



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:13 PM EDT

PDB ID : 3UWX / pdb_00003uwx
Title : Crystal structure of UvrA-UvrB complex
Authors : Pakotiprapha, D.; Jeruzalmi, D.
Deposited on : 2011-12-03
Resolution : 4.40 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

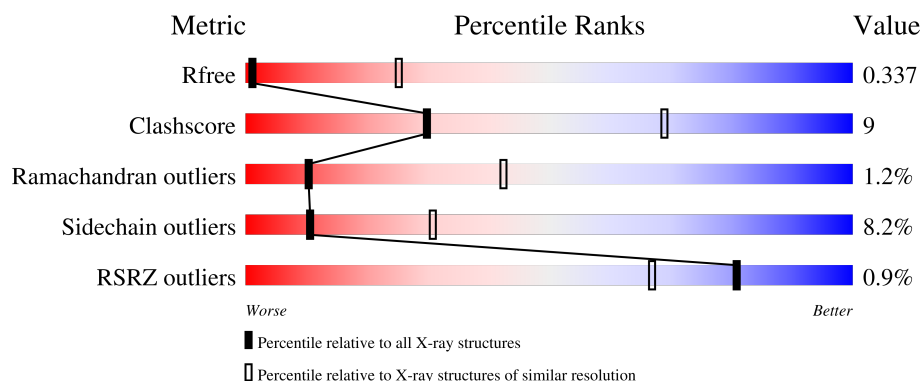
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
Sidechain outliers	187428	1010 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

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	972	% 70% 24% • •
2	B	683	65% 20% • 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12193 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 Excinuclease ABC, A subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	945	7381	4646	1305	1402	28	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP E8SW61
A	-18	GLY	-	expression tag	UNP E8SW61
A	-17	SER	-	expression tag	UNP E8SW61
A	-16	SER	-	expression tag	UNP E8SW61
A	-15	HIS	-	expression tag	UNP E8SW61
A	-14	HIS	-	expression tag	UNP E8SW61
A	-13	HIS	-	expression tag	UNP E8SW61
A	-12	HIS	-	expression tag	UNP E8SW61
A	-11	HIS	-	expression tag	UNP E8SW61
A	-10	HIS	-	expression tag	UNP E8SW61
A	-9	SER	-	expression tag	UNP E8SW61
A	-8	SER	-	expression tag	UNP E8SW61
A	-7	GLY	-	expression tag	UNP E8SW61
A	-6	LEU	-	expression tag	UNP E8SW61
A	-5	VAL	-	expression tag	UNP E8SW61
A	-4	PRO	-	expression tag	UNP E8SW61
A	-3	ARG	-	expression tag	UNP E8SW61
A	-2	GLY	-	expression tag	UNP E8SW61
A	-1	SER	-	expression tag	UNP E8SW61
A	0	HIS	-	expression tag	UNP E8SW61

- Molecule 2 is a protein called UvrABC system protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	595	4809	3031	856	910	12	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-24	MET	-	expression tag	UNP E8SW62
B	-23	GLY	-	expression tag	UNP E8SW62
B	-22	SER	-	expression tag	UNP E8SW62
B	-21	SER	-	expression tag	UNP E8SW62
B	-20	HIS	-	expression tag	UNP E8SW62
B	-19	HIS	-	expression tag	UNP E8SW62
B	-18	HIS	-	expression tag	UNP E8SW62
B	-17	HIS	-	expression tag	UNP E8SW62
B	-16	HIS	-	expression tag	UNP E8SW62
B	-15	HIS	-	expression tag	UNP E8SW62
B	-14	SER	-	expression tag	UNP E8SW62
B	-13	SER	-	expression tag	UNP E8SW62
B	-12	GLY	-	expression tag	UNP E8SW62
B	-11	LEU	-	expression tag	UNP E8SW62
B	-10	VAL	-	expression tag	UNP E8SW62
B	-9	PRO	-	expression tag	UNP E8SW62
B	-8	ARG	-	expression tag	UNP E8SW62
B	-7	GLY	-	expression tag	UNP E8SW62
B	-6	SER	-	expression tag	UNP E8SW62
B	-5	HIS	-	expression tag	UNP E8SW62
B	-3	GLY	-	expression tag	UNP E8SW62
B	-2	PRO	-	expression tag	UNP E8SW62
B	-1	LYS	-	expression tag	UNP E8SW62
B	0	LYS	-	expression tag	UNP E8SW62
B	1	VAL	MET	SEE REMARK 999	UNP E8SW62
B	74	HIS	TYR	SEE REMARK 999	UNP E8SW62

