



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:40 PM GMT

PDB ID : 3UMC  
Title : Crystal Structure of the L-2-Haloacid Dehalogenase PA0810  
Authors : Petit, P.; Chan, P.W.Y.; Savchenko, A.; Yakunin, A.F.; Edwards, E.A.; Pai, E.F.  
Deposited on : 2011-11-13  
Resolution : 2.15 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

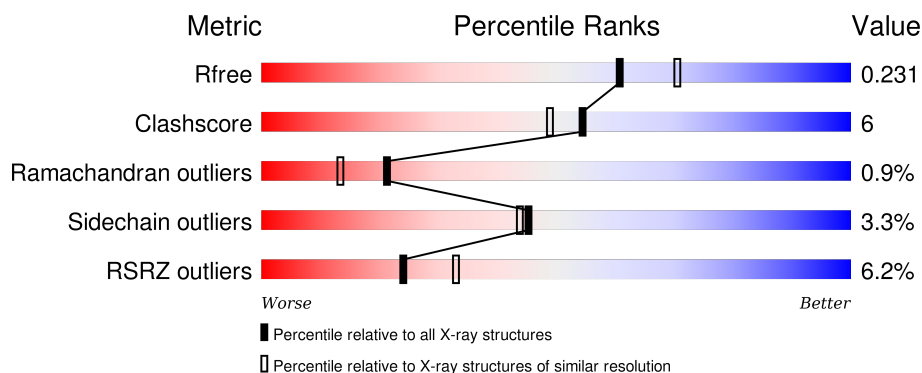
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	254	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 7%</div> </div> </div>
1	B	254	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>• 8%</div> </div> </div>
1	C	254	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>• 8%</div> </div> </div>
1	D	254	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>• 11%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7892 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 haloacid dehalogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	Se	0	0	0
			1883	1206	333	334	4	6			
1	B	234	Total	C	N	O	S	Se	0	0	0
			1854	1183	330	331	4	6			
1	C	233	Total	C	N	O	S	Se	0	0	0
			1849	1180	329	330	4	6			
1	D	227	Total	C	N	O	S	Se	0	0	0
			1815	1160	323	322	4	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MSE	-	EXPRESSION TAG	UNP Q9I5C9
A	-19	GLY	-	EXPRESSION TAG	UNP Q9I5C9
A	-18	SER	-	EXPRESSION TAG	UNP Q9I5C9
A	-17	SER	-	EXPRESSION TAG	UNP Q9I5C9
A	-16	HIS	-	EXPRESSION TAG	UNP Q9I5C9
A	-15	HIS	-	EXPRESSION TAG	UNP Q9I5C9
A	-14	HIS	-	EXPRESSION TAG	UNP Q9I5C9
A	-13	HIS	-	EXPRESSION TAG	UNP Q9I5C9
A	-12	HIS	-	EXPRESSION TAG	UNP Q9I5C9
A	-11	HIS	-	EXPRESSION TAG	UNP Q9I5C9
A	-10	SER	-	EXPRESSION TAG	UNP Q9I5C9
A	-9	SER	-	EXPRESSION TAG	UNP Q9I5C9
A	-8	GLY	-	EXPRESSION TAG	UNP Q9I5C9
A	-7	ARG	-	EXPRESSION TAG	UNP Q9I5C9
A	-6	GLU	-	EXPRESSION TAG	UNP Q9I5C9
A	-5	ASN	-	EXPRESSION TAG	UNP Q9I5C9
A	-4	LEU	-	EXPRESSION TAG	UNP Q9I5C9
A	-3	TYR	-	EXPRESSION TAG	UNP Q9I5C9
A	-2	PHE	-	EXPRESSION TAG	UNP Q9I5C9
A	-1	GLN	-	EXPRESSION TAG	UNP Q9I5C9
A	0	GLY	-	EXPRESSION TAG	UNP Q9I5C9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MSE	-	EXPRESSION TAG	UNP Q9I5C9
B	-19	GLY	-	EXPRESSION TAG	UNP Q9I5C9
B	-18	SER	-	EXPRESSION TAG	UNP Q9I5C9
B	-17	SER	-	EXPRESSION TAG	UNP Q9I5C9
B	-16	HIS	-	EXPRESSION TAG	UNP Q9I5C9
B	-15	HIS	-	EXPRESSION TAG	UNP Q9I5C9
