



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:39 am BST

PDB ID : 3R3U
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

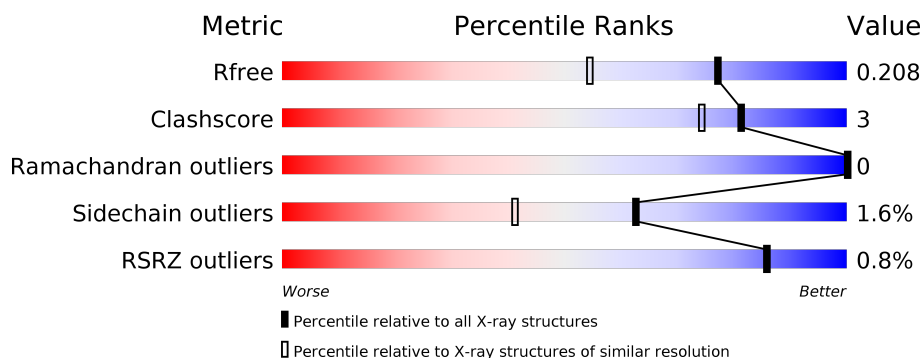
1 Overall quality at a glance

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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (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 on 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 86%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 86% 12% .. </div> </div>
1	B	306	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 84%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 84% 11% . . </div> </div>
1	C	306	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 91%, yellow 7%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 91% 7% . </div> </div>
1	D	306	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 9%, green 88%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 88% 9% . </div> </div>

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 (three-letter code: NI) (formula: Ni).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

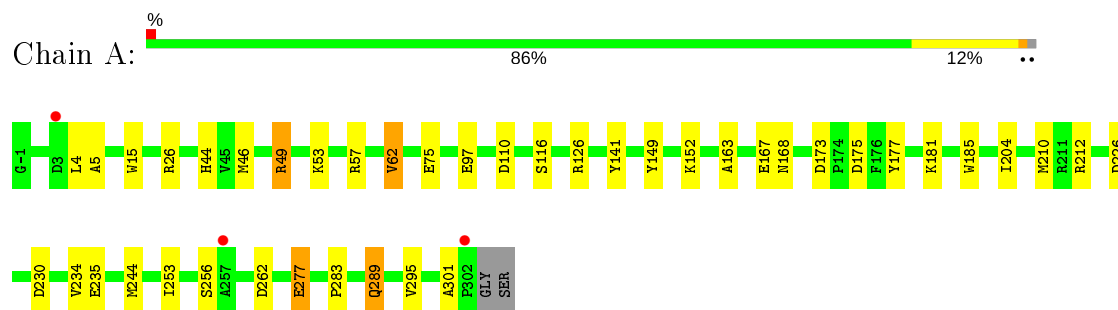
- Molecule 4 is water.

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

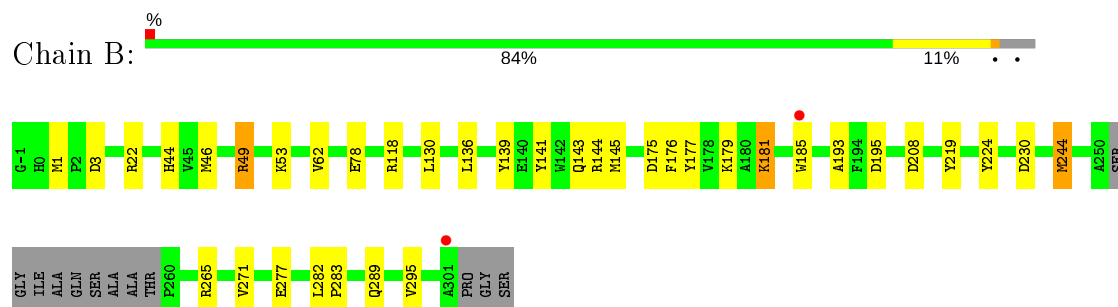
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

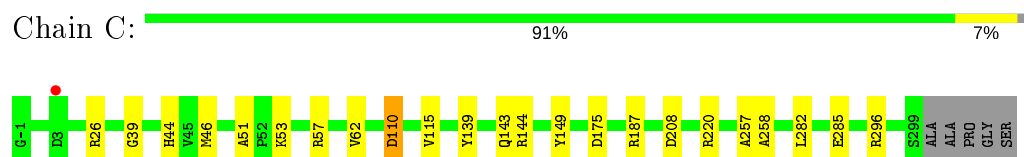
- Molecule 1: Fluoroacetate dehalogenase



