



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:37 PM UTC

PDB ID : 3R3U / pdb_00003r3u
Title : Crystal Structure of the Fluoroacetate Dehalogenase RPA1163 - WT/apo
Authors : Chan, P.W.Y.; Yakunin, A.F.; Edwards, E.A.; Pai, E.F.
Deposited on : 2011-03-16
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

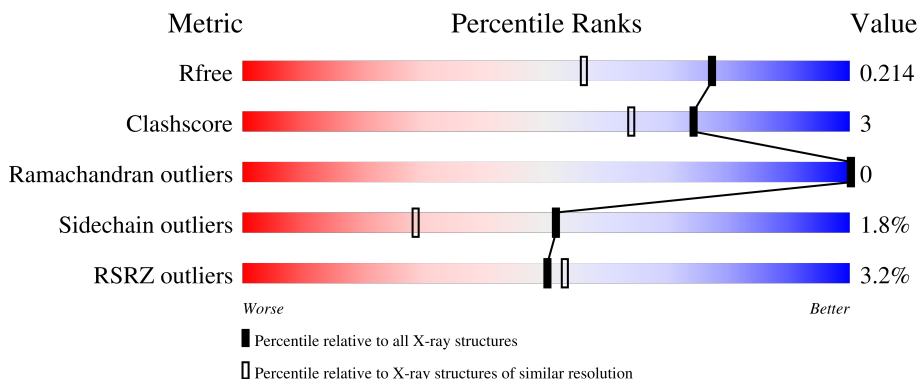
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	306	4% 85% 14% ..
1	B	306	2% 85% 10% ..
1	C	306	2% 88% 10% .
1	D	306	4% 85% 11% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10676 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 Fluoroacetate dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	10	0
			2475	1592	432	441	10			
1	B	294	Total	C	N	O	S	0	5	0
			2383	1536	418	419	10			
1	C	301	Total	C	N	O	S	0	2	0
			2392	1536	419	427	10			
1	D	296	Total	C	N	O	S	0	4	0
			2380	1530	419	422	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q6NAM1
A	0	HIS	-	expression tag	UNP Q6NAM1
A	303	GLY	-	expression tag	UNP Q6NAM1
A	304	SER	-	expression tag	UNP Q6NAM1
B	-1	GLY	-	expression tag	UNP Q6NAM1
B	0	HIS	-	expression tag	UNP Q6NAM1
B	303	GLY	-	expression tag	UNP Q6NAM1
B	304	SER	-	expression tag	UNP Q6NAM1
C	-1	GLY	-	expression tag	UNP Q6NAM1
C	0	HIS	-	expression tag	UNP Q6NAM1
C	303	GLY	-	expression tag	UNP Q6NAM1
C	304	SER	-	expression tag	UNP Q6NAM1
D	-1	GLY	-	expression tag	UNP Q6NAM1
D	0	HIS	-	expression tag	UNP Q6NAM1
D	303	GLY	-	expression tag	UNP Q6NAM1
D	304	SER	-	expression tag	UNP Q6NAM1

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

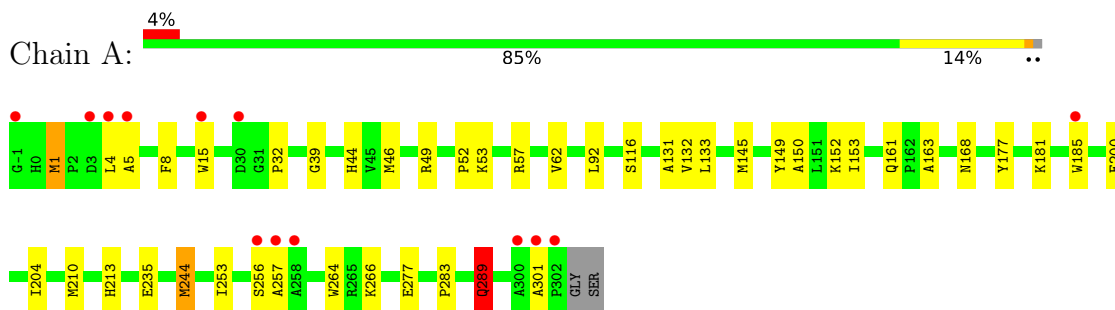
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	276	Total O 276 276	0	0
4	B	297	Total O 297 297	0	0
4	C	256	Total O 256 256	0	0
4	D	210	Total O 210 210	0	0

