



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:15 AM GMT

PDB ID : 3A2N  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

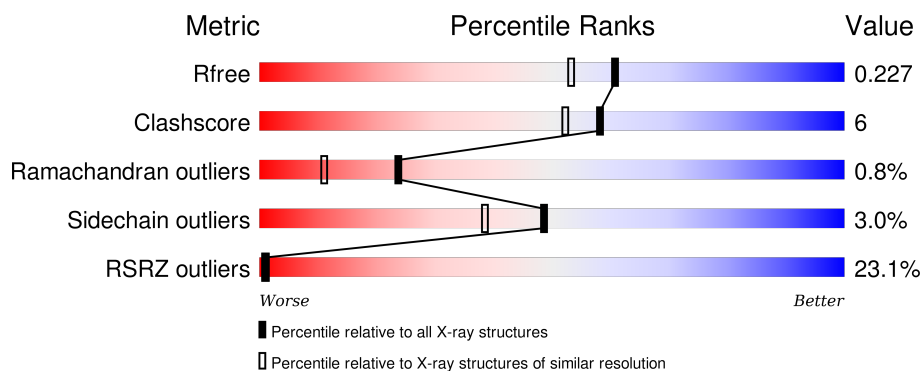
# 1 Overall quality at a glance

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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>18%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>
1	B	312	<div> <div>10%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>• •</div> </div> </div>
1	E	312	<div> <div>44%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• •</div> </div> </div>
1	F	312	<div> <div>16%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>• •</div> </div> </div>

## 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 (three-letter code: CL) (formula: Cl).

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

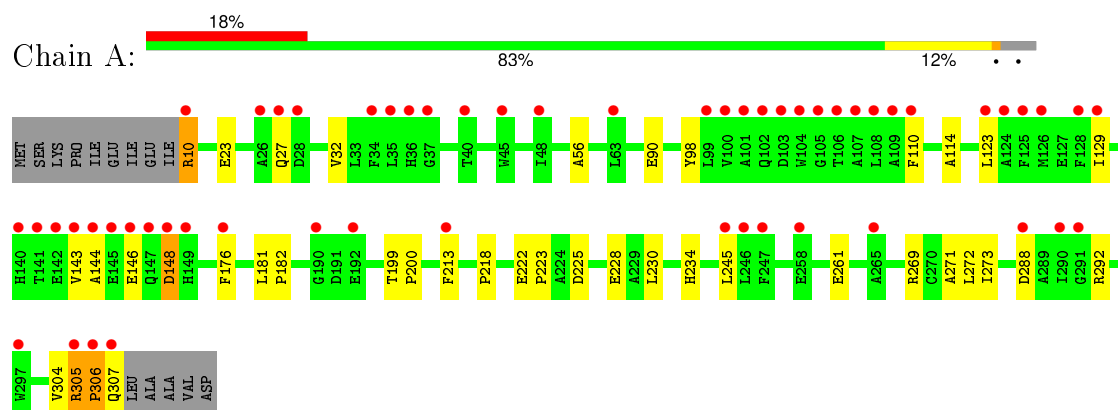
- Molecule 3 is water.

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

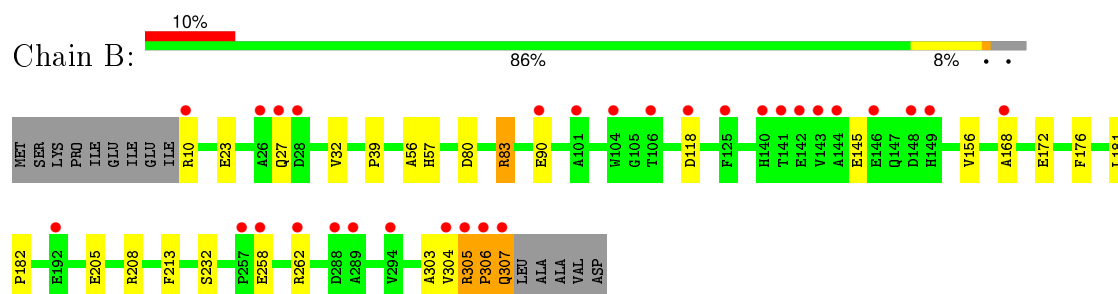
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

