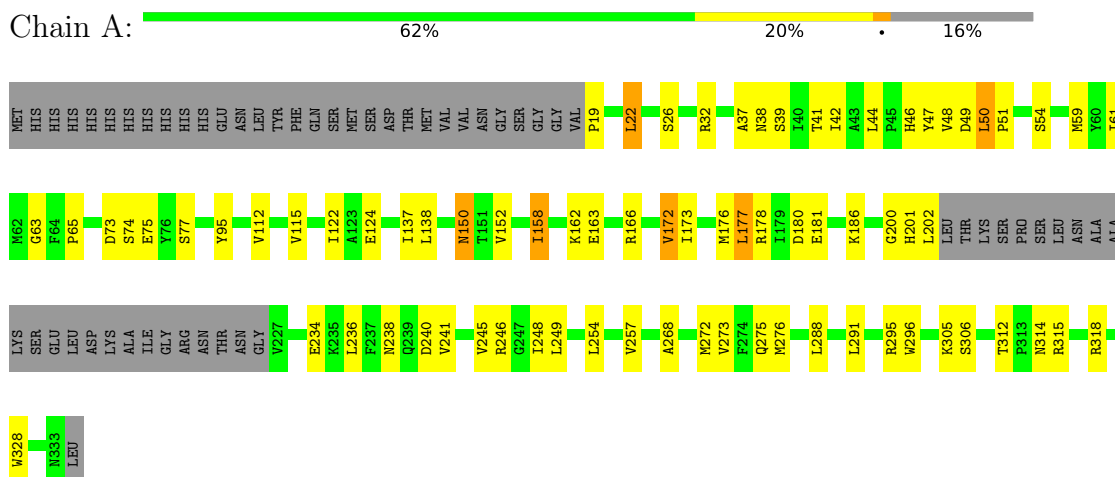
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	28	Total O 28 28	0	0
2	B	27	Total O 27 27	0	0
2	C	9	Total O 9 9	0	0
2	D	11	Total O 11 11	0	0

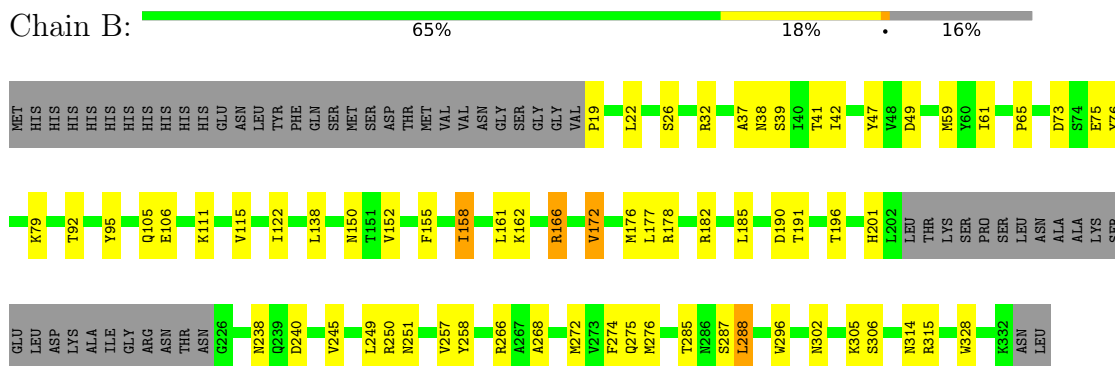
3 Residue-property plots

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.