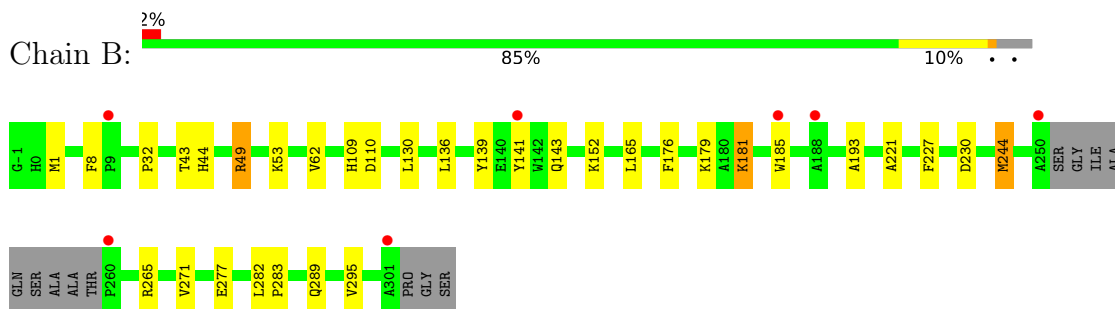
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

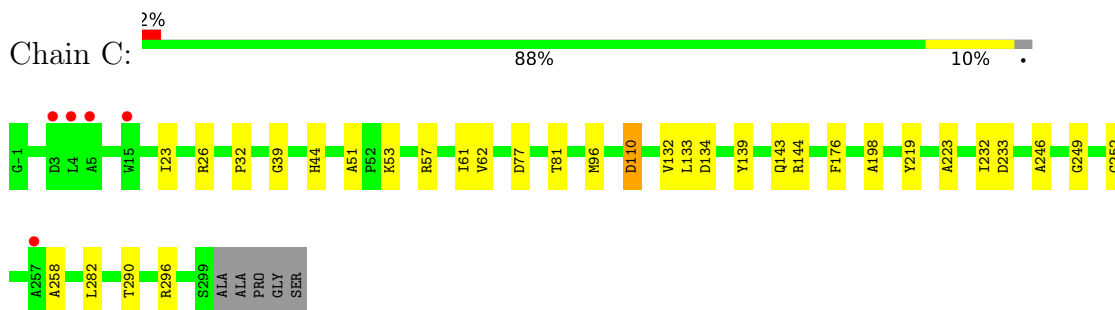
- Molecule 1: Fluoroacetate dehalogenase



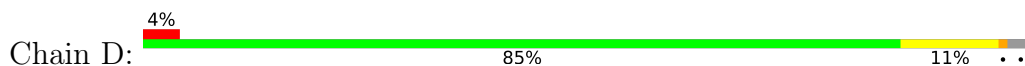
- Molecule 1: Fluoroacetate dehalogenase