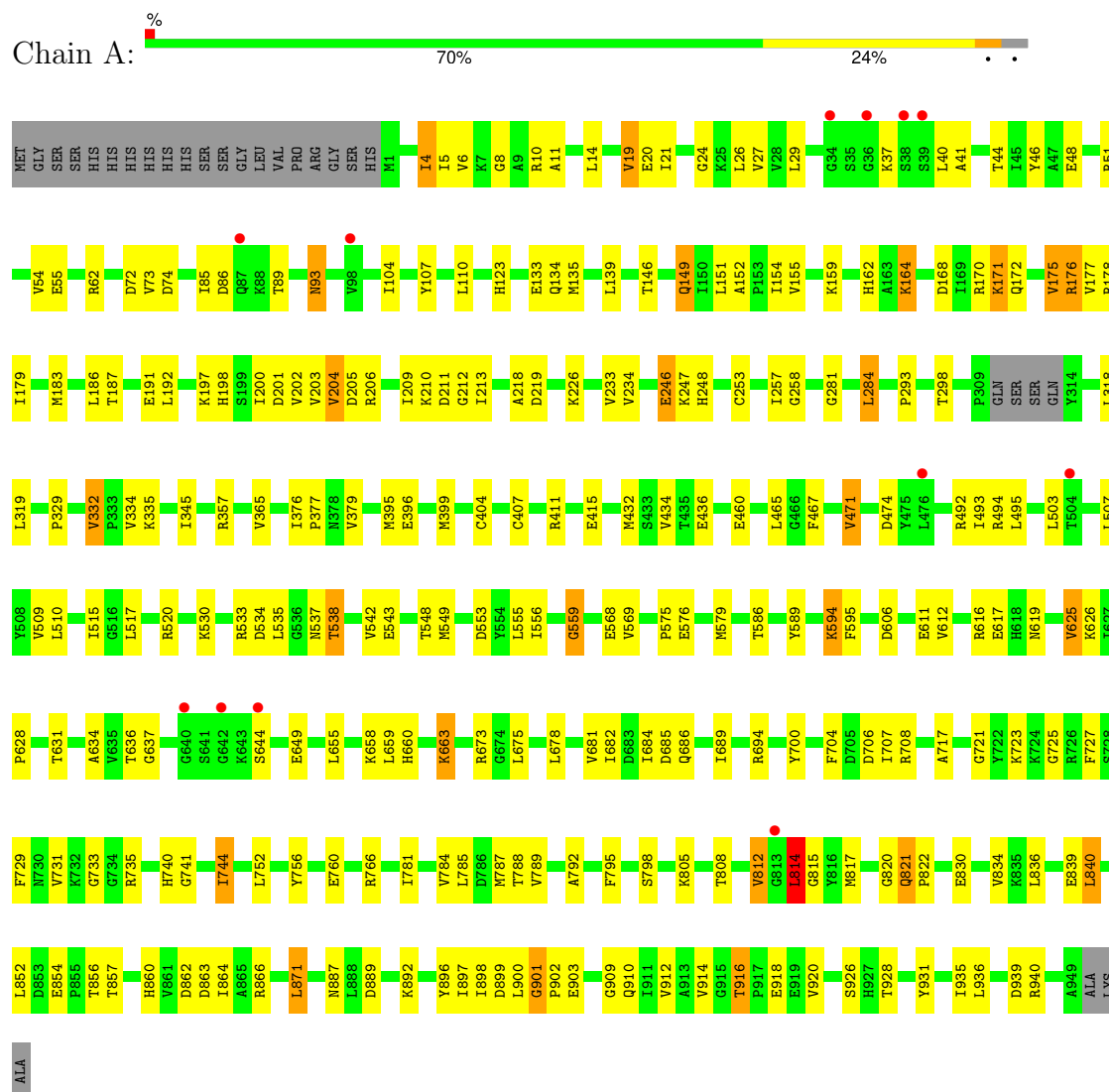
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Zn	0	0
			3	3		

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: Excinuclease ABC, A subunit