B	-14	HIS	-	EXPRESSION TAG	UNP Q9I5C9
B	-13	HIS	-	EXPRESSION TAG	UNP Q9I5C9
B	-12	HIS	-	EXPRESSION TAG	UNP Q9I5C9
B	-11	HIS	-	EXPRESSION TAG	UNP Q9I5C9
B	-10	SER	-	EXPRESSION TAG	UNP Q9I5C9
B	-9	SER	-	EXPRESSION TAG	UNP Q9I5C9
B	-8	GLY	-	EXPRESSION TAG	UNP Q9I5C9
B	-7	ARG	-	EXPRESSION TAG	UNP Q9I5C9
B	-6	GLU	-	EXPRESSION TAG	UNP Q9I5C9
B	-5	ASN	-	EXPRESSION TAG	UNP Q9I5C9
B	-4	LEU	-	EXPRESSION TAG	UNP Q9I5C9
B	-3	TYR	-	EXPRESSION TAG	UNP Q9I5C9
B	-2	PHE	-	EXPRESSION TAG	UNP Q9I5C9
B	-1	GLN	-	EXPRESSION TAG	UNP Q9I5C9
B	0	GLY	-	EXPRESSION TAG	UNP Q9I5C9
C	-20	MSE	-	EXPRESSION TAG	UNP Q9I5C9
C	-19	GLY	-	EXPRESSION TAG	UNP Q9I5C9
C	-18	SER	-	EXPRESSION TAG	UNP Q9I5C9
C	-17	SER	-	EXPRESSION TAG	UNP Q9I5C9
C	-16	HIS	-	EXPRESSION TAG	UNP Q9I5C9
C	-15	HIS	-	EXPRESSION TAG	UNP Q9I5C9
C	-14	HIS	-	EXPRESSION TAG	UNP Q9I5C9
C	-13	HIS	-	EXPRESSION TAG	UNP Q9I5C9
C	-12	HIS	-	EXPRESSION TAG	UNP Q9I5C9
C	-11	HIS	-	EXPRESSION TAG	UNP Q9I5C9
C	-10	SER	-	EXPRESSION TAG	UNP Q9I5C9
C	-9	SER	-	EXPRESSION TAG	UNP Q9I5C9
C	-8	GLY	-	EXPRESSION TAG	UNP Q9I5C9
C	-7	ARG	-	EXPRESSION TAG	UNP Q9I5C9
C	-6	GLU	-	EXPRESSION TAG	UNP Q9I5C9
C	-5	ASN	-	EXPRESSION TAG	UNP Q9I5C9
C	-4	LEU	-	EXPRESSION TAG	UNP Q9I5C9
C	-3	TYR	-	EXPRESSION TAG	UNP Q9I5C9
C	-2	PHE	-	EXPRESSION TAG	UNP Q9I5C9
C	-1	GLN	-	EXPRESSION TAG	UNP Q9I5C9
C	0	GLY	-	EXPRESSION TAG	UNP Q9I5C9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MSE	-	EXPRESSION TAG	UNP Q9I5C9
D	-19	GLY	-	EXPRESSION TAG	UNP Q9I5C9
D	-18	SER	-	EXPRESSION TAG	UNP Q9I5C9
D	-17	SER	-	EXPRESSION TAG	UNP Q9I5C9
D	-16	HIS	-	EXPRESSION TAG	UNP Q9I5C9
D	-15	HIS	-	EXPRESSION TAG	UNP Q9I5C9
D	-14	HIS	-	EXPRESSION TAG	UNP Q9I5C9
D	-13	HIS	-	EXPRESSION TAG	UNP Q9I5C9
D	-12	HIS	-	EXPRESSION TAG	UNP Q9I5C9
D	-11	HIS	-	EXPRESSION TAG	UNP Q9I5C9
D	-10	SER	-	EXPRESSION TAG	UNP Q9I5C9
D	-9	SER	-	EXPRESSION TAG	UNP Q9I5C9
D	-8	GLY	-	EXPRESSION TAG	UNP Q9I5C9
D	-7	ARG	-	EXPRESSION TAG	UNP Q9I5C9
D	-6	GLU	-	EXPRESSION TAG	UNP Q9I5C9
D	-5	ASN	-	EXPRESSION TAG	UNP Q9I5C9
D	-4	LEU	-	EXPRESSION TAG	UNP Q9I5C9
D	-3	TYR	-	EXPRESSION TAG	UNP Q9I5C9
D	-2	PHE	-	EXPRESSION TAG	UNP Q9I5C9
D	-1	GLN	-	EXPRESSION TAG	UNP Q9I5C9
D	0	GLY	-	EXPRESSION TAG	UNP Q9I5C9

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

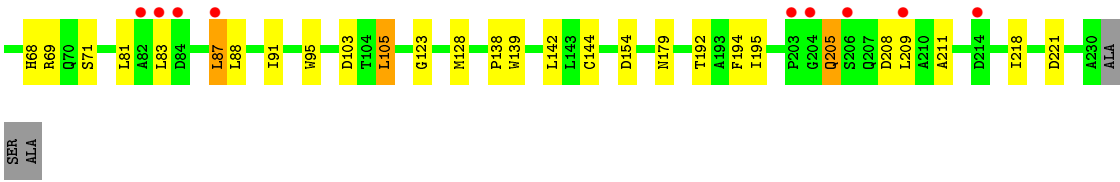
