



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:03 PM UTC

PDB ID : 3A2N / pdb_00003a2n
Title : Crystal structure of DBJA (Wild Type Type II P21)
Authors : Sato, Y.; Senda, T.
Deposited on : 2009-05-23
Resolution : 1.89 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

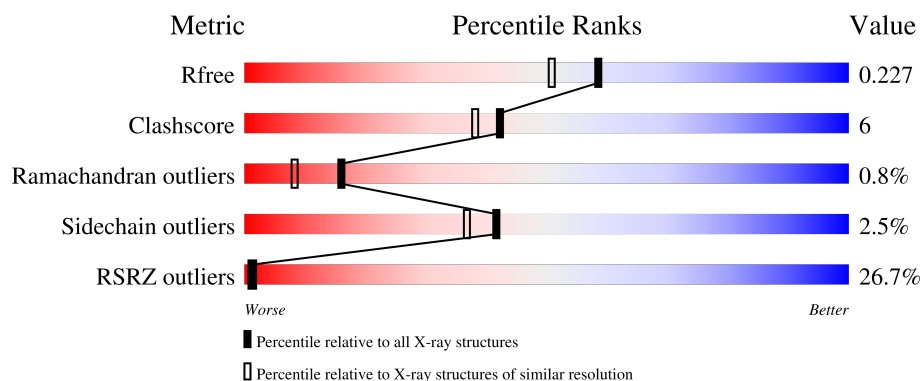
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	312	10% 83% 12% ..
1	B	312	6% 87% 8% ..
1	E	312	79% 77% 17% ..
1	F	312	7% 85% 10% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9801 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 Haloalkane dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2320	1485	415	413	7			
1	B	298	Total	C	N	O	S	0	1	0
			2330	1491	418	414	7			
1	E	298	Total	C	N	O	S	0	0	0
			2320	1485	415	413	7			
1	F	299	Total	C	N	O	S	0	1	0
			2338	1497	419	415	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	VAL	-	SEE REMARK 999	UNP P59337
A	312	ASP	-	SEE REMARK 999	UNP P59337
B	311	VAL	-	SEE REMARK 999	UNP P59337
B	312	ASP	-	SEE REMARK 999	UNP P59337
E	311	VAL	-	SEE REMARK 999	UNP P59337
E	312	ASP	-	SEE REMARK 999	UNP P59337
F	311	VAL	-	SEE REMARK 999	UNP P59337
F	312	ASP	-	SEE REMARK 999	UNP P59337

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	F	1	Total	Cl	0	0
			1	1		

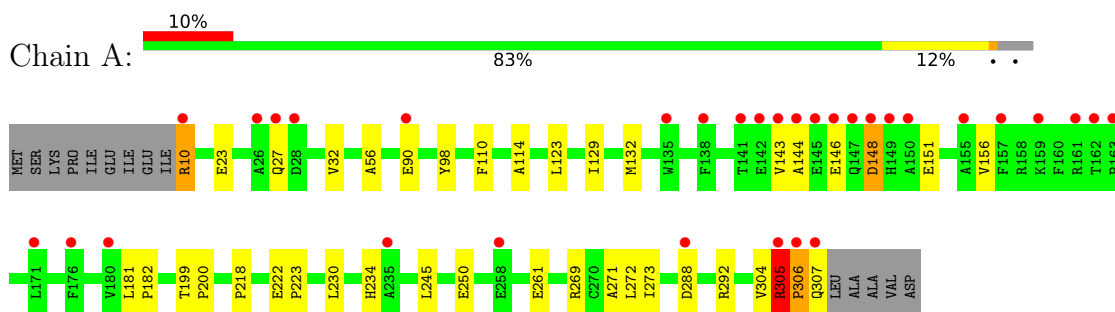
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total 110	O 110	0	0
3	B	162	Total 162	O 162	0	0
3	E	45	Total 45	O 45	0	0
3	F	172	Total 173	O 173	0	1