• Molecule 2: UvrABC system protein B



GLU	E478	L334	P204	E99	MET
GLU	I479	I335	A205	E100	GLY
THR	K480	I336	S206	Y101	SER
GLU	T481		R207		SER
MET		V342	D208	D106	HIS
TYR	R484	T343	E209		HIS
GLU		L344	H210	E110	HIS
ALA	R489		C211	E111	HIS
LYS		I347	I212	K111	HIS
PRO	L493		D213	D112	HIS
ALA	G494	Y351	V214	A113	SER
ALA	K495		E215	K114	SER
ALA	Y496	K358	F216	I115	GLY
MET	D497				LEU
THR	V498	R367	E220	E118	VAL
THR	L499	L372	I224	I119	PRO
GLN				K121	ARG
GLU	R506	R375	V227	L122	GLY
ARG	E507				SER
ARG		F382	L230	S125	HIS
GLU	V517	K385	L235	L130	MET
GLU	A518	I386	E239	R133	GLY
ILE	I519	Y391	H240	R134	LYS
ARG	L520	I392	V241	D135	LYS
LYS		T395	F244		V1
LEU		P396	R252	V139	E12
GLU	R532	G397			Q19
GLU			A259	V142	A40
ALA	M551	S404		S143	
ALA	Y552	P405	I263	E153	T43
LYS		Q410	E264	E156	
ALA	E565	I411	R270		I49
LEU	E566			E166	P59
LEU	T567	T415	Q288	I167	T60
ASP	K568	D419	R291		L61
PHE				I179	V62
GLU	R571	V424	R298	Q180	N66
ARG		Q430	E307	M184	K67
ALA	Y577	I431		D185	
ALA			R316	I186	A70
GLN	K580	L434	P317	D187	G71
LEU	H581	I438	S320	T192	L73
ARG			T321	F193	L74
ASP	V588	R444	L326	R194	
ILE		L449	D327	V195	V86
ILE	E591	K456	P330	D198	E87
PHE	I592		D331	V199	Y88
GLU	R593	I470	D332		
LEU	D594	K471	F333	I202	Y92
LYS	V595			F203	Y93
LYS					D94
ALA	ILE				
ARG	ARG				
ALA	ALA				
GLU	THR				
GLY	ALA				

4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	216.82Å 216.82Å 116.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.06 – 4.40 38.06 – 4.40	Depositor EDS
% Data completeness (in resolution range)	96.7 (38.06-4.40) 85.4 (38.06-4.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 4.44Å)	Xtriage
Refinement program	PHENIX 1.7.2 _869	Depositor
R, R_{free}	0.288 , 0.349 0.275 , 0.337	Depositor DCC
R_{free} test set	900 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	189.5	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 348.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12193	wwPDB-VP
Average B, all atoms (Å ²)	347.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.31	0/7507	0.79	2/10143 (0.0%)
2	B	0.33	0/4892	0.81	4/6612 (0.1%)
All	All	0.32	0/12399	0.80	6/16755 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	GLY	CA-C-N	6.53	125.76	118.97
2	B	397	GLY	C-N-CA	6.53	125.76	118.97
2	B	244	PHE	CA-C-N	5.79	125.79	119.89
2	B	244	PHE	C-N-CA	5.79	125.79	119.89
1	A	821	GLN	CA-C-N	5.34	125.34	119.90
1	A	821	GLN	C-N-CA	5.34	125.34	119.90