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total 122	O 122	0	0
4	B	134	Total 134	O 134	0	0
4	C	133	Total 133	O 133	0	0
4	D	96	Total 96	O 96	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.42Å 123.87Å 125.60Å 90.00° 90.97° 90.00°	Depositor
Resolution (Å)	28.38 – 2.15 28.38 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.8 (28.38-2.15) 97.8 (28.38-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.44 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.190 , 0.236 0.188 , 0.231	Depositor DCC
$R_{free}$ test set	3090 reflections (5.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.8	EDS
Estimated twinning fraction	0.022 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.019 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.011 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.013 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.026 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 60928 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	1.02	2/1927 (0.1%)	0.87	2/2612 (0.1%)
1	B	1.01	2/1896 (0.1%)	0.91	5/2570 (0.2%)
1	C	1.01	0/1891	0.92	2/2563 (0.1%)
1	D	0.97	0/1856	0.88	2/2514 (0.1%)
All	All	1.00	4/7570 (0.1%)	0.90	11/10259 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	ALA	CA-CB	5.37	1.63	1.52
1	A	166	ASP	CB-CG	5.33	1.62	1.51
1	A	99	ARG	CG-CD	5.23	1.65	1.51
1	B	176	ALA	CA-CB	5.19	1.63	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	MSE	CG-SE-CE	-7.08	83.32	98.90
1	A	14	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	B	69	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	B	69	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	D	42	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	C	214	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	216	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	197	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	B	53	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	163	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	D	42	ARG	NE-CZ-NH2	-5.20	117.70	120.30

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	1883	0	1849	24	0
1	B	1854	0	1822	18	0
1	C	1849	0	1817	22	0
1	D	1815	0	1782	33	0
2	A	1	0	0	1	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	122	0	0	3	0
4	B	134	0	0	0	0
4	C	133	0	0	5	0