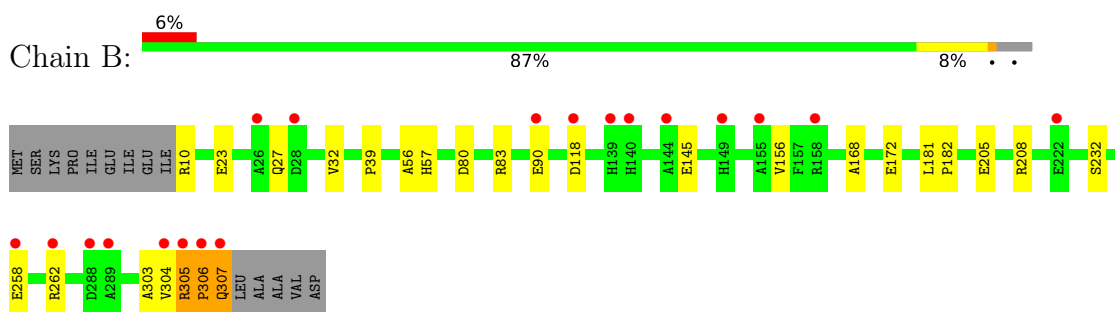
3 Residue-property plots [i](#)

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.

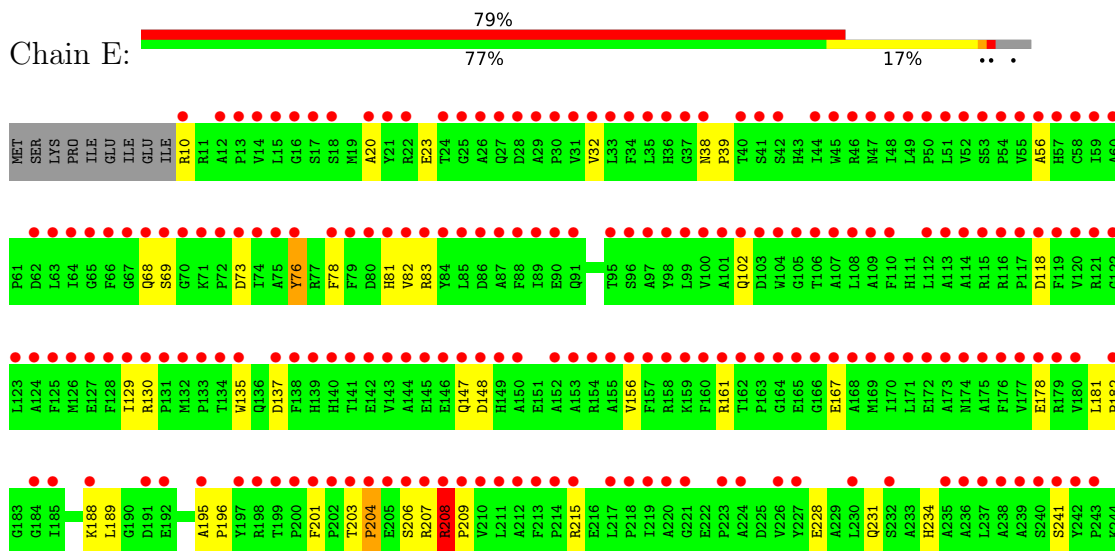
• Molecule 1: Haloalkane dehalogenase

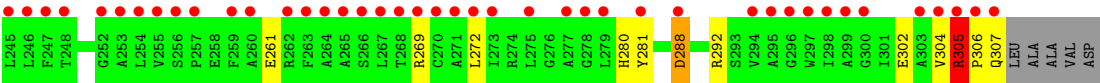


• Molecule 1: Haloalkane dehalogenase

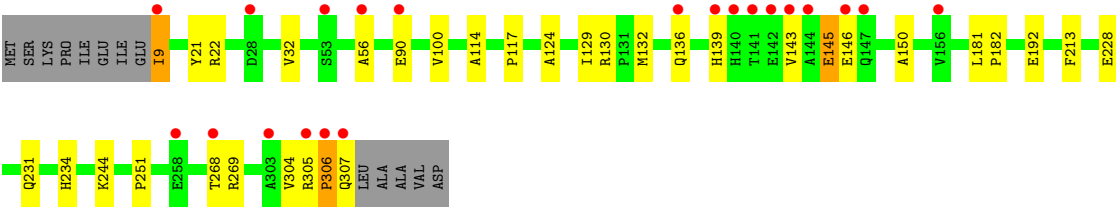
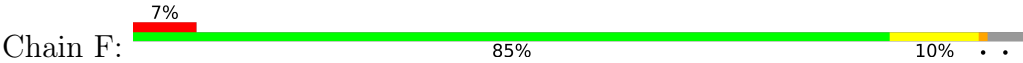


