



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:45 PM GMT

PDB ID : 1GYH
Title : STRUCTURE OF D158A CELLVIBRIO CELLULOSA ALPHA-L-ARABINANASE MUTANT
Authors : Nurizzo, D.; Turkenburg, J.P.; Charnock, S.J.; Roberts, S.M.; Dodson, E.J.; Mckie, V.A.; Taylor, E.J.; Gilbert, H.J.; Davies, G.J.
Deposited on : 2002-04-23
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
<http://wwpdb.org/validation/2016/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
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

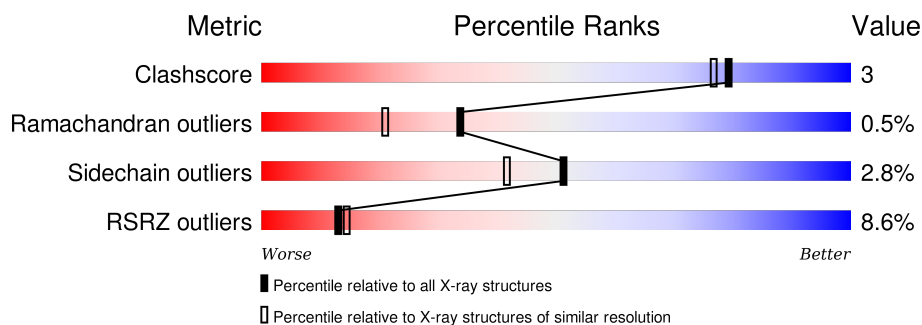
1 Overall quality at a glance

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))
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 ≥ 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	318	<div> <div></div> <div>92% 7% .</div> </div>
1	B	318	<div> <div>3%</div> <div>92% 6% ..</div> </div>
1	C	318	<div> <div>3%</div> <div>94% . .</div> </div>
1	D	318	<div> <div>15%</div> <div>91% 8% ..</div> </div>
1	E	318	<div> <div>8%</div> <div>88% 10% ..</div> </div>
1	F	318	<div> <div>21%</div> <div>86% 12% ..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	1348	-	-	X	X
2	CL	B	1348	-	-	X	X
2	CL	C	1348	-	-	X	X
2	CL	D	1347	-	-	X	X
2	CL	E	1348	-	-	X	X
2	CL	F	1347	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17338 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 ARABINAN ENDO-1,5-ALPHA-L-ARABINOSIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	8	0
			2589	1654	452	477	6			
1	B	317	Total	C	N	O	S	0	11	0
			2592	1658	450	478	6			
1	C	318	Total	C	N	O	S	0	7	0
			2576	1646	444	480	6			
1	D	316	Total	C	N	O	S	0	2	0
			2548	1634	436	471	7			
1	E	318	Total	C	N	O	S	0	3	0
			2570	1647	441	476	6			
1	F	316	Total	C	N	O	S	0	2	0
			2547	1632	436	473	6			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cl	0	0
			1	1		
2	E	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	C	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	447	Total 447	O 447	0	0
3	B	356	Total 356	O 356	0	0
3	C	371	Total 371	O 371	0	0
3	D	277	Total 277	O 277	0	0
3	E	291	Total 291	O 291	0	0
3	F	168	Total 168	O 168	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 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: ARABINAN ENDO-1,5-ALPHA-L-ARABINOSIDASE A



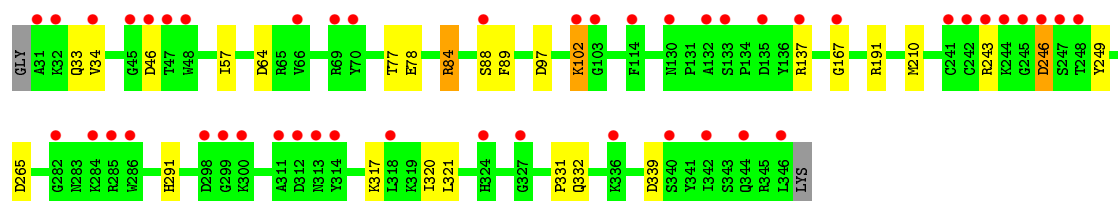
- Molecule 1: ARABINAN ENDO-1,5-ALPHA-L-ARABINOSIDASE A