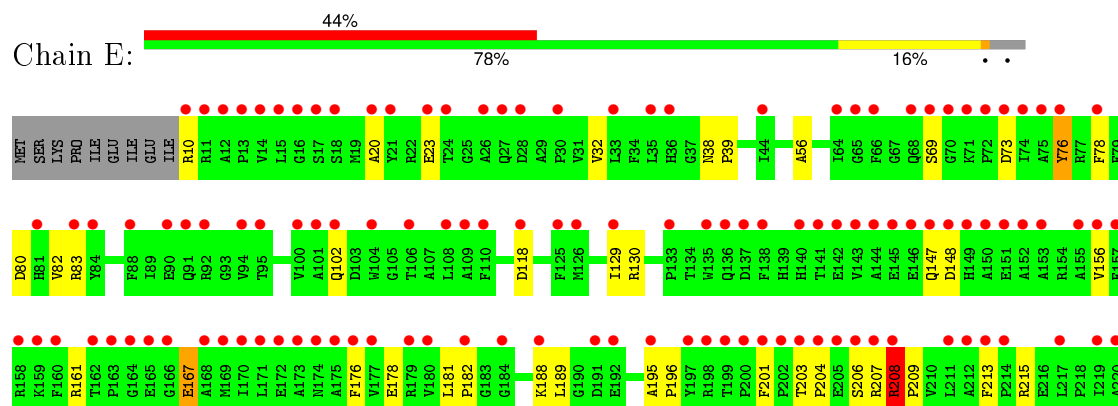
- Molecule 1: Haloalkane dehalogenase

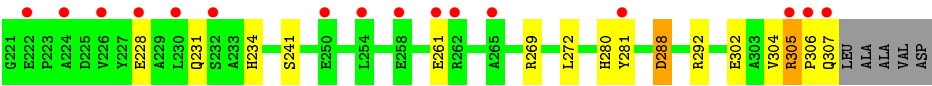


- Molecule 1: Haloalkane dehalogenase

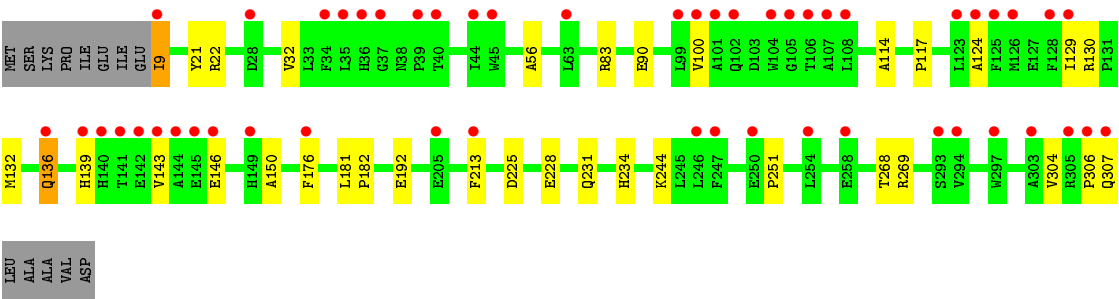
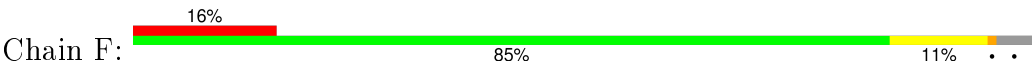


- Molecule 1: Haloalkane dehalogenase





● Molecule 1: Haloalkane dehalogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.53 Å 47.77 Å 99.41 Å 90.00° 93.61° 90.00°	Depositor
Resolution (Å)	32.81 – 1.89 31.49 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.3 (32.81-1.89) 99.3 (31.49-1.89)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.17 (at 1.89 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.192 , 0.228 0.191 , 0.227	Depositor DCC
$R_{free}$ test set	4719 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 53.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 94027 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9801	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.59	0/2388	0.61	1/3252 (0.0%)
1	B	0.65	0/2399	0.66	1/3267 (0.0%)
1	E	0.77	6/2388 (0.3%)	0.69	5/3252 (0.2%)
1	F	0.68	0/2407	0.69	2/3278 (0.1%)
All	All	0.68	6/9582 (0.1%)	0.66	9/13049 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	73	ASP	CG-OD2	12.28	1.53	1.25
1	E	76	TYR	C-O	12.03	1.46	1.23
1	E	73	ASP	CG-OD1	10.18	1.48	1.25
1	E	167	GLU	CD-OE1	8.03	1.34	1.25
1	E	208	ARG	CZ-NH1	6.38	1.41	1.33
1	E	76	TYR	CG-CD1	5.92	1.46	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	73	ASP	CB-CG-OD1	-11.52	107.94	118.30
1	E	76	TYR	CB-CG-CD2	-8.35	115.99	121.00
1	E	80	ASP	CB-CG-OD1	7.92	125.42	118.30
1	E	208	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	E	76	TYR	CG-CD2-CE2	-6.24	116.31	121.30
1	F	83	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	225	ASP	CB-CG-OD1	5.54	123.29	118.30
1	B	83	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	F	225	ASP	CB-CG-OD1	5.10	122.89	118.30