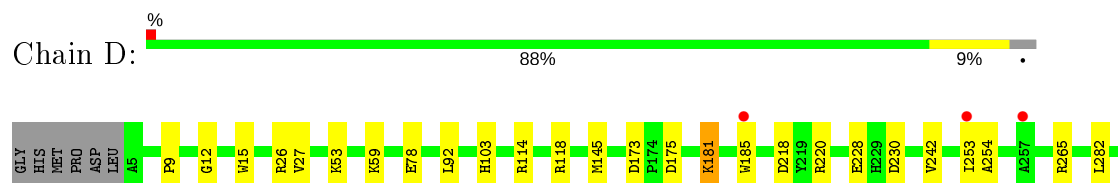
- Molecule 1: Fluoroacetate dehalogenase



- Molecule 1: Fluoroacetate dehalogenase



- Molecule 1: Fluoroacetate dehalogenase



Q289	
A300	
ALA	
PRO	
GLY	
SER	

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 0.177 , 0.208	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 , 44.5	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

5.1 Standard geometry

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	1.29	10/2559 (0.4%)	1.12	15/3488 (0.4%)
1	B	1.28	6/2463 (0.2%)	1.15	13/3351 (0.4%)
1	C	1.23	3/2470 (0.1%)	1.15	13/3363 (0.4%)
1	D	1.22	3/2458 (0.1%)	1.15	16/3346 (0.5%)
All	All	1.26	22/9950 (0.2%)	1.14	57/13548 (0.4%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	GLU	CG-CD	7.01	1.62	1.51
1	B	295	VAL	CB-CG1	6.25	1.66	1.52
1	C	285	GLU	CB-CG	-6.16	1.40	1.52
1	A	277	GLU	CB-CG	6.16	1.63	1.52
1	A	97	GLU	CB-CG	-6.14	1.40	1.52
1	A	234	VAL	CB-CG2	-5.92	1.40	1.52
1	B	224	TYR	CE1-CZ	-5.76	1.31	1.38
1	D	254	ALA	CA-CB	5.76	1.64	1.52
1	A	163	ALA	CA-CB	5.62	1.64	1.52
1	B	219	TYR	CE1-CZ	-5.60	1.31	1.38
1	A	116	SER	CA-CB	-5.58	1.44	1.52
1	A	75	GLU	CG-CD	5.41	1.60	1.51
1	C	115	VAL	CB-CG2	-5.40	1.41	1.52
1	A	75	GLU	CB-CG	-5.40	1.41	1.52
1	A	295	VAL	CB-CG1	5.39	1.64	1.52
1	A	141	TYR	CE2-CZ	-5.37	1.31	1.38
1	D	242	VAL	CB-CG2	5.37	1.64	1.52
1	C	51	ALA	CA-CB	5.34	1.63	1.52
1	D	78	GLU	CG-CD	5.31	1.59	1.51
1	B	177	TYR	CD1-CE1	5.20	1.47	1.39
1	B	144	ARG	CB-CG	-5.12	1.38	1.52
1	A	62	VAL	CB-CG2	5.02	1.63	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	MET	CG-SD-CE	-10.40	83.55	100.20
1	B	208	ASP	CB-CG-OD1	10.14	127.42	118.30
1	D	114	ARG	NE-CZ-NH1	-9.96	115.32	120.30
1	B	49	ARG	NE-CZ-NH2	9.32	124.96	120.30
1	C	175	ASP	CB-CG-OD1	8.96	126.36	118.30
1	B	49	ARG	NE-CZ-NH1	-8.82	115.89	120.30
1	A	244	MET	CG-SD-CE	-8.31	86.91	100.20
1	C	57	ARG	NE-CZ-NH1	-7.93	116.33	120.30
1	D	230	ASP	CB-CG-OD1	7.51	125.06	118.30
1	D	114	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	D	218	ASP	CB-CG-OD1	-7.29	111.73	118.30
1	C	187	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	C	175	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	D	118	ARG	NE-CZ-NH2	7.21	123.91	120.30
1	B	1	MET	CG-SD-CE	-7.20	88.68	100.20
1	C	57	ARG	NE-CZ-NH2	7.19	123.90	120.30
1	A	49	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	B	3	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	210	MET	CG-SD-CE	-6.75	89.39	100.20
1	C	187	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	175	ASP	CB-CG-OD1	6.53	124.18	118.30
1	B	175	ASP	CB-CG-OD1	6.52	124.17	118.30
1	C	26	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	A	26	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	D	282	LEU	CA-CB-CG	6.35	129.91	115.30
1	D	145	MET	CG-SD-CE	6.27	110.23	100.20
1	C	208	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	262	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	D	26	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	B	22	ARG	NE-CZ-NH1	-6.03	117.28	120.30
1	A	212	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	D	175	ASP	CB-CG-OD1	5.86	123.57	118.30
1	D	265	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	B	195	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	262	ASP	CB-CG-OD1	5.83	123.55	118.30
1	D	92	LEU	CB-CG-CD2	5.83	120.90	111.00
1	A	110	ASP	CB-CG-OD1	5.74	123.46	118.30
1	B	46	MET	CG-SD-CE	-5.70	91.08	100.20
1	D	220	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	C	208	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	C	220	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	A	226	ASP	CB-CG-OD2	-5.48	113.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	GLU	OE1-CD-OE2	-5.47	116.73	123.30
1	C	110	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	126	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	C	46	MET	CG-SD-CE	-5.41	91.55	100.20
1	A	212	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	B	144	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	B	145	MET	CG-SD-CE	5.19	108.50	100.20
1	D	173	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	173	ASP	CB-CG-OD1	5.18	122.97	118.30
1	B	118	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	D	26	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	D	103	HIS	CB-CA-C	5.08	120.57	110.40
1	D	228	GLU	OE1-CD-OE2	-5.08	117.20	123.30
1	C	257	ALA	N-CA-CB	-5.04	103.04	110.10
1	A	230	ASP	CB-CG-OD1	5.04	122.83	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	2475	0	2374	18	0
1	B	2383	0	2293	18	0
1	C	2392	0	2308	5	0
1	D	2380	0	2293	9	0
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	5	0
4	B	297	0	0	3	0
4	C	256	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	210	0	0	2	0
All	All	10676	0	9268	49	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 (49) 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:NE2	1:D:289[B]:GLN:H	1.98	0.61
1:A:289:GLN:H	1:A:289:GLN:HE21	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
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: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:C:144:ARG:HE	1:C:258:ALA:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:TYR:HB2	1:B:230:ASP:HB3	1.99	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: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:B:136:LEU:HB2	1:B:141:TYR:CE1	2.54	0.42
1:B:181:LYS:HD3	1:B:181:LYS:HA	1.86	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%)	242 (98%)	6 (2%)	49	24
1	B	240/242 (99%)	238 (99%)	2 (1%)	81	70
1	C	242/242 (100%)	238 (98%)	4 (2%)	60	38
1	D	239/242 (99%)	235 (98%)	4 (2%)	60	38
All	All	969/968 (100%)	953 (98%)	16 (2%)	62	38