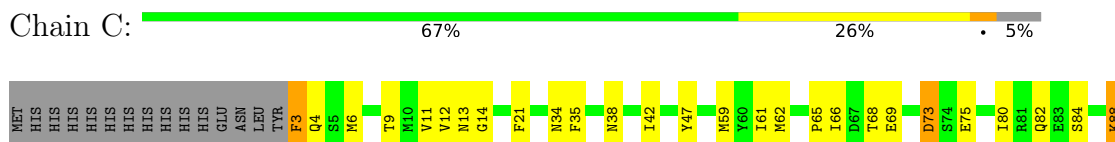
• Molecule 1: Pesticin, Lysozyme Chimera

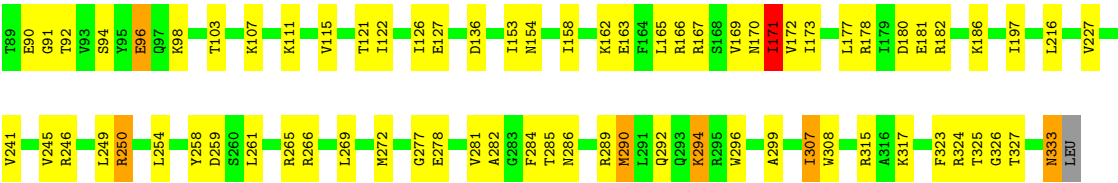


• Molecule 1: Pesticin, Lysozyme Chimera

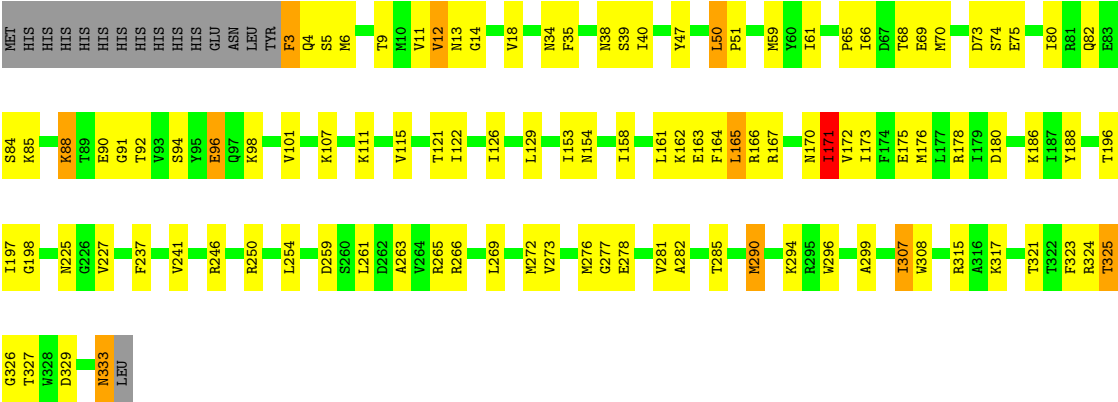


• Molecule 1: Pesticin, Lysozyme Chimera





• Molecule 1: Pesticin, Lysozyme Chimera



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	108.43Å 108.43Å 109.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.80 – 2.60 29.80 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.80-2.60) 99.9 (29.80-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1038)	Depositor
R, R_{free}	0.199 , 0.251 0.204 , 0.255	Depositor DCC
R_{free} test set	2254 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l 0.479 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9875	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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	0.43	0/2304	0.83	4/3116 (0.1%)
1	B	0.43	0/2328	0.80	0/3146
1	C	0.40	0/2674	0.81	4/3606 (0.1%)
1	D	0.41	0/2646	0.81	6/3572 (0.2%)
All	All	0.42	0/9952	0.81	14/13440 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	13	ASN	N-CA-C	6.80	121.24	113.15
1	C	13	ASN	N-CA-C	6.23	120.38	113.21
1	C	35	PHE	CB-CA-C	-6.05	109.00	117.23
1	C	171	ILE	CB-CA-C	-5.74	104.39	112.14
1	D	35	PHE	CB-CA-C	-5.73	109.98	116.63
1	A	312	THR	CA-C-N	5.58	125.25	119.05
1	A	312	THR	C-N-CA	5.58	125.25	119.05
1	C	14	GLY	N-CA-C	5.37	118.98	111.19
1	A	50	LEU	CA-C-N	5.19	125.44	119.83
1	A	50	LEU	C-N-CA	5.19	125.44	119.83
1	D	14	GLY	N-CA-C	5.06	118.53	111.19
1	D	171	ILE	CB-CA-C	-5.03	104.37	112.16
1	D	50	LEU	CA-C-N	5.02	126.11	119.84
1	D	50	LEU	C-N-CA	5.02	126.11	119.84

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	2269	0	2212	40	0
1	B	2292	0	2253	37	0
1	C	2633	0	2645	56	0
1	D	2606	0	2604	56	0
2	A	28	0	0	3	0
2	B	27	0	0	4	0
2	C	9	0	0	1	0
2	D	11	0	0	0	0
All	All	9875	0	9714	178	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 9.