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	32	0
1	E	2320	0	2268	38	0
1	F	2338	0	2285	31	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	109	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 (109) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:F:268:THR:HG22	1:F:269:ARG:HD2	1.90	0.53
1:B:32:VAL:HG23	1:B:56:ALA:HB1	1.91	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:A:222:GLU:HA	1:A:223:PRO:C	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:E:203:THR:O	1:E:206:SER:N	2.42	0.50
1:A:218:PRO:HG3	1:A:230:LEU:HD12	1.92	0.50
1:E:288:ASP:O	1:E:292:ARG:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:10:ARG:NH1	1:B:23:GLU:OE1	2.48	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: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:F:136:GLN:CD	1:F:136:GLN:H	2.21	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: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: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: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:130:ARG:O	1:F:132:MET:HG3	2.19	0.43
1:A:304:VAL:HG23	1:B:304:VAL:HG21	2.00	0.43
1:A:32:VAL:HG23	1:A:56:ALA:HB1	2.01	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:F:228:GLU:HA	1:F:231:GLN:HE21	1.82	0.42
1:E:261:GLU:HA	1:E:272:LEU:HD22	1.99	0.42
1:E:167:GLU:CD	1:E:215:ARG:HH22	2.23	0.42
1:E:78:PHE:O	1:E:82:VAL:HG23	2.19	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:146:GLU:HG3	1:F:251:PRO:HB2	2.03	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: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:E:241:SER:O	1:E:269:ARG:HD2	2.20	0.40
1:A:10:ARG:NH1	1:A:23:GLU:H	2.19	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	296/312 (95%)	282 (95%)	12 (4%)	2 (1%)	26	14
1	B	297/312 (95%)	287 (97%)	8 (3%)	2 (1%)	26	14
1	E	296/312 (95%)	281 (95%)	11 (4%)	4 (1%)	14	4
1	F	298/312 (96%)	289 (97%)	8 (3%)	1 (0%)	46	35
All	All	1187/1248 (95%)	1139 (96%)	39 (3%)	9 (1%)	24	11

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	ALA

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Mol	Chain	Res	Type
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%)	39	27
1	B	233/244 (96%)	224 (96%)	9 (4%)	39	27
1	E	232/244 (95%)	227 (98%)	5 (2%)	60	53
1	F	234/244 (96%)	229 (98%)	5 (2%)	61	55
All	All	931/976 (95%)	903 (97%)	28 (3%)	48	38

All (28) 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	176	PHE
1	A	213	PHE
1	A	228	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	176	PHE
1	B	205	GLU
1	B	213	PHE
1	B	232	SER
1	B	307	GLN
1	E	156	VAL
1	E	176	PHE
1	E	208	ARG
1	E	213	PHE
1	E	288	ASP
1	F	9	ILE
1	F	136	GLN
1	F	176	PHE
1	F	192	GLU
1	F	213	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	HIS
1	A	234	HIS
1	B	231	GLN
1	B	234	HIS
1	B	307	GLN
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 [i](#)

There are no carbohydrates 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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	298/312 (95%)	1.11	56 (18%) <b>2</b> <b>2</b>	20, 26, 39, 55	0
1	B	298/312 (95%)	0.84	30 (10%) <b>9</b> <b>10</b>	18, 23, 33, 51	0
1	E	298/312 (95%)	2.23	138 (46%) <b>0</b> <b>0</b>	24, 39, 60, 64	0
1	F	299/312 (95%)	0.96	51 (17%) <b>2</b> <b>2</b>	15, 20, 33, 58	0
All	All	1193/1248 (95%)	1.29	275 (23%) <b>1</b> <b>1</b>	15, 25, 48, 64	0

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	307	GLN	11.5
1	A	306	PRO	10.7
1	B	306	PRO	9.6
1	B	307	GLN	9.4
1	F	307	GLN	9.4
1	E	203	THR	9.0
1	E	211	LEU	8.7
1	E	143	VAL	8.7
1	F	306	PRO	8.6
1	A	307	GLN	8.0
1	E	306	PRO	8.0
1	E	144	ALA	7.6
1	E	170	ILE	7.3
1	A	148	ASP	7.1
1	E	14	VAL	7.0
1	E	148	ASP	6.9
1	E	205	GLU	6.8
1	E	168	ALA	6.7
1	A	144	ALA	6.3
1	E	73	ASP	6.1
1	E	160	PHE	6.1