• Molecule 1: Haloalkane dehalogenase





● Molecule 1: Haloalkane dehalogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.53Å 47.77Å 99.41Å 90.00° 93.61° 90.00°	Depositor
Resolution (Å)	32.81 – 1.89 32.81 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.3 (32.81-1.89) 99.2 (32.81-1.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.17 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.192 , 0.228 0.191 , 0.227	Depositor DCC
R_{free} test set	4719 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9801	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0884e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

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	0.73	0/2388	0.83	4/3252 (0.1%)
1	B	0.80	0/2399	0.83	0/3267
1	E	0.94	8/2388 (0.3%)	0.91	2/3252 (0.1%)
1	F	0.82	0/2407	0.88	0/3278
All	All	0.82	8/9582 (0.1%)	0.86	6/13049 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	76	TYR	C-O	17.54	1.46	1.23
1	E	73	ASP	CG-OD2	14.87	1.53	1.25
1	E	73	ASP	CG-OD1	12.32	1.48	1.25
1	E	81	HIS	CE1-NE2	7.66	1.40	1.32
1	E	81	HIS	CG-CD2	6.55	1.43	1.35
1	E	208	ARG	CZ-NH1	6.14	1.41	1.32
1	E	68	GLN	C-N	5.72	1.41	1.33
1	E	76	TYR	CA-C	5.34	1.60	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	MET	CA-C-N	5.30	125.36	119.32
1	A	132	MET	C-N-CA	5.30	125.36	119.32
1	E	305	ARG	CA-C-N	-5.03	114.77	119.85
1	E	305	ARG	C-N-CA	-5.03	114.77	119.85
1	A	305	ARG	CA-C-N	5.03	126.13	119.84
1	A	305	ARG	C-N-CA	5.03	126.13	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	2320	0	2268	28	0
1	B	2330	0	2274	33	0
1	E	2320	0	2268	40	0
1	F	2338	0	2285	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	F	1	0	0	0	0
3	A	110	0	0	1	0
3	B	162	0	0	3	0
3	E	45	0	0	3	0
3	F	173	0	0	2	0
All	All	9801	0	9095	115	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 6.