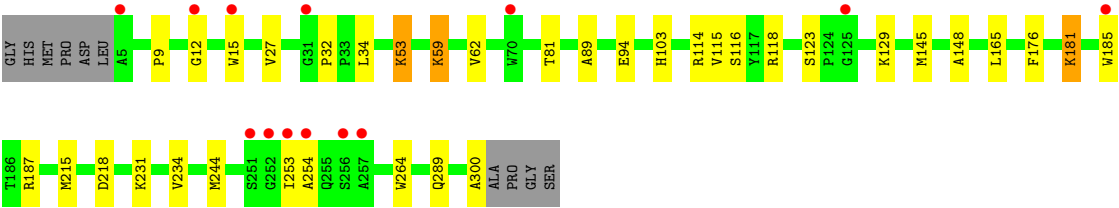


- Molecule 1: Fluoroacetate dehalogenase



- Molecule 1: Fluoroacetate dehalogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.23Å 122.70Å 132.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.17 – 1.60 90.08 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (90.17-1.60) 99.7 (90.08-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.170 , 0.202 (Not available) , 0.214	Depositor DCC
R_{free} test set	8616 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10676	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: NI, 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	1.51	14/2559 (0.5%)	1.25	7/3488 (0.2%)
1	B	1.51	8/2463 (0.3%)	1.28	8/3351 (0.2%)
1	C	1.52	13/2470 (0.5%)	1.29	6/3363 (0.2%)
1	D	1.54	18/2458 (0.7%)	1.33	11/3346 (0.3%)
All	All	1.52	53/9950 (0.5%)	1.29	32/13548 (0.2%)

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	32	PRO	CA-C	12.55	1.58	1.51
1	A	32	PRO	CA-C	10.77	1.59	1.52
1	C	232	ILE	CA-CB	-8.86	1.44	1.54
1	A	163	ALA	CA-CB	7.29	1.64	1.53
1	D	215	MET	N-CA	7.29	1.55	1.46
1	C	23	ILE	CA-CB	-7.24	1.45	1.54
1	D	254	ALA	CA-CB	7.20	1.64	1.53
1	C	51	ALA	CA-CB	7.12	1.63	1.53
1	B	165	LEU	C-O	-6.53	1.18	1.24
1	B	8	PHE	C-O	-6.51	1.16	1.24
1	D	123	SER	CA-C	6.38	1.60	1.52
1	C	290	THR	C-O	-6.37	1.16	1.24
1	D	32	PRO	CA-C	6.25	1.55	1.51
1	D	123	SER	N-CA	6.24	1.53	1.46
1	C	81	THR	CA-CB	6.20	1.62	1.53
1	D	145	MET	C-O	6.19	1.31	1.23
1	C	232	ILE	N-CA	6.13	1.53	1.46
1	D	231	LYS	N-CA	-6.00	1.38	1.46
1	D	59	LYS	C-O	-5.98	1.16	1.24
1	D	81	THR	CA-CB	5.97	1.60	1.53
1	A	257	ALA	CA-CB	5.91	1.61	1.53
1	D	116	SER	CA-C	-5.85	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	VAL	CA-CB	-5.74	1.47	1.54
1	B	227	PHE	C-O	5.72	1.30	1.24
1	D	114	ARG	CA-C	5.72	1.60	1.52
1	A	39	GLY	N-CA	-5.64	1.40	1.44
1	C	249	GLY	C-O	-5.61	1.18	1.24
1	A	150	ALA	N-CA	5.61	1.53	1.46
1	D	115	VAL	CA-CB	-5.61	1.48	1.54
1	A	161	GLN	N-CA	5.60	1.53	1.45
1	D	176	PHE	CA-C	5.59	1.60	1.52
1	A	116	SER	CA-CB	-5.54	1.44	1.53
1	D	129	LYS	N-CA	5.53	1.52	1.45
1	A	92	LEU	CA-C	5.52	1.60	1.52