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Mol	Chain	Res	Type	RSRZ
1	E	16	GLY	6.1
1	E	174	ASN	6.0
1	E	142	GLU	6.0
1	E	208	ARG	6.0
1	E	70	GLY	5.8
1	B	28	ASP	5.8
1	E	201	PHE	5.6
1	E	169	MET	5.5
1	E	10	ARG	5.4
1	E	176	PHE	5.4
1	E	173	ALA	5.3
1	E	171	LEU	5.3
1	E	206	SER	5.3
1	B	305	ARG	5.3
1	E	84	TYR	5.3
1	A	28	ASP	5.2
1	E	164	GLY	5.1
1	A	145	GLU	5.1
1	E	197	TYR	5.1
1	E	74	ILE	5.1
1	E	162	THR	5.0
1	E	219	ILE	5.0
1	A	142	GLU	5.0
1	E	200	PRO	4.9
1	A	26	ALA	4.8
1	A	100	VAL	4.8
1	E	159	LYS	4.7
1	B	27	GLN	4.7
1	A	35	LEU	4.6
1	A	146	GLU	4.6
1	F	35	LEU	4.6
1	E	217	LEU	4.6
1	A	143	VAL	4.5
1	E	76	TYR	4.5
1	F	305	ARG	4.5
1	E	65	GLY	4.5
1	E	152	ALA	4.5
1	A	27	GLN	4.4
1	E	191	ASP	4.4
1	E	179	ARG	4.4
1	E	18	SER	4.3
1	E	202	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	150	ALA	4.3
1	E	27	GLN	4.2
1	E	28	ASP	4.2
1	E	226	VAL	4.2
1	F	144	ALA	4.2
1	E	172	GLU	4.1
1	A	305	ARG	4.1
1	E	145	GLU	4.1
1	E	204	PRO	4.1
1	B	26	ALA	4.1
1	F	125	PHE	4.1
1	E	258	GLU	4.1
1	A	147	GLN	4.0
1	A	125	PHE	4.0
1	B	118	ASP	3.9
1	B	144	ALA	3.9
1	E	17	SER	3.9
1	E	13	PRO	3.9
1	A	104	TRP	3.9
1	E	146	GLU	3.9
1	E	133	PRO	3.8
1	F	101	ALA	3.8
1	F	100	VAL	3.8
1	F	258	GLU	3.7
1	E	184	GLY	3.7
1	E	136	GLN	3.7
1	A	124	ALA	3.7
1	E	213	PHE	3.7
1	E	12	ALA	3.6
1	E	104	TRP	3.6
1	A	37	GLY	3.6
1	A	101	ALA	3.6
1	E	157	PHE	3.6
1	A	149	HIS	3.5
1	F	28	ASP	3.5
1	E	92	ARG	3.5
1	A	106	THR	3.5
1	E	175	ALA	3.5
1	E	149	HIS	3.5
1	E	24	THR	3.5
1	B	143	VAL	3.5
1	F	104	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	15	LEU	3.5
1	E	21	TYR	3.4
1	E	305	ARG	3.4
1	E	35	LEU	3.4
1	E	78	PHE	3.4
1	A	245	LEU	3.4
1	E	199	THR	3.4
1	E	214	PRO	3.4
1	F	143	VAL	3.4
1	E	220	ALA	3.3
1	B	149	HIS	3.3
1	F	37	GLY	3.3
1	B	142	GLU	3.3
1	F	146	GLU	3.3
1	E	94	VAL	3.3
1	F	126	MET	3.3
1	E	163	PRO	3.3
1	E	109	ALA	3.2
1	A	109	ALA	3.2
1	F	63	LEU	3.2
1	A	141	THR	3.2
1	F	254	LEU	3.2
1	B	141	THR	3.1
1	F	9	ILE	3.1
1	A	63	LEU	3.1
1	A	34	PHE	3.1
1	F	106	THR	3.1
1	E	129	ILE	3.1
1	B	262	ARG	3.1
1	E	95	THR	3.0
1	E	261	GLU	3.0
1	F	123	LEU	3.0
1	A	126	MET	3.0
1	B	140	HIS	3.0
1	E	147	GLN	3.0
1	B	288	ASP	3.0
1	A	213	PHE	3.0
1	F	129	ILE	3.0
1	E	212	ALA	2.9
1	F	145	GLU	2.9
1	A	105	GLY	2.9
1	E	75	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	66	PHE	2.9
1	A	99	LEU	2.9
1	A	247	PHE	2.9
1	A	258	GLU	2.8
1	F	205	GLU	2.8
1	F	108	LEU	2.8