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	7381	0	7458	147	0
2	B	4809	0	4839	68	0
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12193	0	12297	209	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 (209) 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:176:ARG:HB3	1:A:203:VAL:HB	1.61	0.80
1:A:168:ASP:HA	1:A:171:LYS:HB3	1.69	0.75
1:A:432:MET:HE2	1:A:436:GLU:HB3	1.68	0.75
2:B:74:HIS:CE1	2:B:88:TYR:HA	2.22	0.75
1:A:634:ALA:HB3	1:A:897:ILE:HG22	1.70	0.71
2:B:484:ARG:HH11	2:B:484:ARG:HB3	1.57	0.70
2:B:316:ARG:NH2	2:B:321:THR:O	2.25	0.69
1:A:151:LEU:HB2	1:A:233:VAL:HB	1.74	0.68
1:A:789:VAL:HB	1:A:815:GLY:HA2	1.77	0.67
1:A:146:THR:H	1:A:209:ILE:HB	1.60	0.67
2:B:74:HIS:CE1	2:B:139:VAL:HB	2.31	0.65
1:A:162:HIS:HA	1:A:164:LYS:HE2	1.79	0.65
1:A:812:VAL:HG22	1:A:836:LEU:HD12	1.79	0.65
2:B:66:ASN:ND2	2:B:507:GLU:OE2	2.29	0.65
2:B:484:ARG:HH21	2:B:506:ARG:HD3	1.61	0.65
1:A:682:ILE:HG21	1:A:839:GLU:HG2	1.77	0.64
1:A:85:ILE:HG23	1:A:494:ARG:HG2	1.79	0.64
1:A:248:HIS:ND1	1:A:258:GLY:O	2.26	0.64
2:B:264:GLU:OE2	2:B:298:ARG:NH1	2.30	0.62
1:A:729:PHE:HE1	1:A:766:ARG:HB3	1.64	0.62
2:B:74:HIS:HE1	2:B:88:TYR:HA	1.64	0.61
2:B:49:ILE:HG12	2:B:392:ILE:HD11	1.83	0.61
1:A:24:GLY:H	1:A:538:THR:HB	1.67	0.60
2:B:185:ASP:HA	2:B:194:ARG:HD3	1.83	0.60
1:A:54:VAL:HG11	1:A:752:LEU:HD11	1.82	0.60
1:A:123:HIS:HE1	1:A:253:CYS:HB3	1.67	0.59
2:B:419:ASP:O	2:B:571:ARG:NH1	2.28	0.58
1:A:139:LEU:HD22	1:A:234:VAL:HG11	1.85	0.58
1:A:329:PRO:HG2	1:A:332:VAL:HG21	1.86	0.58
2:B:60:THR:HG22	2:B:334:LEU:HB3	1.86	0.57
2:B:112:ASP:OD1	2:B:113:ALA:N	2.37	0.57
2:B:484:ARG:NH2	2:B:506:ARG:HB2	2.19	0.57
1:A:29:LEU:HD23	1:A:556:ILE:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:GLU:HB2	2:B:138:ILE:HG12	1.87	0.57
1:A:179:ILE:HG23	1:A:200:ILE:HG12	1.86	0.57
2:B:489:ARG:NH1	2:B:593:ARG:O	2.37	0.57
1:A:10:ARG:NH2	1:A:72:ASP:OD1	2.38	0.56
1:A:660:HIS:HE1	1:A:681:VAL:H	1.52	0.56
1:A:852:LEU:HD11	1:A:871:LEU:HD11	1.86	0.56
1:A:8:GLY:O	1:A:10:ARG:NH1	2.38	0.56
1:A:284:LEU:HD22	1:A:399:MET:HE3	1.87	0.56
1:A:694:ARG:HA	1:A:729:PHE:HE2	1.70	0.55
1:A:781:ILE:HA	1:A:784:VAL:HG12	1.88	0.55
1:A:379:VAL:HG13	1:A:395:MET:HE3	1.89	0.55
1:A:636:THR:HG21	1:A:928:THR:HG21	1.88	0.55
2:B:214:VAL:HG23	2:B:224:ILE:HG12	1.89	0.54
2:B:184:ASN:ND2	2:B:187:ASP:O	2.40	0.54
1:A:55:GLU:HG2	1:A:62:ARG:HG3	1.89	0.54