1	C	223	ALA	CA-CB	-5.52	1.44	1.53
1	B	110	ASP	C-O	-5.49	1.19	1.24
1	D	148	ALA	N-CA	-5.46	1.39	1.46
1	C	110	ASP	CA-C	5.44	1.57	1.53
1	A	213	HIS	N-CA	-5.43	1.39	1.46
1	A	8	PHE	C-O	-5.43	1.17	1.24
1	A	131	ALA	N-CA	5.41	1.52	1.46
1	A	52	PRO	N-CA	5.40	1.54	1.47
1	C	246	ALA	CA-CB	5.35	1.60	1.53
1	B	43	THR	CA-CB	5.33	1.60	1.53
1	B	295	VAL	CA-CB	-5.32	1.48	1.54
1	A	289	GLN	CD-NE2	5.26	1.44	1.33
1	C	252	GLY	N-CA	5.18	1.51	1.45
1	D	218	ASP	CA-C	5.17	1.59	1.52
1	B	109	HIS	C-O	5.10	1.29	1.24
1	D	234	VAL	CA-C	-5.10	1.46	1.52
1	C	219	TYR	N-CA	5.09	1.52	1.46
1	C	32	PRO	CA-C	5.07	1.54	1.51
1	D	34	LEU	N-CA	5.01	1.52	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	PRO	O-C-N	11.04	126.39	121.31
1	B	244	MET	CG-SD-CE	-7.88	83.55	100.90
1	D	123	SER	CA-C-N	6.77	126.72	119.28
1	D	123	SER	C-N-CA	6.77	126.72	119.28
1	B	49	ARG	NE-CZ-NH2	6.40	124.96	119.20
1	A	244	MET	CG-SD-CE	-6.36	86.91	100.90
1	D	114	ARG	NE-CZ-NH1	-6.18	115.32	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	187	ARG	N-CA-C	6.18	117.68	111.07
1	D	103	HIS	CB-CA-C	6.01	120.57	109.70
1	A	133	LEU	CA-C-N	5.63	130.14	122.19
1	A	133	LEU	C-N-CA	5.63	130.14	122.19
1	B	49	ARG	NE-CZ-NH1	-5.61	115.89	121.50
1	D	89	ALA	N-CA-C	-5.56	105.12	111.07
1	B	1	MET	CG-SD-CE	-5.55	88.68	100.90
1	D	165	LEU	CA-C-N	-5.53	113.33	119.19
1	D	165	LEU	C-N-CA	-5.53	113.33	119.19
1	B	152	LYS	N-CA-C	5.45	117.03	111.14
1	C	233	ASP	N-CA-C	5.36	116.80	111.07
1	D	114	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	D	94	GLU	N-CA-C	5.31	117.76	111.33
1	B	221	ALA	CA-C-N	5.30	126.76	120.14
1	B	221	ALA	C-N-CA	5.30	126.76	120.14
1	A	210	MET	CG-SD-CE	-5.23	89.39	100.90
1	D	118	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A	200	GLU	N-CA-C	5.22	116.97	111.28
1	C	57	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	C	26	ARG	O-C-N	-5.20	117.11	123.19
1	C	134	ASP	N-CA-C	5.18	118.73	111.74
1	C	57	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	C	198	ALA	N-CA-C	-5.12	105.78	111.36
1	A	1	MET	CA-C-N	5.01	124.99	120.03
1	A	1	MET	C-N-CA	5.01	124.99	120.03