1	E	20	ALA	2.8
1	F	303	ALA	2.8
1	E	108	LEU	2.8
1	A	192	GLU	2.8
1	E	88	PHE	2.8
1	E	166	GLY	2.8
1	E	254	LEU	2.8
1	E	141	THR	2.8
1	F	149	HIS	2.8
1	A	10	ARG	2.8
1	B	90	GLU	2.7
1	E	265	ALA	2.7
1	E	180	VAL	2.7
1	E	72	PRO	2.7
1	F	247	PHE	2.7
1	A	288	ASP	2.7
1	B	148	ASP	2.7
1	B	258	GLU	2.7
1	E	177	VAL	2.7
1	F	34	PHE	2.7
1	E	44	ILE	2.6
1	F	294	VAL	2.6
1	E	118	ASP	2.6
1	A	107	ALA	2.6
1	E	155	ALA	2.6
1	E	91	GLN	2.6
1	E	138	PHE	2.6
1	E	100	VAL	2.6
1	E	101	ALA	2.6
1	A	128	PHE	2.6
1	E	110	PHE	2.6
1	E	207	ARG	2.6
1	F	140	HIS	2.6
1	B	257	PRO	2.6
1	F	297	TRP	2.6
1	F	136	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	71	LYS	2.6
1	A	40	THR	2.6
1	F	99	LEU	2.5
1	A	48	ILE	2.5
1	A	190	GLY	2.5
1	F	105	GLY	2.5
1	A	176	PHE	2.5
1	E	188	LYS	2.5
1	A	45	TRP	2.5
1	E	232	SER	2.5
1	E	156	VAL	2.5
1	E	198	ARG	2.5
1	E	228	GLU	2.5
1	F	102	GLN	2.5
1	A	103	ASP	2.5
1	A	129	ILE	2.5
1	E	224	ALA	2.5
1	E	262	ARG	2.4
1	E	195	ALA	2.4
1	F	39	PRO	2.4
1	A	108	LEU	2.4
1	F	213	PHE	2.4
1	E	23	GLU	2.4
1	F	176	PHE	2.4
1	A	246	LEU	2.4
1	A	110	PHE	2.4
1	F	107	ALA	2.4
1	E	36	HIS	2.4
1	A	297	TRP	2.4
1	E	151	GLU	2.4
1	E	11	ARG	2.4
1	E	81	HIS	2.4
1	E	102	GLN	2.3
1	F	44	ILE	2.3
1	F	40	THR	2.3
1	E	182	PRO	2.3
1	E	64	ILE	2.3
1	B	104	TRP	2.3
1	F	246	LEU	2.3
1	E	68	GLN	2.3
1	B	294	VAL	2.3
1	E	83	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	158	ARG	2.3
1	E	90	GLU	2.3
1	F	128	PHE	2.3
1	E	165	GLU	2.2
1	E	222	GLU	2.2
1	E	30	PRO	2.2
1	E	69	SER	2.2
1	F	124	ALA	2.2
1	A	123	LEU	2.2
1	A	102	GLN	2.2
1	F	293	SER	2.2
1	F	36	HIS	2.2
1	B	192	GLU	2.2
1	F	142	GLU	2.2
1	B	10	ARG	2.2
1	B	106	THR	2.2
1	E	153	ALA	2.2
1	F	139[A]	HIS	2.2
1	E	281	TYR	2.2
1	E	106	THR	2.2
1	E	137	ASP	2.1
1	E	192	GLU	2.1
1	E	125	PHE	2.1
1	E	33	LEU	2.1
1	F	250	GLU	2.1
1	E	26	ALA	2.1
1	A	290	ILE	2.1
1	A	291	GLY	2.1
1	A	265	ALA	2.1
1	B	101	ALA	2.1
1	B	289	ALA	2.1
1	F	141	THR	2.1
1	A	140	HIS	2.1
1	F	45	TRP	2.1
1	E	230	LEU	2.1
1	E	250	GLU	2.1
1	B	304	VAL	2.1
1	B	125	PHE	2.0
1	E	135	TRP	2.0
1	A	36	HIS	2.0
1	B	146	GLU	2.0
1	B	168	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	140	HIS	2.0
1	E	126	MET	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	F	313	1/1	1.00	0.06	-3.74	10,10,10,10	0
2	CL	A	313	1/1	0.99	0.04	-4.37	15,15,15,15	0
2	CL	B	313	1/1	0.99	0.05	-4.70	12,12,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.