All (115) 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:E:188:LYS:HD3	3:E:327:HOH:O	1.57	1.00
1:B:305:ARG:HB2	1:B:306:PRO:HD2	1.44	1.00
1:E:304:VAL:HG21	1:F:304:VAL:HG23	1.63	0.81
1:F:9:ILE:HG23	1:F:21:TYR:O	1.80	0.81
1:B:307:GLN:HG3	1:F:117:PRO:HB3	1.65	0.79
1:E:304:VAL:CG2	1:F:304:VAL:HG23	2.14	0.78
1:B:83:ARG:HD3	3:B:407:HOH:O	1.85	0.76
1:A:269:ARG:HH22	1:B:307:GLN:NE2	1.87	0.73
1:A:304:VAL:CG2	1:B:304:VAL:HG23	2.20	0.72
1:B:258:GLU:HG2	1:B:262:ARG:NH1	2.04	0.71
1:A:304:VAL:HG21	1:B:304:VAL:HG23	1.73	0.70
1:B:208:ARG:HB2	3:B:396:HOH:O	1.92	0.70
1:F:9:ILE:HG21	1:F:22:ARG:HG3	1.75	0.69
1:B:305:ARG:CB	1:B:306:PRO:HD2	2.22	0.69
1:F:90:GLU:HG2	3:F:433:HOH:O	1.93	0.68
1:B:306:PRO:HA	1:F:114:ALA:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:HB3	1:A:182:PRO:HD3	1.77	0.66
1:B:10:ARG:CZ	1:B:23:GLU:OE1	2.44	0.66
1:E:302:GLU:O	1:E:305:ARG:HG2	1.95	0.66
1:A:304:VAL:CG2	1:B:304:VAL:CG2	2.75	0.64
1:E:304:VAL:O	1:E:305:ARG:O	2.17	0.63
1:E:305:ARG:HB2	1:E:306:PRO:CD	2.29	0.62
1:B:258:GLU:HG2	1:B:262:ARG:HH11	1.64	0.62
1:F:146:GLU:HG3	1:F:251:PRO:CB	2.31	0.60
1:B:181:LEU:HB3	1:B:182:PRO:HD3	1.82	0.60
1:A:269:ARG:NH2	1:B:307:GLN:HB2	2.16	0.60
1:E:188:LYS:HE3	1:E:189:LEU:O	2.01	0.60
1:E:83:ARG:HD2	3:E:350:HOH:O	2.02	0.58
1:F:9:ILE:HG21	1:F:22:ARG:CG	2.33	0.58
1:A:269:ARG:HD3	1:B:303:ALA:O	2.03	0.57
1:E:228:GLU:HA	1:E:231:GLN:HE21	1.68	0.57
1:B:90:GLU:HG2	3:B:362:HOH:O	2.05	0.57
1:A:222:GLU:HA	1:A:223:PRO:C	2.29	0.57
1:E:201:PHE:HB3	1:E:207:ARG:HG2	1.87	0.57
1:E:304:VAL:CG2	1:F:304:VAL:CG2	2.81	0.56
1:B:307:GLN:HG3	1:F:117:PRO:CB	2.35	0.56
1:A:288:ASP:O	1:A:292:ARG:HG2	2.07	0.55
1:E:161:ARG:HA	1:E:215:ARG:HG2	1.89	0.55
1:F:139[B]:HIS:ND1	1:F:150:ALA:HA	2.21	0.55
1:B:80:ASP:OD1	1:B:83:ARG:NH2	2.39	0.54
1:A:304:VAL:HG23	1:B:304:VAL:CG2	2.38	0.54
1:A:114:ALA:O	1:E:307:GLN:N	2.41	0.54
1:F:130:ARG:NH1	3:F:414:HOH:O	2.36	0.54
1:B:32:VAL:HG23	1:B:56:ALA:HB1	1.91	0.53
1:F:268:THR:HG22	1:F:269:ARG:HD2	1.90	0.53
1:B:304:VAL:O	1:B:305:ARG:O	2.26	0.53
1:B:305:ARG:HB2	1:B:306:PRO:CD	2.29	0.53
1:B:307:GLN:N	1:F:114:ALA:O	2.36	0.52
1:B:305:ARG:CB	1:B:306:PRO:CD	2.88	0.52
1:E:102:GLN:NE2	1:E:281:TYR:HA	2.26	0.51
1:E:305:ARG:HB2	1:E:306:PRO:HD2	1.93	0.50
1:A:218:PRO:HG3	1:A:230:LEU:HD12	1.92	0.50
1:E:203:THR:O	1:E:206:SER:N	2.42	0.50
1:E:288:ASP:O	1:E:292:ARG:HG2	2.12	0.50
1:F:136:GLN:H	1:F:136:GLN:CD	2.21	0.49
1:A:305:ARG:HB2	1:A:306:PRO:HD2	1.92	0.49
1:E:38:ASN:OD1	1:E:39:PRO:HA	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:ILE:CG2	1:F:22:ARG:HG3	2.42	0.49
1:A:269:ARG:HH22	1:B:307:GLN:HE21	1.57	0.49
1:F:143:VAL:HG11	1:F:146:GLU:HG2	1.94	0.49