1:A:520:ARG:HA	1:A:931:TYR:CZ	2.43	0.54
1:A:467:PHE:O	1:A:471:VAL:HG23	2.08	0.54
1:A:559:GLY:N	1:A:568:GLU:O	2.40	0.53
1:A:178:ARG:HA	1:A:183:MET:HA	1.90	0.53
2:B:156:GLU:OE1	2:B:252:ARG:NH2	2.40	0.53
1:A:170:ARG:HB2	1:A:186:LEU:HD22	1.90	0.53
1:A:404:CYS:HB3	1:A:407:CYS:SG	2.49	0.53
2:B:185:ASP:OD2	2:B:185:ASP:N	2.34	0.52
1:A:177:VAL:HG12	1:A:202:VAL:HG22	1.91	0.52
1:A:549:MET:HE1	1:A:586:THR:HG21	1.90	0.52
1:A:434:VAL:HB	1:A:474:ASP:HA	1.92	0.52
1:A:543:GLU:HG3	1:A:548:THR:HG21	1.90	0.52
1:A:731:VAL:O	1:A:735:ARG:HG2	2.09	0.52
2:B:78:LYS:HA	2:B:86:VAL:HG21	1.90	0.52
1:A:107:TYR:CZ	1:A:460:GLU:HG2	2.45	0.52
1:A:611:GLU:HB2	1:A:673:ARG:HB2	1.91	0.51
2:B:415:THR:HG21	2:B:588:VAL:HG13	1.92	0.51
1:A:4:ILE:HG23	1:A:21:ILE:HB	1.92	0.51
1:A:204:VAL:HG12	2:B:197:GLY:HA3	1.92	0.51
1:A:863:ASP:OD2	1:A:866:ARG:NH2	2.44	0.51
1:A:576:GLU:HA	1:A:579:MET:HE2	1.93	0.51
1:A:44:THR:HG23	1:A:73:VAL:HG21	1.92	0.51
1:A:495:LEU:HD13	1:A:510:LEU:HD21	1.91	0.50
1:A:619:ASN:O	1:A:909:GLY:HA3	2.11	0.50
1:A:172:GLN:O	2:B:196:ARG:NH2	2.42	0.50
1:A:902:PRO:HD3	1:A:912:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:LYS:O	1:A:534:ASP:N	2.43	0.50
1:A:10:ARG:HA	1:A:14:LEU:HB2	1.94	0.49
2:B:449:LEU:HB2	2:B:517:VAL:HG22	1.93	0.49
1:A:735:ARG:NH1	1:A:740:HIS:HA	2.26	0.49
1:A:48:GLU:CD	1:A:51:ARG:HH12	2.21	0.49
1:A:636:THR:OG1	1:A:637:GLY:N	2.43	0.49
1:A:659:LEU:HD12	1:A:681:VAL:HG23	1.95	0.49
2:B:142:VAL:HG12	2:B:347:LEU:HD12	1.94	0.49
1:A:898:ILE:HG23	1:A:914:VAL:HG12	1.95	0.49
1:A:856:THR:HG21	1:A:887:ASN:HD22	1.77	0.49
1:A:175:VAL:HG21	2:B:215:GLU:CD	2.38	0.48
2:B:196:ARG:HB2	2:B:199:VAL:HB	1.93	0.48
1:A:897:ILE:HG13	1:A:920:VAL:HG21	1.95	0.48
2:B:59:PRO:HG2	2:B:330:PRO:HG2	1.95	0.48
2:B:202:ILE:O	2:B:204:PRO:HD3	2.14	0.48
1:A:93:ASN:OD1	1:A:93:ASN:N	2.46	0.48
1:A:6:VAL:HG13	1:A:19:VAL:HG13	1.95	0.48
1:A:735:ARG:HD2	1:A:741:GLY:HA3	1.95	0.48
1:A:830:GLU:O	1:A:834:VAL:HG23	2.13	0.48
1:A:37:LYS:HD2	1:A:542:VAL:HG13	1.96	0.47
1:A:293:PRO:HG3	1:A:663:LYS:NZ	2.29	0.47
1:A:694:ARG:HA	1:A:729:PHE:CE2	2.48	0.47
1:A:396:GLU:HA	1:A:399:MET:HE2	1.95	0.47
1:A:814:LEU:HB3	1:A:815:GLY:H	1.55	0.47
1:A:594:LYS:HE3	1:A:595:PHE:H	1.79	0.47
2:B:99:GLU:OE2	2:B:367:ARG:NH2	2.45	0.47
1:A:293:PRO:HG3	1:A:663:LYS:HZ1	1.79	0.47
2:B:110:GLU:HB3	2:B:112:ASP:H	1.80	0.47
2:B:395:THR:HB	2:B:532:ARG:HG2	1.97	0.47
1:A:171:LYS:NZ	2:B:230:LEU:O	2.47	0.47