All (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LEU:HB3	1:B:158:ILE:HG13	1.53	0.91
1:B:314:ASN:ND2	2:B:425:HOH:O	2.04	0.90
1:B:92:THR:O	2:B:410:HOH:O	1.95	0.84
1:A:138:LEU:HB3	1:A:158:ILE:HG13	1.60	0.83
1:C:265:ARG:NH2	1:C:324:ARG:O	2.15	0.80
1:C:325:THR:O	1:C:327:THR:N	2.15	0.79
1:D:290:MET:HE3	1:D:299:ALA:HA	1.64	0.78
1:D:65:PRO:HG2	1:D:115:VAL:HB	1.65	0.78
1:C:65:PRO:HG2	1:C:115:VAL:HB	1.65	0.77
1:D:69:GLU:HB2	1:D:111:LYS:HB2	1.65	0.77
1:C:290:MET:HE3	1:C:299:ALA:HA	1.72	0.71
1:A:314:ASN:ND2	2:A:409:HOH:O	2.23	0.71
1:D:186:LYS:HG2	1:D:227:VAL:HG22	1.71	0.71
1:B:274:PHE:O	2:B:419:HOH:O	2.10	0.70
1:C:69:GLU:HB2	1:C:111:LYS:HB2	1.75	0.67
1:A:47:TYR:CE1	1:A:59:MET:HG3	2.30	0.66
1:C:158:ILE:HG13	1:C:162:LYS:HD2	1.79	0.65
1:C:6:MET:HG2	1:D:4:GLN:NE2	2.13	0.64
1:C:186:LYS:HG2	1:C:227:VAL:HG22	1.79	0.63
1:D:122:ILE:HG23	1:D:165:LEU:HG	1.81	0.61
1:B:95:TYR:HA	1:B:122:ILE:HD12	1.82	0.61
1:D:50:LEU:HD12	1:D:51:PRO:HD2	1.82	0.61
1:D:307:ILE:HD12	1:D:308:TRP:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:TYR:CE1	1:B:59:MET:HG3	2.36	0.60
1:D:170:ASN:HA	1:D:173:ILE:HD12	1.85	0.59
1:A:95:TYR:HA	1:A:122:ILE:HD12	1.84	0.59
1:B:26:SER:HB3	1:C:9:THR:HG22	1.84	0.59
1:D:265:ARG:NH2	1:D:324:ARG:O	2.36	0.58
1:A:180:ASP:OD1	1:A:318:ARG:NH1	2.37	0.58
1:C:292:GLN:HB3	2:C:405:HOH:O	2.04	0.57
1:D:261:LEU:HD22	1:D:265:ARG:HD3	1.87	0.57
1:D:272:MET:HE2	1:D:308:TRP:CH2	2.39	0.57
1:B:176:MET:HE1	1:B:268:ALA:HA	1.86	0.57
1:D:158:ILE:HG13	1:D:162:LYS:HD2	1.85	0.57
1:A:245:VAL:O	1:A:249:LEU:HG	2.04	0.57
1:A:32:ARG:HG3	1:B:32:ARG:HD2	1.87	0.57
1:C:307:ILE:HD12	1:C:308:TRP:H	1.70	0.56
1:A:201:HIS:ND1	1:A:240:ASP:OD2	2.31	0.56
1:D:4:GLN:HE22	1:D:6:MET:HG3	1.70	0.56
1:C:91:GLY:N	1:C:167:ARG:HH22	2.05	0.55
1:C:4:GLN:HE22	1:C:6:MET:HG3	1.72	0.55
1:D:92:THR:HG21	1:D:171:ILE:HD11	1.89	0.55
1:C:92:THR:HG21	1:C:171:ILE:HD11	1.89	0.55