4	D	96	0	0	3	0
All	All	7892	0	7270	94	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 (94) 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:-4:LEU:HD12	4:A:428:HOH:O	1.74	0.87
1:A:140:ASP:HB3	1:C:129:LEU:CD2	2.09	0.83
1:D:36:CYS:O	1:D:39:LEU:HD12	1.85	0.75
1:C:65:ASP:OD2	4:C:324:HOH:O	2.06	0.74
1:A:140:ASP:HB3	1:C:129:LEU:HD21	1.75	0.69
1:C:68:HIS:NE2	4:C:341:HOH:O	2.28	0.67
1:D:69:ARG:HH21	1:D:88:LEU:HD23	1.62	0.65
1:B:127:LEU:O	1:B:127:LEU:HD23	1.97	0.65
1:B:83:LEU:HD22	1:B:87:LEU:HD23	1.80	0.64
1:C:78:GLU:OE2	4:C:321:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ASP:HB2	4:D:524:HOH:O	2.01	0.60
1:A:80:GLY:O	1:A:81:LEU:HD13	2.02	0.58
1:D:205:GLN:O	1:D:209:LEU:HD11	2.04	0.58
1:B:127:LEU:HD22	1:B:128:MSE:HE2	1.84	0.58
1:A:39:LEU:HD23	1:A:75:LEU:CD1	2.34	0.57
1:C:109:HIS:ND1	1:C:112:LYS:NZ	2.46	0.57
1:D:59:ALA:HB1	1:D:60:PRO:HD2	1.88	0.56
1:C:96:HIS:CD2	1:C:127:LEU:HD13	2.41	0.56
1:D:83:LEU:HB2	1:D:88:LEU:HD13	1.87	0.55
1:B:63:HIS:CE1	1:B:66:GLN:HG3	2.42	0.55
1:D:69:ARG:NH2	1:D:88:LEU:HD23	2.21	0.55
1:B:83:LEU:HD22	1:B:87:LEU:CD2	2.38	0.54
1:B:4:ILE:HG12	1:B:173:MSE:HE2	1.89	0.54
1:A:173:MSE:HE1	1:A:229:LEU:HD11	1.91	0.53
1:B:127:LEU:C	1:B:127:LEU:HD23	2.29	0.53
1:A:53:ARG:HG3	1:A:58:GLN:HB3	1.90	0.53
1:A:129:LEU:CD2	1:C:140:ASP:HB3	2.39	0.52
1:D:211:ALA:HB2	1:D:218:ILE:CD1	2.40	0.52
1:D:195:ILE:O	1:D:195:ILE:HG22	2.09	0.51
1:D:24:GLN:O	1:D:26:LEU:N	2.43	0.51
1:C:70:GLN:HG3	1:C:71:SER:N	2.25	0.50
1:D:59:ALA:HB1	1:D:60:PRO:CD	2.41	0.50
1:B:63:HIS:HB2	1:B:124:ASN:HB3	1.94	0.50
1:D:9:PHE:CE1	1:D:128:MSE:HE1	2.46	0.50
1:A:51:MSE:HE3	1:A:55:ARG:NH2	2.27	0.50
1:A:15:TRP:CH2	1:A:44:ARG:HG2	2.47	0.49
2:A:234:CL:CL	4:A:560:HOH:O	2.57	0.49
1:A:77:GLY:O	1:A:78:GLU:C	2.51	0.49
1:C:105:LEU:HD21	4:C:330:HOH:O	2.13	0.49
1:A:39:LEU:CD2	1:A:75:LEU:CD1	2.90	0.49
1:D:194:PHE:HB3	1:D:218:ILE:HD13	1.95	0.48
1:D:179:ASN:ND2	1:D:208:ASP:OD1	2.37	0.48
1:B:46:GLN:C	1:B:49:PRO:HD2	2.33	0.48
1:A:63:HIS:HB2	1:A:124:ASN:HB3	1.95	0.48
1:B:83:LEU:CD2	1:B:87:LEU:HD23	2.43	0.47
1:C:128:MSE:HE2	1:C:128:MSE:HA	1.95	0.47
1:D:87:LEU:CD1	1:D:91:ILE:HD11	2.45	0.47
1:D:128:MSE:HG3	1:D:144:CYS:SG	2.54	0.47
1:C:44:ARG:HA	1:C:47:TYR:CE1	2.50	0.47
1:D:105:LEU:HB2	4:D:271:HOH:O	2.15	0.47
1:D:83:LEU:HD12	1:D:88:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:ASP:OD2	4:D:311:HOH:O	2.20	0.46