2:B:153:GLU:OE2	2:B:252:ARG:HG3	2.15	0.47
2:B:507:GLU:H	2:B:507:GLU:CD	2.21	0.47
1:A:731:VAL:HG12	1:A:733:GLY:H	1.80	0.47
1:A:889:ASP:HA	1:A:892:LYS:HE2	1.96	0.47
1:A:492:ARG:NH1	1:A:515:ILE:O	2.48	0.46
1:A:685:ASP:OD1	1:A:686:GLN:N	2.48	0.46
1:A:281:GLY:HA3	1:A:411:ARG:HG2	1.98	0.46
1:A:533:ARG:NH1	1:A:553:ASP:OD1	2.49	0.46
1:A:520:ARG:NH1	1:A:903:GLU:OE2	2.45	0.46
1:A:684:ILE:HD13	1:A:836:LEU:HA	1.96	0.46
1:A:104:ILE:HD13	1:A:465:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:PRO:HG3	1:A:896:TYR:CG	2.50	0.46
1:A:21:ILE:HG23	1:A:27:VAL:HG21	1.98	0.46
1:A:507:LEU:HA	1:A:538:THR:HG23	1.97	0.46
2:B:382:PHE:O	2:B:386:ILE:HG13	2.15	0.46
1:A:5:ILE:HG12	1:A:20:GLU:HG2	1.98	0.45
1:A:660:HIS:CE1	1:A:681:VAL:H	2.33	0.45
1:A:357:ARG:HH21	1:A:365:VAL:HG21	1.81	0.45
2:B:88:TYR:HB3	2:B:122:LEU:HD13	1.98	0.45
1:A:655:LEU:HB3	1:A:681:VAL:HG21	1.98	0.45
2:B:438:ILE:HD13	2:B:498:VAL:HG21	1.97	0.45
1:A:612:VAL:HG23	1:A:625:VAL:H	1.82	0.45
1:A:916:THR:HG23	1:A:918:GLU:H	1.79	0.45
1:A:123:HIS:CE1	1:A:253:CYS:HB3	2.51	0.45
1:A:549:MET:HB3	1:A:555:LEU:HD11	1.99	0.45
1:A:704:PHE:O	1:A:708:ARG:HG3	2.17	0.45
1:A:689:ILE:HG23	1:A:700:TYR:CD2	2.52	0.45
2:B:317:PRO:O	2:B:320:SER:OG	2.28	0.45
1:A:684:ILE:HB	1:A:852:LEU:HD22	2.00	0.44
2:B:212:ILE:HG12	2:B:241:VAL:HG21	2.00	0.44
1:A:192:LEU:HB3	1:A:198:HIS:NE2	2.33	0.44
1:A:727:PHE:HB3	1:A:781:ILE:HD12	2.00	0.44
2:B:484:ARG:HH11	2:B:484:ARG:CB	2.27	0.44
1:A:46:TYR:HB2	1:A:509:VAL:HG21	2.00	0.44
1:A:135:MET:O	1:A:139:LEU:HG	2.18	0.44
1:A:257:ILE:HD13	1:A:415:GLU:HB2	2.00	0.44
1:A:376:ILE:HB	1:A:377:PRO:HD3	2.00	0.44
1:A:717:ALA:O	1:A:721:GLY:N	2.50	0.44
2:B:43:THR:HG21	2:B:410:GLN:HG2	2.00	0.44
1:A:319:LEU:HD23	1:A:319:LEU:HA	1.85	0.44
1:A:575:PRO:O	1:A:579:MET:HB2	2.17	0.44
1:A:784:VAL:HA	1:A:787:MET:HG3	1.98	0.44
1:A:936:LEU:O	1:A:940:ARG:HB2	2.17	0.44
1:A:589:TYR:OH	1:A:862:ASP:OD1	2.31	0.43
1:A:744:ILE:HG21	1:A:756:TYR:HB3	2.01	0.43
2:B:520:LEU:HA	2:B:552:TYR:HB2	2.00	0.43
2:B:70:ALA:C	2:B:74:HIS:HD2	2.26	0.43
2:B:471:LYS:HB3	2:B:496:TYR:HA	2.01	0.43
1:A:29:LEU:HD12	1:A:41:ALA:HB2	2.00	0.43
1:A:175:VAL:HG22	2:B:213:ARG:NH2	2.34	0.43
2:B:438:ILE:HG21	2:B:470:ILE:HD13	2.01	0.43
2:B:40:ALA:O	2:B:43:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:THR:HB	1:A:209:ILE:HG13	2.00	0.43
1:A:787:MET:HE1	1:A:795:PHE:HB2	2.01	0.43