1:B:201:HIS:ND1	1:B:240:ASP:OD2	2.28	0.55
1:D:325:THR:O	1:D:327:THR:N	2.34	0.55
1:A:201:HIS:CD2	1:A:236:LEU:HD13	2.43	0.54
1:C:261:LEU:HD22	1:C:265:ARG:HD3	1.90	0.54
1:D:94:SER:OG	1:D:96:GLU:OE1	2.26	0.53
1:B:65:PRO:HG2	1:B:115:VAL:HB	1.89	0.53
1:B:245:VAL:O	1:B:249:LEU:HG	2.08	0.53
1:A:54:SER:O	1:A:150:ASN:ND2	2.42	0.52
1:D:167:ARG:O	1:D:171:ILE:HG13	2.09	0.52
1:C:84:SER:HB3	1:C:153:ILE:HG12	1.91	0.52
1:C:167:ARG:O	1:C:171:ILE:HG13	2.10	0.52
1:D:277:GLY:O	1:D:281:VAL:HG23	2.10	0.52
1:A:65:PRO:HG2	1:A:115:VAL:HB	1.91	0.52
1:A:124:GLU:OE2	1:D:3:PHE:HZ	1.93	0.52
1:C:296:TRP:HB3	1:C:324:ARG:HA	1.91	0.52
1:D:296:TRP:HB3	1:D:324:ARG:HA	1.92	0.52
1:C:170:ASN:HA	1:C:173:ILE:HD12	1.90	0.52
1:B:166:ARG:HB3	1:B:238:ASN:ND2	2.25	0.51
1:C:272:MET:HE3	1:C:323:PHE:HE1	1.75	0.51
1:D:47:TYR:HE1	1:D:59:MET:HE2	1.75	0.51
1:C:290:MET:HB3	1:C:299:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:THR:OG1	1:D:329:ASP:OD1	2.29	0.50
1:D:272:MET:HE3	1:D:323:PHE:HE1	1.76	0.50
1:D:290:MET:HB3	1:D:299:ALA:HB2	1.94	0.50
1:A:172:VAL:HB	1:A:328:TRP:CZ2	2.45	0.50
1:B:172:VAL:HB	1:B:328:TRP:CZ2	2.46	0.50
1:C:59:MET:SD	1:C:66:ILE:HD11	2.52	0.50
1:A:46:HIS:HD2	2:A:402:HOH:O	1.93	0.50
1:C:122:ILE:HG23	1:C:165:LEU:HG	1.93	0.49
1:C:73:ASP:OD1	1:C:73:ASP:N	2.44	0.49
1:A:112:VAL:HG21	1:D:40:ILE:O	2.13	0.49
1:C:272:MET:HE2	1:C:308:TRP:CH2	2.47	0.49
1:A:74:SER:HB3	1:A:77:SER:HB2	1.94	0.49
1:D:59:MET:SD	1:D:66:ILE:HD11	2.52	0.49
1:C:258:TYR:CE2	1:C:266:ARG:HB3	2.48	0.48
1:A:181:GLU:OE1	1:A:200:GLY:HA3	2.13	0.48
1:B:185:LEU:HD12	1:B:185:LEU:H	1.79	0.48
1:D:91:GLY:N	1:D:167:ARG:HH22	2.12	0.48
1:D:197:ILE:HG12	1:D:198:GLY:H	1.78	0.47
1:A:32:ARG:CZ	1:B:37:ALA:HB2	2.44	0.47
1:D:321:THR:HG23	1:D:324:ARG:HH12	1.78	0.47
1:D:101:VAL:HG11	1:D:129:LEU:HD21	1.96	0.47
1:D:88:LYS:HE3	1:D:154:ASN:O	2.14	0.47
1:B:305:LYS:HG3	1:B:306:SER:N	2.30	0.47
1:C:286:ASN:HA	1:C:289:ARG:NH1	2.30	0.47