1:A:261:GLU:HA	1:A:272:LEU:HD22	1.95	0.49
1:A:90:GLU:HG2	3:A:332:HOH:O	2.13	0.49
1:A:306:PRO:O	1:A:307:GLN:HB2	2.13	0.48
1:F:146:GLU:HG3	1:F:251:PRO:HB3	1.95	0.48
1:B:27:GLN:HG2	1:B:57:HIS:CE1	2.49	0.48
1:A:110:PHE:HE1	1:A:123:LEU:HD21	1.79	0.48
1:F:32:VAL:HG23	1:F:56:ALA:HB1	1.95	0.48
1:E:167:GLU:CD	1:E:215:ARG:HH22	2.23	0.47
1:A:129:ILE:O	1:A:234:HIS:HE1	1.97	0.47
1:A:148:ASP:N	1:A:148:ASP:OD1	2.48	0.47
1:B:10:ARG:NH1	1:B:23:GLU:OE1	2.48	0.47
1:F:143:VAL:CG1	1:F:146:GLU:HG2	2.45	0.47
1:A:32:VAL:HG22	1:A:98:TYR:HB2	1.97	0.46
1:F:244:LYS:HE2	1:F:268:THR:O	2.15	0.46
1:E:130:ARG:HA	1:E:234:HIS:CE1	2.51	0.46
1:E:102:GLN:NE2	1:E:280:HIS:O	2.48	0.45
1:E:304:VAL:HG23	1:F:304:VAL:CG2	2.47	0.45
1:E:188:LYS:HD2	1:E:189:LEU:N	2.32	0.45
1:F:136:GLN:CD	1:F:136:GLN:N	2.75	0.45
1:E:76:TYR:CE2	1:E:209:PRO:HG3	2.52	0.45
1:E:181:LEU:HB3	1:E:182:PRO:HD3	1.99	0.44
1:B:307:GLN:C	1:F:117:PRO:HB3	2.42	0.44
1:E:208:ARG:HB3	1:E:209:PRO:HD3	2.00	0.43
1:A:304:VAL:CG2	1:B:304:VAL:HG21	2.47	0.43
1:E:135:TRP:C	1:E:137:ASP:H	2.27	0.43
1:F:268:THR:HG22	1:F:269:ARG:CD	2.48	0.43
1:B:168:ALA:O	1:B:172:GLU:HB3	2.18	0.43
1:A:245:LEU:HD12	1:A:271:ALA:HB3	2.01	0.43
1:F:305:ARG:O	1:F:306:PRO:C	2.61	0.43
1:F:130:ARG:O	1:F:132:MET:HG3	2.19	0.43
1:A:32:VAL:HG23	1:A:56:ALA:HB1	2.01	0.43
1:A:304:VAL:HG23	1:B:304:VAL:HG21	2.00	0.43
1:E:203:THR:O	1:E:204:PRO:C	2.61	0.43
1:E:32:VAL:HG23	1:E:56:ALA:HB1	2.01	0.43
1:F:129:ILE:O	1:F:234:HIS:HE1	2.02	0.43
1:E:261:GLU:HA	1:E:272:LEU:HD22	1.99	0.42
1:F:228:GLU:HA	1:F:231:GLN:HE21	1.82	0.42
1:E:78:PHE:O	1:E:82:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:ALA:HB3	1:E:196:PRO:HD3	2.02	0.42
1:F:181:LEU:HB3	1:F:182:PRO:HD3	2.00	0.42
1:E:20:ALA:H	1:E:69:SER:HA	1.85	0.42
1:E:10:ARG:CZ	1:E:23:GLU:HB3	2.50	0.42
1:F:145:GLU:H	1:F:145:GLU:CD	2.28	0.42
1:E:102:GLN:HE22	1:E:281:TYR:HA	1.83	0.41
1:B:305:ARG:HG3	1:B:306:PRO:N	2.35	0.41
1:E:129:ILE:O	1:E:234:HIS:HE1	2.03	0.41
1:E:269:ARG:HH21	1:F:307:GLN:HG2	1.85	0.41
1:F:146:GLU:HG3	1:F:251:PRO:HB2	2.03	0.41
1:E:178:GLU:O	1:E:182:PRO:HG2	2.20	0.41
1:F:100:VAL:HA	1:F:124:ALA:O	2.21	0.41
1:A:199:THR:N	1:A:200:PRO:CD	2.84	0.41
1:A:245:LEU:HG	1:A:273:ILE:CD1	2.50	0.41
1:E:118:ASP:HB2	3:E:316:HOH:O	2.20	0.40
1:A:10:ARG:NH1	1:A:23:GLU:H	2.19	0.40
1:E:241:SER:O	1:E:269:ARG:HD2	2.20	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	296/312 (95%)	282 (95%)	12 (4%)	2 (1%)	18	10
1	B	297/312 (95%)	287 (97%)	8 (3%)	2 (1%)	18	10
1	E	296/312 (95%)	281 (95%)	11 (4%)	4 (1%)	9	3
1	F	298/312 (96%)	289 (97%)	8 (3%)	1 (0%)	36	29
All	All	1187/1248 (95%)	1139 (96%)	39 (3%)	9 (1%)	16	8