1:A:503:LEU:O	1:A:537:ASN:ND2	2.34	0.43
1:A:805:LYS:O	1:A:808:THR:OG1	2.28	0.43
2:B:62:VAL:HG13	2:B:139:VAL:HG22	2.01	0.43
2:B:130:LEU:HD23	2:B:130:LEU:HA	1.90	0.43
1:A:159:LYS:HG3	1:A:197:LYS:HG2	2.01	0.43
1:A:171:LYS:HE2	1:A:171:LYS:HB2	1.82	0.43
1:A:788:THR:O	1:A:792:ALA:N	2.46	0.43
2:B:358:LYS:HB3	2:B:372:LEU:HD23	2.01	0.43
1:A:86:ASP:OD2	1:A:89:THR:HG22	2.19	0.42
1:A:298:THR:HA	1:A:332:VAL:O	2.19	0.42
2:B:307:GLU:H	2:B:307:GLU:CD	2.26	0.42
2:B:101:TYR:OH	2:B:106:ASP:OD1	2.35	0.42
1:A:706:ASP:OD1	1:A:706:ASP:N	2.52	0.42
1:A:152:ALA:O	1:A:154:ILE:N	2.53	0.42
2:B:351:TYR:HE1	2:B:375:ARG:HD2	1.85	0.42
1:A:723:LYS:C	1:A:725:GLY:H	2.27	0.42
1:A:860:HIS:O	1:A:864:ILE:HG12	2.20	0.42
2:B:259:ALA:O	2:B:263:ILE:HG13	2.18	0.42
2:B:404:SER:HA	2:B:405:PRO:HD3	1.92	0.42
2:B:430:GLN:HG3	2:B:431:ILE:HD12	2.02	0.42
1:A:785:LEU:HG	1:A:820:GLY:HA3	2.00	0.42
1:A:899:ASP:OD1	1:A:926:SER:OG	2.28	0.42
1:A:471:VAL:HG12	1:A:492:ARG:HD2	2.02	0.42
2:B:419:ASP:HB3	2:B:567:THR:HG23	2.01	0.42
1:A:151:LEU:HB3	1:A:201:ASP:HB3	2.02	0.42
1:A:892:LYS:NZ	1:A:939:ASP:OD2	2.53	0.42
1:A:206:ARG:NH2	2:B:216:PHE:O	2.53	0.41
1:A:535:LEU:HD12	1:A:535:LEU:HA	1.83	0.41
2:B:125:SER:HA	2:B:206:SER:HB2	2.02	0.41
1:A:149:GLN:HE22	1:A:183:MET:HE1	1.86	0.41
1:A:854:GLU:O	1:A:857:THR:HG22	2.20	0.41
2:B:495:LYS:HE2	2:B:495:LYS:HB3	1.75	0.41
1:A:689:ILE:HD11	1:A:834:VAL:HB	2.02	0.41
1:A:808:THR:HG22	1:A:840:LEU:HD12	2.01	0.41
1:A:133:GLU:HG2	1:A:134:GLN:N	2.35	0.41
1:A:589:TYR:HA	1:A:594:LYS:O	2.20	0.41
1:A:821:GLN:HA	1:A:822:PRO:HD3	1.90	0.41
1:A:901:GLY:N	1:A:910:GLN:O	2.54	0.41
1:A:6:VAL:CG1	1:A:19:VAL:HG13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:LEU:HD11	2:B:391:TYR:CE2	2.56	0.41
1:A:658:LYS:HB3	1:A:675:LEU:HD21	2.02	0.41
2:B:519:ILE:HB	2:B:551:MET:HG2	2.03	0.41
1:A:248:HIS:HB3	1:A:257:ILE:HG22	2.02	0.41
1:A:164:LYS:H	1:A:164:LYS:HG3	1.53	0.41
2:B:62:VAL:HG22	2:B:139:VAL:HG13	2.02	0.41
1:A:329:PRO:HG2	1:A:332:VAL:CG2	2.49	0.40
2:B:135:ASP:OD1	2:B:135:ASP:N	2.53	0.40
1:A:211:ASP:O	1:A:213:ILE:N	2.54	0.40
1:A:205:ASP:OD1	1:A:206:ARG:N	2.55	0.40
2:B:327:ASP:OD1	2:B:385:LYS:HE3	2.22	0.40
2:B:577:TYR:CZ	2:B:581:HIS:CE1	3.10	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	941/972 (97%)	855 (91%)	72 (8%)	14 (2%)	8	38
2	B	593/683 (87%)	557 (94%)	32 (5%)	4 (1%)	18	55
All	All	1534/1655 (93%)	1412 (92%)	104 (7%)	18 (1%)	10	42