1:C:181:GLU:O	1:C:182:ARG:HB2	2.14	0.47
1:C:197:ILE:HG21	1:C:216:LEU:HD13	1.96	0.47
1:D:70:MET:HE2	1:D:74:SER:HB2	1.97	0.47
1:D:254:LEU:HD21	1:D:282:ALA:HA	1.97	0.46
1:B:258:TYR:O	1:B:266:ARG:NH1	2.48	0.46
1:A:163:GLU:OE2	1:A:238:ASN:ND2	2.49	0.46
1:C:94:SER:OG	1:C:96:GLU:OE1	2.31	0.46
1:A:248:ILE:HD11	1:A:273:VAL:HG21	1.98	0.46
1:C:277:GLY:O	1:C:281:VAL:HG23	2.15	0.46
1:A:59:MET:HE3	1:A:61:ILE:HB	1.98	0.46
1:C:88:LYS:HE3	1:C:154:ASN:O	2.15	0.46
1:D:269:LEU:O	1:D:273:VAL:HG23	2.15	0.46
1:D:69:GLU:HB3	1:D:80:ILE:HD13	1.97	0.46
1:C:325:THR:O	1:C:325:THR:OG1	2.20	0.45
1:A:19:PRO:HB2	1:A:22:LEU:HD23	1.98	0.45
1:C:294:LYS:HB3	1:C:296:TRP:CZ2	2.51	0.45
1:C:254:LEU:HD21	1:C:282:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:TYR:CE2	1:D:196:THR:HB	2.52	0.45
1:D:263:ALA:HA	1:D:266:ARG:HB2	1.99	0.45
1:A:158:ILE:HD13	1:A:162:LYS:HG3	1.98	0.45
1:C:69:GLU:HB3	1:C:80:ILE:HD13	1.98	0.45
1:D:276:MET:HE2	1:D:276:MET:HB3	1.75	0.45
1:B:302:ASN:O	1:B:305:LYS:HG2	2.18	0.44
1:C:47:TYR:HE1	1:C:59:MET:HE2	1.82	0.44
1:C:90:GLU:C	1:C:167:ARG:HH22	2.25	0.44
1:C:166:ARG:HH21	1:C:170:ASN:HD21	1.66	0.44
1:B:39:SER:O	1:B:42:ILE:HG12	2.18	0.43
1:C:269:LEU:HD12	1:C:269:LEU:HA	1.86	0.43
1:A:272:MET:O	1:A:276:MET:HG2	2.17	0.43
1:C:42:ILE:O	1:C:62:MET:N	2.43	0.43
1:A:254:LEU:O	1:A:257:VAL:HG12	2.19	0.43
1:A:50:LEU:HA	1:A:51:PRO:HD3	1.85	0.43
1:B:190:ASP:HB3	1:B:196:THR:HG21	2.01	0.43
1:B:249:LEU:C	1:B:251:ASN:H	2.25	0.43
1:C:284:PHE:O	1:C:286:ASN:N	2.52	0.43
1:C:307:ILE:HD12	1:C:308:TRP:N	2.33	0.43
1:D:90:GLU:C	1:D:167:ARG:HH22	2.27	0.43
1:C:333:ASN:N	1:C:333:ASN:OD1	2.51	0.43
1:A:38:ASN:OD1	1:C:3:PHE:HB2	2.18	0.43
1:B:158:ILE:HD12	1:B:162:LYS:HE3	2.01	0.43
1:B:275:GLN:HB2	1:B:315:ARG:CZ	2.49	0.43
1:C:98:LYS:HE2	1:C:121:THR:HG22	2.01	0.43
1:D:307:ILE:HD12	1:D:308:TRP:N	2.31	0.43
1:B:105:GLN:OE1	2:B:423:HOH:O	2.21	0.43
1:D:12:VAL:HG13	1:D:18:VAL:HB	2.01	0.43