All (16) residues with a non-rotameric sidechain are listed below:

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	GLN
1	B	289	GLN

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 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	304/306 (99%)	-0.59	3 (0%) 82 82	11, 18, 29, 40	0
1	B	294/306 (96%)	-0.61	2 (0%) 87 87	10, 16, 29, 39	0
1	C	301/306 (98%)	-0.58	1 (0%) 94 93	12, 19, 30, 51	0
1	D	296/306 (96%)	-0.42	3 (1%) 82 82	14, 22, 37, 50	0
All	All	1195/1224 (97%)	-0.55	9 (0%) 86 86	10, 19, 32, 51	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	ASP	5.1
1	D	253	ILE	3.4
1	D	257	ALA	3.3
1	A	257	ALA	3.1
1	B	301	ALA	3.1
1	A	3[A]	ASP	2.5
1	A	302	PRO	2.4
1	D	185[A]	TRP	2.1
1	B	185[A]	TRP	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. 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	0.06	30,30,30,30	0
3	CL	A	306	1/1	0.97	0.04	32,32,32,32	0
3	CL	C	306	1/1	0.98	0.06	38,38,38,38	0
2	NI	C	305	1/1	0.98	0.05	28,28,28,28	0
2	NI	A	305	1/1	0.99	0.06	21,21,21,21	0
3	CL	B	306	1/1	0.99	0.05	26,26,26,26	0
2	NI	B	305	1/1	1.00	0.06	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.