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	901	GLY
1	A	212	GLY
1	A	559	GLY
1	A	617	GLU
1	A	798	SER
2	B	112	ASP

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Mol	Chain	Res	Type
1	A	74	ASP
1	A	204	VAL
1	A	606	ASP
2	B	143	SER
2	B	180	GLN
1	A	11	ALA
1	A	218	ALA
1	A	814	LEU
2	B	113	ALA
1	A	246	GLU
1	A	247	LYS
1	A	334	VAL

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	796/818 (97%)	748 (94%)	48 (6%)	17	39
2	B	523/592 (88%)	463 (88%)	60 (12%)	5	20
All	All	1319/1410 (94%)	1211 (92%)	108 (8%)	10	31

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	19	VAL
1	A	26	LEU
1	A	40	LEU
1	A	93	ASN
1	A	110	LEU
1	A	149	GLN
1	A	155	VAL
1	A	164	LYS
1	A	171	LYS
1	A	175	VAL

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Mol	Chain	Res	Type
1	A	176	ARG
1	A	187	THR
1	A	191	GLU
1	A	210	LYS
1	A	219	ASP
1	A	226	LYS
1	A	246	GLU
1	A	284	LEU
1	A	318	LEU
1	A	332	VAL
1	A	335	LYS
1	A	345	ILE
1	A	471	VAL
1	A	493	ILE
1	A	517	LEU
1	A	538	THR
1	A	569	VAL
1	A	594	LYS
1	A	616	ARG
1	A	625	VAL
1	A	626	LYS
1	A	631	THR
1	A	644	SER
1	A	649	GLU
1	A	663	LYS
1	A	678	LEU
1	A	707	ILE
1	A	744	ILE
1	A	760	GLU
1	A	812	VAL
1	A	814	LEU
1	A	817	MET
1	A	840	LEU
1	A	871	LEU
1	A	900	LEU
1	A	916	THR
1	A	935	ILE
2	B	12	GLU
2	B	19	GLN
2	B	49	ILE
2	B	62	VAL
2	B	67	LYS

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Mol	Chain	Res	Type
2	B	72	GLN
2	B	92	TYR
2	B	93	TYR
2	B	94	ASP
2	B	114	LYS
2	B	115	ILE
2	B	118	GLU
2	B	120	ASP
2	B	133	ARG
2	B	134	ARG
2	B	166	GLU
2	B	167	ILE
2	B	179	ILE
2	B	180	GLN
2	B	185	ASP
2	B	186	ILE
2	B	187	ASP
2	B	192	THR
2	B	208	ASP
2	B	210	HIS
2	B	212	ILE
2	B	220	GLU
2	B	227	VAL
2	B	235	LEU
2	B	239	GLU
2	B	270	ARG
2	B	288	GLN
2	B	291	ARG
2	B	326	LEU
2	B	336	ILE
2	B	342	VAL
2	B	347	LEU
2	B	358	LYS
2	B	411	ILE
2	B	424	VAL
2	B	444	ARG
2	B	456	LYS
2	B	471	LYS
2	B	478	GLU
2	B	479	ILE
2	B	481	THR
2	B	484	ARG

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Mol	Chain	Res	Type
2	B	489	ARG
2	B	493	LEU
2	B	499	LEU
2	B	506	ARG
2	B	507	GLU
2	B	558	LYS
2	B	561	GLU
2	B	565	GLN
2	B	568	LYS
2	B	580	LYS
2	B	588	VAL
2	B	591	GLU
2	B	592	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	134	GLN
1	A	195	ASN
1	A	302	HIS
1	A	660	HIS
2	B	19	GLN
2	B	74	HIS
2	B	104	GLN
2	B	116	ASN
2	B	288	GLN
2	B	346	GLN
2	B	565	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	945/972 (97%)	-0.24	12 (1%) 75 60	250, 336, 486, 771	0
2	B	595/683 (87%)	-0.32	2 (0%) 90 80	252, 325, 437, 576	0
All	All	1540/1655 (93%)	-0.27	14 (0%) 81 67	250, 332, 468, 771	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	644	SER	4.1
1	A	476	LEU	3.6
1	A	36	GLY	3.3
1	A	34	GLY	2.9
2	B	434	LEU	2.9
1	A	98	VAL	2.8
2	B	332	ASP	2.8
1	A	642	GLY	2.6
1	A	813	GLY	2.6
1	A	38	SER	2.5
1	A	504	THR	2.3
1	A	87	GLN	2.3
1	A	640	GLY	2.2
1	A	39	SER	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	1006	1/1	0.95	0.08	550,550,550,550	0
3	ZN	A	1004	1/1	0.97	0.04	550,550,550,550	0
3	ZN	A	1005	1/1	0.98	0.06	550,550,550,550	0

6.5 Other polymers [i](#)

There are no such residues in this entry.