1:C:21:PHE:CD2	1:C:136:ASP:HB3	2.54	0.42
1:C:180:ASP:CG	1:C:315:ARG:HG3	2.44	0.42
1:A:39:SER:O	1:A:42:ILE:HG12	2.20	0.42
1:B:155:PHE:CD2	1:B:161:LEU:HD12	2.55	0.42
1:B:272:MET:O	1:B:276:MET:HG2	2.19	0.42
1:B:257:VAL:HG11	1:B:288:LEU:CD2	2.50	0.42
1:A:241:VAL:O	1:A:245:VAL:HG23	2.19	0.42
1:A:37:ALA:HB2	1:B:32:ARG:CZ	2.49	0.42
1:A:257:VAL:HG11	1:A:288:LEU:CD2	2.48	0.42
1:D:237:PHE:O	1:D:241:VAL:HG23	2.20	0.42
1:D:333:ASN:N	1:D:333:ASN:OD1	2.52	0.42
1:B:38:ASN:OD1	1:D:3:PHE:HB2	2.19	0.42
1:A:177:LEU:HD12	1:A:177:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLN:HB2	1:A:315:ARG:CZ	2.50	0.42
1:A:158:ILE:HD12	1:A:162:LYS:HE3	2.01	0.41
1:B:158:ILE:HD13	1:B:162:LYS:HG3	2.01	0.41
1:C:245:VAL:O	1:C:249:LEU:HG	2.20	0.41
1:C:286:ASN:HA	1:C:289:ARG:HH12	1.85	0.41
1:D:180:ASP:HB3	1:D:315:ARG:NE	2.35	0.41
1:C:126:ILE:HG12	1:C:165:LEU:HB3	2.02	0.41
1:C:180:ASP:HB3	1:C:315:ARG:NE	2.36	0.41
1:A:63:GLY:N	2:A:426:HOH:O	2.24	0.41
1:B:79:LYS:HE3	1:B:79:LYS:HB2	1.94	0.41
1:A:61:ILE:HD12	1:A:61:ILE:HA	1.91	0.41
1:D:84:SER:HB3	1:D:153:ILE:HG12	2.03	0.41
1:D:98:LYS:HE2	1:D:121:THR:HG22	2.01	0.41
1:D:321:THR:HG23	1:D:324:ARG:NH1	2.36	0.41
1:A:26:SER:HB3	1:D:9:THR:HG22	2.01	0.41
1:D:85:LYS:HA	1:D:85:LYS:HD3	1.87	0.41
1:B:59:MET:HE3	1:B:61:ILE:HB	2.03	0.41
1:B:158:ILE:HD13	1:B:158:ILE:O	2.21	0.41
1:C:250:ARG:H	1:C:250:ARG:HG2	1.66	0.41
1:A:305:LYS:HG3	1:A:306:SER:N	2.36	0.41
1:D:161:LEU:O	1:D:164:PHE:HB3	2.20	0.41
1:B:75:GLU:HG2	1:B:76:TYR:CG	2.56	0.40
1:C:241:VAL:O	1:C:245:VAL:HG23	2.20	0.40
1:D:4:GLN:NE2	1:D:5:SER:C	2.79	0.40
1:A:176:MET:HE1	1:A:268:ALA:HA	2.03	0.40
1:B:106:GLU:HG2	1:B:111:LYS:HG2	2.03	0.40
1:C:6:MET:HG3	1:D:6:MET:HG2	2.04	0.40
1:C:290:MET:HE2	1:C:290:MET:HB2	1.69	0.40
1:D:126:ILE:HD13	1:D:166:ARG:HD2	2.03	0.40
1:A:172:VAL:HG23	1:A:173:ILE:HD12	2.03	0.40
1:B:19:PRO:HB2	1:B:22:LEU:HD13	2.04	0.40
1:D:273:VAL:HG13	1:D:278:GLU:HG3	2.04	0.40