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	ALA
1	B	305	ARG
1	E	148	ASP
1	E	305	ARG
1	F	306	PRO
1	A	306	PRO
1	B	306	PRO
1	E	147	GLN
1	E	204	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	232/244 (95%)	223 (96%)	9 (4%)	28	21
1	B	233/244 (96%)	226 (97%)	7 (3%)	36	30
1	E	232/244 (95%)	229 (99%)	3 (1%)	61	61
1	F	234/244 (96%)	230 (98%)	4 (2%)	53	52
All	All	931/976 (95%)	908 (98%)	23 (2%)	42	37

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	27	GLN
1	A	143	VAL
1	A	146	GLU
1	A	148	ASP
1	A	151	GLU
1	A	156	VAL
1	A	250	GLU
1	A	305	ARG
1	B	39	PRO
1	B	118	ASP
1	B	145	GLU
1	B	156	VAL

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Mol	Chain	Res	Type
1	B	205	GLU
1	B	232	SER
1	B	307	GLN
1	E	156	VAL
1	E	208	ARG
1	E	288	ASP
1	F	9	ILE
1	F	145	GLU
1	F	192	GLU
1	F	213	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	234	HIS
1	B	234	HIS
1	E	81	HIS
1	E	111	HIS
1	E	139	HIS
1	E	231	GLN
1	E	234	HIS
1	F	231	GLN
1	F	234	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	298/312 (95%)	0.90	32 (10%)	11 11	20, 26, 39, 55	0
1	B	298/312 (95%)	0.52	19 (6%)	25 27	14, 23, 33, 51	1 (0%)
1	E	298/312 (95%)	3.38	246 (82%)	0 0	24, 39, 60, 64	0
1	F	299/312 (95%)	0.53	21 (7%)	22 24	13, 20, 33, 58	1 (0%)
All	All	1193/1248 (95%)	1.34	318 (26%)	1 1	13, 25, 48, 64	2 (0%)