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	2475	0	2374	22	0
1	B	2383	0	2293	18	0
1	C	2392	0	2308	9	0
1	D	2380	0	2293	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	276	0	0	6	0
4	B	297	0	0	3	0
4	C	256	0	0	0	0
4	D	210	0	0	3	0
All	All	10676	0	9268	59	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 3.

All (59) 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[B]:LEU:HD21	1:A:204:ILE:CD1	1.81	1.08
1:A:4[B]:LEU:CD2	1:A:204:ILE:HD12	1.85	1.06
1:A:4[B]:LEU:HD21	1:A:204:ILE:HD12	0.93	0.87
1:B:176[A]:PHE:HZ	4:B:1254:HOH:O	1.62	0.81
1:D:289[B]:GLN:HE21	1:D:289[B]:GLN:H	1.30	0.78
4:A:421:HOH:O	1:B:176[A]:PHE:CE1	2.37	0.78
1:B:181:LYS:HD2	1:B:185[B]:TRP:CZ2	2.19	0.77
4:A:421:HOH:O	1:B:176[A]:PHE:HE1	1.67	0.76
1:A:5[B]:ALA:HB2	4:A:479:HOH:O	1.87	0.73
1:D:181:LYS:HD2	1:D:185[A]:TRP:CZ2	2.32	0.65
1:A:235:GLU:OE1	4:A:497:HOH:O	2.15	0.64
1:B:277:GLU:H	1:B:289:GLN:HE22	1.45	0.64
1:B:176[A]:PHE:CZ	4:B:1254:HOH:O	2.45	0.62
1:D:289[B]:GLN:H	1:D:289[B]:GLN:NE2	1.98	0.61
1:A:289:GLN:HE21	1:A:289:GLN:H	1.49	0.60
1:B:265[B]:ARG:HG2	1:B:271:VAL:CG1	2.33	0.59
1:C:44:HIS:HB2	1:C:62:VAL:HG12	1.84	0.59
1:D:289[B]:GLN:HE21	1:D:289[B]:GLN:N	1.98	0.59
1:A:4[B]:LEU:CD2	1:A:204:ILE:CD1	2.63	0.58
1:D:53:LYS:HB2	4:D:657:HOH:O	2.04	0.56
1:A:57:ARG:NH2	1:A:301:ALA:HB3	2.21	0.56
1:A:177:TYR:CZ	1:A:181:LYS:HE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185[B]:TRP:HZ3	1:D:253:ILE:HG12	1.72	0.55
1:A:49:ARG:HD2	4:A:651:HOH:O	2.07	0.54
1:B:265[B]:ARG:HG2	1:B:271:VAL:HG13	1.93	0.51
1:A:168:ASN:ND2	1:B:176[B]:PHE:CE1	2.78	0.51
1:A:152:LYS:HG3	1:A:185[B]:TRP:HZ2	1.77	0.49
1:A:177:TYR:OH	1:A:181:LYS:HE2	2.12	0.49
1:D:181:LYS:NZ	4:D:515:HOH:O	2.40	0.48
1:A:44:HIS:HB2	1:A:62:VAL:HG12	1.96	0.48
1:D:12:GLY:N	1:D:27:VAL:O	2.44	0.48
1:B:130:LEU:O	1:B:244:MET:HA	2.15	0.47
1:A:1:MET:HE3	4:A:375:HOH:O	2.16	0.46
1:C:144:ARG:HE	1:C:258:ALA:HB2	1.81	0.46
1:B:139:TYR:HB2	1:B:230:ASP:HB3	1.99	0.44
1:D:244:MET:HE1	1:D:264:TRP:CZ3	2.51	0.44
1:C:132:VAL:C	1:C:133:LEU:HD12	2.43	0.44
1:C:144:ARG:NE	1:C:258:ALA:HB2	2.33	0.44
1:A:46:MET:CE	1:A:283:PRO:HG2	2.47	0.44
1:C:61:ILE:HD13	1:C:96:MET:HE1	1.99	0.44
1:A:244:MET:HE1	1:A:264:TRP:CE3	2.53	0.44
1:B:139:TYR:CE2	1:B:143:GLN:HG3	2.53	0.44
1:C:139:TYR:CE2	1:C:143:GLN:HG3	2.54	0.43
1:A:289:GLN:H	1:A:289:GLN:NE2	2.15	0.43
1:D:181:LYS:HA	1:D:181:LYS:HD3	1.75	0.43
1:C:77:ASP:C	1:C:77:ASP:OD2	2.60	0.43
1:A:244:MET:HE1	1:A:264:TRP:CZ3	2.54	0.42
1:B:136:LEU:HB2	1:B:141:TYR:CE1	2.54	0.42
1:B:181:LYS:HA	1:B:181:LYS:HD3	1.86	0.41
1:C:176:PHE:CD2	1:C:176:PHE:C	2.98	0.41
1:A:145:MET:HE1	1:A:153:ILE:HD11	2.02	0.41
1:A:253:ILE:O	1:A:256:SER:HB2	2.20	0.41
1:B:179:LYS:NZ	4:B:816:HOH:O	2.45	0.41
1:B:44:HIS:HB2	1:B:62:VAL:HG12	2.03	0.41
1:C:39:GLY:HA3	1:C:110:ASP:HB3	2.02	0.41
1:D:300:ALA:HB3	4:D:724:HOH:O	2.20	0.40
1:B:49:ARG:NH1	1:B:193:ALA:O	2.54	0.40
1:A:57:ARG:HH22	1:A:301:ALA:HB3	1.86	0.40
1:B:282:LEU:HB2	1:B:283:PRO:HD3	2.03	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	312/306 (102%)	305 (98%)	7 (2%)	0	100	100
1	B	295/306 (96%)	291 (99%)	4 (1%)	0	100	100
1	C	301/306 (98%)	291 (97%)	10 (3%)	0	100	100
1	D	298/306 (97%)	287 (96%)	11 (4%)	0	100	100
All	All	1206/1224 (98%)	1174 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	248/242 (102%)	241 (97%)	7 (3%)	38	15
1	B	240/242 (99%)	238 (99%)	2 (1%)	73	59
1	C	242/242 (100%)	239 (99%)	3 (1%)	63	43
1	D	239/242 (99%)	233 (98%)	6 (2%)	42	18
All	All	969/968 (100%)	951 (98%)	18 (2%)	51	27