1:D:43:TRP:HE1	1:D:71:SER:HG	1.62	0.46
1:A:81:LEU:HD22	1:A:81:LEU:N	2.31	0.45
1:C:23:PHE:HB3	1:C:36:CYS:SG	2.56	0.45
1:B:6:PHE:HE2	1:B:117:LEU:HD22	1.82	0.45
1:C:109:HIS:O	1:C:112:LYS:HG2	2.16	0.45
1:C:123:GLY:HA3	1:C:128:MSE:HE3	1.99	0.45
1:A:0:GLY:O	1:A:2:ARG:HG3	2.17	0.45
1:D:23:PHE:O	1:D:26:LEU:HB3	2.17	0.44
1:D:39:LEU:HD12	1:D:40:THR:H	1.82	0.44
1:B:127:LEU:C	1:B:127:LEU:CD2	2.86	0.44
1:D:27:GLU:O	1:D:29:GLU:N	2.51	0.44
1:D:27:GLU:C	1:D:29:GLU:H	2.22	0.43
1:C:123:GLY:O	1:C:144:CYS:HB3	2.17	0.43
1:C:96:HIS:CD2	1:C:127:LEU:CD1	3.02	0.43
1:A:183:LYS:NZ	4:A:452:HOH:O	2.32	0.43
1:D:68:HIS:ND1	1:D:95:TRP:CD1	2.87	0.43
1:D:81:LEU:HA	1:D:81:LEU:HD13	1.90	0.43
1:C:63:HIS:HA	1:C:151:TYR:OH	2.19	0.42
1:D:123:GLY:O	1:D:144:CYS:HB3	2.19	0.42
1:A:112:LYS:O	1:C:133:ARG:NH1	2.52	0.42
1:A:49:PRO:O	1:A:53:ARG:HB2	2.20	0.42
1:B:143:LEU:HD13	1:B:161:ALA:HB1	2.00	0.42
1:A:83:LEU:HD22	1:A:87:LEU:HB3	2.01	0.42
1:B:173:MSE:HE1	1:B:229:LEU:HD11	2.01	0.42
1:C:163:ARG:NH2	4:C:355:HOH:O	2.52	0.42
1:A:19:LEU:HD21	1:A:95:TRP:CE2	2.55	0.42
1:B:159:LEU:HD11	1:B:188:LEU:HD22	2.02	0.42
1:B:42:ARG:HA	1:B:45:GLN:HG2	2.00	0.42
1:C:63:HIS:HB2	1:C:124:ASN:HB3	2.03	0.41
1:D:103:ASP:CG	1:D:221:ASP:HB2	2.40	0.41
1:A:123:GLY:O	1:A:144:CYS:HB3	2.20	0.41
1:D:19:LEU:HD21	1:D:95:TRP:CZ2	2.55	0.41
1:D:17:SER:O	1:D:21:GLU:HB3	2.20	0.41
1:D:87:LEU:CD1	1:D:91:ILE:CD1	2.99	0.41
1:C:59:ALA:HB1	1:C:60:PRO:HD2	2.03	0.41
1:D:205:GLN:HG2	1:D:209:LEU:HD21	2.03	0.41
1:D:139:TRP:CD1	1:D:142:LEU:HD21	2.56	0.40
1:A:193:ALA:HA	1:A:217:LEU:O	2.22	0.40
1:A:63:HIS:CE1	1:A:66:GLN:HG3	2.56	0.40
1:A:47:TYR:O	1:A:51:MSE:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MSE:HE3	1:B:1:MSE:HB3	2.00	0.40
1:B:81:LEU:HD13	1:B:81:LEU:HA	1.93	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	234/254 (92%)	223 (95%)	10 (4%)	1 (0%)	39	34
1	B	232/254 (91%)	228 (98%)	4 (2%)	0	100	100
1	C	231/254 (91%)	223 (96%)	7 (3%)	1 (0%)	39	34
1	D	223/254 (88%)	210 (94%)	7 (3%)	6 (3%)	6	1
All	All	920/1016 (91%)	884 (96%)	28 (3%)	8 (1%)	21	13

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	24	GLN
1	A	-1	GLN
1	D	25	ALA
1	D	27	GLU
1	D	205	GLN
1	C	28	ARG
1	D	28	ARG
1	D	138	PRO

### 5.3.2 Protein sidechains [i](#)

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	190/198 (96%)	185 (97%)	5 (3%)	54	55