There are no symmetry-related clashes.

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	287/347 (83%)	269 (94%)	18 (6%)	0	100	100
1	B	287/347 (83%)	270 (94%)	15 (5%)	2 (1%)	18	38
1	C	329/347 (95%)	307 (93%)	19 (6%)	3 (1%)	14	30
1	D	329/347 (95%)	304 (92%)	22 (7%)	3 (1%)	14	30
All	All	1232/1388 (89%)	1150 (93%)	74 (6%)	8 (1%)	21	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	326	GLY
1	C	34	ASN
1	C	285	THR
1	D	34	ASN
1	D	285	THR
1	B	250	ARG
1	B	182	ARG
1	D	326	GLY

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	237/306 (78%)	215 (91%)	22 (9%)	8	18
1	B	244/306 (80%)	229 (94%)	15 (6%)	17	37
1	C	288/306 (94%)	259 (90%)	29 (10%)	7	15
1	D	282/306 (92%)	252 (89%)	30 (11%)	6	14
All	All	1051/1224 (86%)	955 (91%)	96 (9%)	9	19

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	41	THR
1	A	44	LEU
1	A	48	VAL
1	A	49	ASP
1	A	73	ASP
1	A	75	GLU
1	A	137	ILE
1	A	150	ASN
1	A	152	VAL
1	A	158	ILE
1	A	166	ARG
1	A	172	VAL
1	A	177	LEU
1	A	178	ARG
1	A	186	LYS
1	A	202	LEU
1	A	234	GLU
1	A	246	ARG
1	A	291	LEU
1	A	295	ARG
1	A	296	TRP
1	B	41	THR
1	B	49	ASP
1	B	73	ASP
1	B	150	ASN
1	B	152	VAL
1	B	158	ILE
1	B	166	ARG
1	B	172	VAL
1	B	177	LEU
1	B	178	ARG
1	B	191	THR
1	B	285	THR
1	B	287	SER
1	B	288	LEU
1	B	296	TRP
1	C	3	PHE
1	C	11	VAL
1	C	12	VAL
1	C	38	ASN
1	C	61	ILE
1	C	68	THR

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Mol	Chain	Res	Type
1	C	73	ASP
1	C	75	GLU
1	C	82	GLN
1	C	88	LYS
1	C	96	GLU
1	C	103	THR
1	C	107	LYS
1	C	127	GLU
1	C	163	GLU
1	C	169	VAL
1	C	171	ILE
1	C	172	VAL
1	C	177	LEU
1	C	178	ARG
1	C	246	ARG
1	C	250	ARG
1	C	259	ASP
1	C	278	GLU
1	C	290	MET
1	C	294	LYS
1	C	307	ILE
1	C	317	LYS
1	C	333	ASN
1	D	3	PHE
1	D	11	VAL
1	D	12	VAL
1	D	38	ASN
1	D	39	SER
1	D	61	ILE
1	D	68	THR
1	D	73	ASP
1	D	75	GLU
1	D	82	GLN
1	D	88	LYS
1	D	96	GLU
1	D	107	LYS
1	D	163	GLU
1	D	165	LEU
1	D	171	ILE
1	D	172	VAL
1	D	175	GLU
1	D	176	MET

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Mol	Chain	Res	Type
1	D	178	ARG
1	D	225	ASN
1	D	246	ARG
1	D	250	ARG
1	D	259	ASP
1	D	290	MET
1	D	294	LYS
1	D	307	ILE
1	D	317	LYS
1	D	325	THR
1	D	333	ASN

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	238	ASN
1	C	4	GLN
1	C	140	ASN
1	C	170	ASN
1	C	225	ASN
1	C	251	ASN
1	D	4	GLN
1	D	251	ASN

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	291/347 (83%)	-1.14	0 100 100	46, 77, 133, 171	0
1	B	291/347 (83%)	-1.14	0 100 100	44, 78, 140, 162	0
1	C	331/347 (95%)	-1.05	0 100 100	56, 90, 136, 153	0
1	D	331/347 (95%)	-1.05	0 100 100	54, 89, 134, 167	0
All	All	1244/1388 (89%)	-1.09	0 100 100	44, 85, 137, 171	0

There are no RSRZ outliers to report.

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.