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15[A]	TRP
1	A	15[B]	TRP

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Mol	Chain	Res	Type
1	A	53	LYS
1	A	149	TYR
1	A	266	LYS
1	A	277	GLU
1	A	289	GLN
1	B	53	LYS
1	B	181	LYS
1	C	53	LYS
1	C	282	LEU
1	C	296	ARG
1	D	9	PRO
1	D	15	TRP
1	D	53	LYS
1	D	59	LYS
1	D	62	VAL
1	D	181	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	A	161	GLN
1	A	289	GLN
1	B	272	GLN
1	B	289	GLN
1	C	79	GLN
1	D	79	GLN
1	D	101	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 7 ligands modelled in this entry, 7 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 [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(Å²)	Q<0.9
1	A	304/306 (99%)	-0.17	13 (4%)	40	41	9, 17, 29, 40	10 (3%)
1	B	294/306 (96%)	-0.29	7 (2%)	59	63	6, 16, 29, 39	5 (1%)
1	C	301/306 (98%)	-0.08	5 (1%)	69	72	7, 19, 30, 51	2 (0%)
1	D	296/306 (96%)	0.26	13 (4%)	39	40	8, 22, 37, 50	4 (1%)
All	All	1195/1224 (97%)	-0.07	38 (3%)	50	53	6, 19, 32, 51	21 (1%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	253	ILE	5.0
1	A	257	ALA	4.6
1	C	4	LEU	4.1
1	D	185[A]	TRP	4.0
1	D	257	ALA	3.9
1	D	5	ALA	3.5
1	A	302	PRO	3.5
1	C	3	ASP	3.5
1	A	5[A]	ALA	3.4
1	A	3[A]	ASP	3.4
1	D	252	GLY	3.4
1	D	254	ALA	3.3
1	B	185[A]	TRP	3.2
1	D	125	GLY	3.2
1	B	301	ALA	3.2
1	A	300	ALA	3.1
1	D	251	SER	2.7
1	A	301	ALA	2.7
1	D	15	TRP	2.7
1	C	257	ALA	2.6
1	D	12	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	4[A]	LEU	2.5
1	A	256	SER	2.5
1	C	5	ALA	2.4
1	B	260	PRO	2.4
1	D	31	GLY	2.3
1	B	250	ALA	2.3
1	A	258	ALA	2.3
1	B	141	TYR	2.3
1	C	15	TRP	2.2
1	B	188	ALA	2.1
1	A	-1	GLY	2.1
1	A	15[A]	TRP	2.1
1	A	30	ASP	2.1
1	B	9	PRO	2.1
1	D	70	TRP	2.1
1	A	185[A]	TRP	2.0
1	D	256	SER	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
3	CL	D	305	1/1	0.95	0.08	30,30,30,30	0
3	CL	A	306	1/1	0.97	0.07	32,32,32,32	0
3	CL	C	306	1/1	0.97	0.12	38,38,38,38	0
2	NI	C	305	1/1	0.97	0.05	28,28,28,28	0
3	CL	B	306	1/1	0.98	0.10	26,26,26,26	0
2	NI	A	305	1/1	0.99	0.03	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NI	B	305	1/1	1.00	0.02	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.