1	B	187/198 (94%)	184 (98%)	3 (2%)	70	76
1	C	187/198 (94%)	180 (96%)	7 (4%)	41	38
1	D	184/198 (93%)	174 (95%)	10 (5%)	27	22
All	All	748/792 (94%)	723 (97%)	25 (3%)	45	44

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-4	LEU
1	A	48	LYS
1	A	81	LEU
1	A	87	LEU
1	A	153	PRO
1	B	65	ASP
1	B	69	ARG
1	B	81	LEU
1	C	33	THR
1	C	44	ARG
1	C	45	GLN
1	C	65	ASP
1	C	105	LEU
1	C	180	TYR
1	C	207	GLN
1	D	19	LEU
1	D	21	GLU
1	D	34	LEU
1	D	39	LEU
1	D	56	ASN
1	D	58	GLN
1	D	65	ASP
1	D	87	LEU
1	D	105	LEU
1	D	192	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	63	HIS
1	D	56	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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	230/254 (90%)	0.18	18 (7%)	16 22	8, 21, 60, 73	0
1	B	228/254 (89%)	0.00	7 (3%)	52 62	13, 24, 55, 65	0
1	C	227/254 (89%)	0.13	12 (5%)	30 40	11, 25, 57, 76	0
1	D	221/254 (87%)	0.35	19 (8%)	13 19	12, 31, 63, 78	0
All	All	906/1016 (89%)	0.16	56 (6%)	24 33	8, 26, 60, 78	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	THR	7.4
1	C	31	GLY	5.9
1	C	32	GLY	5.3
1	A	-4	LEU	4.8
1	A	49	PRO	4.7
1	D	206	SER	4.7
1	A	-1	GLN	4.1
1	B	31	GLY	4.1
1	D	0	GLY	4.1
1	D	87	LEU	3.9
1	A	-2	PHE	3.6
1	A	59	ALA	3.5
1	A	-3	TYR	3.5
1	A	0	GLY	3.4
1	D	214	ASP	3.4
1	C	232	SER	3.3
1	B	83	LEU	3.2
1	C	204	GLY	3.1
1	C	28	ARG	3.0
1	C	59	ALA	2.9
1	D	60	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	82	ALA	2.8
1	B	233	ALA	2.7
1	B	82	ALA	2.7
1	A	58	GLN	2.7
1	D	25	ALA	2.7
1	D	56	ASN	2.7
1	A	31	GLY	2.6
1	D	37	VAL	2.6
1	D	36	CYS	2.6
1	A	81	LEU	2.5
1	A	82	ALA	2.5
1	C	203	PRO	2.5
1	D	82	ALA	2.5
1	D	29	GLU	2.5
1	D	204	GLY	2.5
1	D	84	ASP	2.4
1	D	203	PRO	2.4
1	A	53	ARG	2.4
1	C	0	GLY	2.3
1	A	28	ARG	2.3
1	A	46	GLN	2.3
1	A	29	GLU	2.3
1	A	50	ALA	2.3
1	B	119	ALA	2.3
1	D	8	VAL	2.2
1	A	143	LEU	2.2
1	D	209	LEU	2.2
1	A	56	ASN	2.2
1	D	83	LEU	2.2
1	C	84	ASP	2.2
1	D	28	ARG	2.1
1	C	119	ALA	2.1
1	B	8	VAL	2.1
1	D	26	LEU	2.1
1	B	32	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	B	234	1/1	0.99	0.19	0.49	32,32,32,32	0
2	CL	C	234	1/1	0.98	0.17	0.39	36,36,36,36	0
2	CL	A	234	1/1	0.99	0.15	-0.18	37,37,37,37	0
2	CL	D	234	1/1	0.97	0.14	-0.29	40,40,40,40	0
3	NA	C	235	1/1	0.93	0.07	-2.25	37,37,37,37	0
3	NA	D	235	1/1	0.94	0.04	-4.66	45,45,45,45	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.