All (318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	307	GLN	8.6
1	E	134	THR	7.6
1	B	306	PRO	7.3
1	E	128	PHE	7.2
1	E	132	MET	7.0
1	E	203	THR	7.0
1	E	160	PHE	6.9
1	A	306	PRO	6.9
1	E	74	ILE	6.9
1	E	125	PHE	6.8
1	E	76	TYR	6.8
1	E	129	ILE	6.8
1	E	14	VAL	6.7
1	E	177	VAL	6.3
1	F	306	PRO	6.2
1	E	306	PRO	6.2
1	F	307	GLN	6.1
1	B	307	GLN	6.1
1	E	98	TYR	6.0
1	E	70	GLY	6.0
1	E	124	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	F	9	ILE	5.8
1	E	55	VAL	5.7
1	B	305	ARG	5.7
1	E	168	ALA	5.6
1	E	182	PRO	5.6
1	E	122	GLY	5.5
1	A	141	THR	5.4
1	E	206	SER	5.4
1	E	26	ALA	5.3
1	E	108	LEU	5.3
1	E	170	ILE	5.3
1	E	176	PHE	5.2
1	E	51	LEU	5.2
1	E	171	LEU	5.2
1	E	33	LEU	5.2
1	E	226	VAL	5.2
1	E	131	PRO	5.1
1	A	307	GLN	5.0
1	E	201	PHE	5.0
1	A	143	VAL	5.0
1	E	79	PHE	5.0
1	E	34	PHE	5.0
1	E	143	VAL	4.9
1	E	119	PHE	4.9
1	E	75	ALA	4.9
1	E	96	SER	4.8
1	E	123	LEU	4.8
1	E	149	HIS	4.8
1	E	184	GLY	4.8
1	E	21	TYR	4.8
1	E	117	PRO	4.7
1	E	200	PRO	4.7
1	E	255	VAL	4.7
1	E	106	THR	4.7
1	E	305	ARG	4.7
1	E	18	SER	4.7
1	E	109	ALA	4.7
1	E	127	GLU	4.7
1	E	156	VAL	4.6
1	E	13	PRO	4.6
1	E	30	PRO	4.6
1	E	144	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	195	ALA	4.6
1	E	165	GLU	4.6
1	E	167	GLU	4.6
1	E	146	GLU	4.5
1	E	47	ASN	4.5
1	E	82	VAL	4.5
1	E	44	ILE	4.5
1	E	54	PRO	4.5
1	E	299	ALA	4.5
1	E	102	GLN	4.5
1	E	268	THR	4.5
1	E	150	ALA	4.5
1	E	264	ALA	4.4
1	E	105	GLY	4.4
1	E	267	LEU	4.4
1	E	130	ARG	4.4
1	E	16	GLY	4.4
1	E	110	PHE	4.4
1	E	213	PHE	4.4
1	E	72	PRO	4.4
1	E	212	ALA	4.4
1	A	28	ASP	4.3
1	E	275	LEU	4.3
1	E	133	PRO	4.3
1	E	113	ALA	4.3
1	E	252	GLY	4.3
1	E	162	THR	4.2
1	E	42	SER	4.2
1	E	153	ALA	4.2
1	E	204	PRO	4.2
1	E	208	ARG	4.2
1	E	56	ALA	4.2
1	E	107	ALA	4.2
1	E	35	LEU	4.2
1	E	100	VAL	4.2
1	E	24	THR	4.2
1	E	87	ALA	4.1
1	E	97	ALA	4.1
1	E	214	PRO	4.1
1	E	12	ALA	4.1
1	E	50	PRO	4.1
1	E	159	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	258	GLU	4.1
1	E	272	LEU	4.0
1	E	148	ASP	4.0
1	E	126	MET	4.0
1	E	32	VAL	4.0
1	E	173	ALA	4.0
1	E	114	ALA	4.0
1	E	271	ALA	4.0
1	E	25	GLY	3.9
1	E	197	TYR	3.9
1	E	223	PRO	3.9
1	E	135	TRP	3.8
1	F	303	ALA	3.8
1	E	157	PHE	3.8
1	E	69	SER	3.8
1	E	49	LEU	3.8
1	A	26	ALA	3.8
1	E	101	ALA	3.8
1	E	31	VAL	3.7
1	E	118	ASP	3.7
1	E	191	ASP	3.7
1	E	253	ALA	3.7
1	E	120	VAL	3.7
1	E	138	PHE	3.7
1	E	296	GLY	3.7
1	E	202	PRO	3.7
1	E	155	ALA	3.7
1	E	219	ILE	3.7
1	E	273	ILE	3.7
1	E	38	ASN	3.7
1	E	158	ARG	3.7
1	E	81	HIS	3.6
1	E	288	ASP	3.6
1	E	265	ALA	3.6
1	E	164	GLY	3.6
1	E	48	ILE	3.6
1	E	103	ASP	3.6
1	E	10	ARG	3.6
1	E	185	ILE	3.6
1	E	141	THR	3.6
1	E	78	PHE	3.6
1	E	99	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	175	ALA	3.5
1	E	205	GLU	3.5
1	E	112	LEU	3.5
1	E	95	THR	3.4
1	E	104	TRP	3.4
1	E	139	HIS	3.4
1	E	245	LEU	3.4
1	A	142	GLU	3.4
1	E	145	GLU	3.4
1	A	144	ALA	3.4
1	E	235	ALA	3.4
1	E	163	PRO	3.4
1	E	270	CYS	3.4
1	E	65	GLY	3.3
1	E	166	GLY	3.3
1	B	304	VAL	3.3
1	E	20	ALA	3.3
1	E	64	ILE	3.3
1	E	169	MET	3.3
1	E	66	PHE	3.3
1	B	288	ASP	3.3
1	F	305	ARG	3.3
1	E	174	ASN	3.3
1	E	217	LEU	3.3
1	E	121	ARG	3.3
1	E	84	TYR	3.2
1	E	147	GLN	3.2
1	E	239	ALA	3.2
1	E	199	THR	3.2
1	E	83	ARG	3.2
1	F	144	ALA	3.2
1	E	40	THR	3.2
1	E	254	LEU	3.2
1	E	192	GLU	3.2
1	E	240	SER	3.2
1	F	146	GLU	3.2
1	E	243	PRO	3.2
1	E	36	HIS	3.2
1	A	163	PRO	3.1
1	B	118	ASP	3.1
1	E	90	GLU	3.1
1	E	137	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	71	LYS	3.1
1	E	116	ARG	3.1
1	E	260	ALA	3.1
1	E	179	ARG	3.1
1	A	148	ASP	3.0
1	E	230	LEU	3.0
1	E	297	TRP	3.0
1	E	37	GLY	3.0
1	E	88	PHE	3.0
1	E	58	CYS	3.0
1	B	144	ALA	3.0
1	A	27	GLN	3.0
1	E	263	PHE	3.0
1	E	238	ALA	3.0
1	E	45	TRP	2.9
1	E	178	GLU	2.9
1	E	53	SER	2.9
1	E	161	ARG	2.9
1	F	28	ASP	2.9
1	E	180	VAL	2.9
1	E	227	TYR	2.9
1	E	188	LYS	2.9
1	E	73	ASP	2.9
1	E	89	ILE	2.9
1	F	143	VAL	2.9
1	E	210	VAL	2.8
1	E	140	HIS	2.8
1	E	29	ALA	2.8
1	A	147	GLN	2.8
1	E	220	ALA	2.8
1	E	224	ALA	2.8
1	E	85	LEU	2.8
1	E	142	GLU	2.8
1	E	209	PRO	2.8
1	E	17	SER	2.8
1	E	152	ALA	2.8
1	E	211	LEU	2.8
1	B	26	ALA	2.7
1	A	258	GLU	2.7
1	E	236	ALA	2.7
1	E	242	TYR	2.7
1	A	305	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	68	GLN	2.7
1	E	115	ARG	2.7
1	B	222	GLU	2.7
1	E	278	GLY	2.7
1	E	80	ASP	2.7
1	F	141	THR	2.7
1	E	237	LEU	2.7
1	E	246	LEU	2.7
1	E	266	SER	2.6
1	B	149	HIS	2.6
1	F	140	HIS	2.6
1	E	294	VAL	2.6
1	A	10	ARG	2.6
1	A	138	PHE	2.6
1	E	279	LEU	2.6
1	A	145	GLU	2.6
1	E	277	ALA	2.6
1	A	288	ASP	2.6
1	E	304	VAL	2.6
1	F	268	THR	2.6
1	E	218	PRO	2.5
1	A	157	PHE	2.5
1	B	262	ARG	2.5
1	F	53	SER	2.5
1	B	155	ALA	2.5
1	E	207	ARG	2.5
1	E	232	SER	2.5
1	F	136	GLN	2.5
1	A	150	ALA	2.5
1	E	303	ALA	2.5
1	E	248	THR	2.4
1	B	158	ARG	2.4
1	E	67	GLY	2.4
1	E	198	ARG	2.4
1	E	300	GLY	2.4
1	E	63	LEU	2.4
1	B	28	ASP	2.4
1	E	46	ARG	2.4
1	E	86	ASP	2.3
1	E	281	TYR	2.3
1	A	146	GLU	2.3
1	E	256	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	215	ARG	2.3
1	E	15	LEU	2.3
1	E	259	PHE	2.3
1	B	139[A]	HIS	2.3
1	E	60	ALA	2.3
1	E	172	GLU	2.3
1	B	140	HIS	2.3
1	F	139[A]	HIS	2.3
1	E	22	ARG	2.3
1	E	262	ARG	2.3
1	E	41	SER	2.3
1	E	52	VAL	2.3
1	A	135	TRP	2.2
1	E	27	GLN	2.2
1	A	180	VAL	2.2
1	A	149	HIS	2.2
1	E	269	ARG	2.2
1	A	159	LYS	2.2
1	B	90	GLU	2.2
1	F	147	GLN	2.2
1	E	62	ASP	2.2
1	A	155	ALA	2.2
1	F	56	ALA	2.2
1	A	176	PHE	2.2
1	E	298	ILE	2.2
1	E	257	PRO	2.2
1	A	235	ALA	2.2
1	B	289	ALA	2.2
1	A	161	ARG	2.2
1	E	247	PHE	2.1
1	A	162	THR	2.1
1	B	258	GLU	2.1
1	E	59	ILE	2.1
1	F	90	GLU	2.1
1	F	142	GLU	2.1
1	E	91	GLN	2.1
1	A	90	GLU	2.1
1	E	57	HIS	2.1
1	F	156	VAL	2.1
1	A	171	LEU	2.1
1	E	28	ASP	2.1
1	E	241	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	154	ARG	2.0
1	E	295	ALA	2.0
1	E	221	GLY	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](#)

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(Å ²)	Q<0.9
2	CL	A	313	1/1	0.97	0.10	15,15,15,15	0
2	CL	B	313	1/1	0.99	0.12	12,12,12,12	0
2	CL	F	313	1/1	0.99	0.09	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.