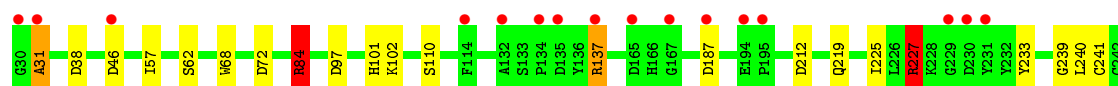
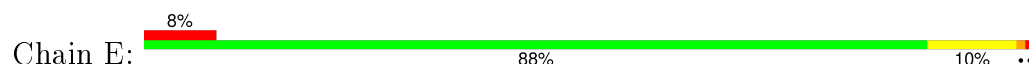
- Molecule 1: ARABINAN ENDO-1,5-ALPHA-L-ARABINOSIDASE A

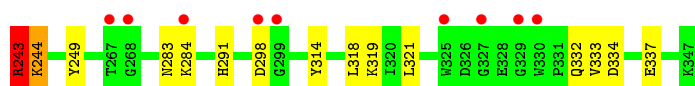


- Molecule 1: ARABINAN ENDO-1,5-ALPHA-L-ARABINOSIDASE A

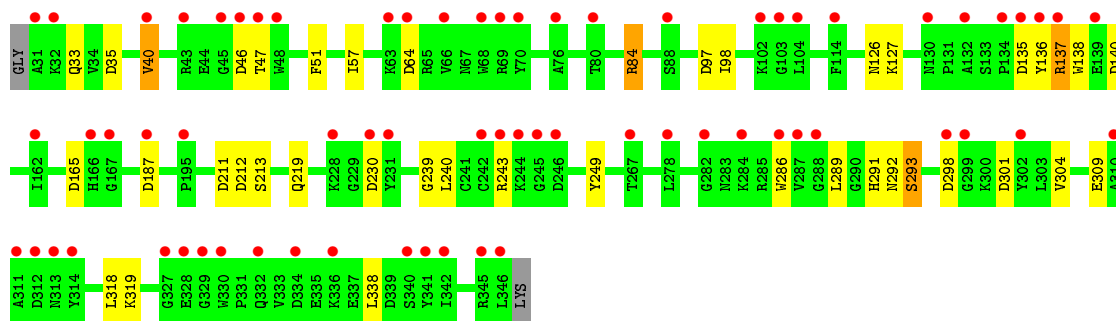
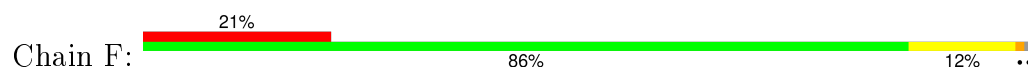


- Molecule 1: ARABINAN ENDO-1,5-ALPHA-L-ARABINOSIDASE A





● Molecule 1: ARABINAN ENDO-1,5-ALPHA-L-ARABINOSIDASE A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.56 Å 79.56 Å 132.40 Å 88.83° 89.58° 83.58°	Depositor
Resolution (Å)	20.00 – 1.89 19.85 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.6 (20.00-1.89) 96.3 (19.85-1.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 1.89 Å)	Xtriage
Refinement program	REFMAC 5.1.13	Depositor
R, R_{free}	0.147 , 0.203 0.148 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 70.4	EDS
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 154823 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17338	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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, 0.375 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	0.86	2/2712 (0.1%)	0.98	14/3679 (0.4%)
1	B	0.77	0/2729	0.94	15/3702 (0.4%)
1	C	0.79	2/2692 (0.1%)	0.91	12/3656 (0.3%)
1	D	0.73	1/2636 (0.0%)	0.88	9/3584 (0.3%)
1	E	0.74	1/2664 (0.0%)	0.92	14/3619 (0.4%)
1	F	0.63	0/2635	0.86	12/3582 (0.3%)
All	All	0.76	6/16068 (0.0%)	0.92	76/21822 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	30	GLY	N-CA	-8.36	1.33	1.46
1	A	30	GLY	N-CA	-7.63	1.34	1.46
1	A	31	ALA	CA-CB	-7.44	1.36	1.52
1	D	191	ARG	CG-CD	-6.38	1.36	1.51
1	C	31	ALA	CA-CB	-5.67	1.40	1.52
1	E	333	VAL	CB-CG2	-5.04	1.42	1.52

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188[A]	ASP	CB-CG-OD2	12.28	129.35	118.30
1	A	188[B]	ASP	CB-CG-OD2	12.28	129.35	118.30
1	B	165[A]	ASP	CB-CG-OD2	9.41	126.77	118.30
1	B	165[B]	ASP	CB-CG-OD2	9.41	126.77	118.30
1	D	84	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	D	84	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	C	312	ASP	CB-CG-OD2	7.34	124.91	118.30
1	B	140	ASP	CB-CG-OD2	7.28	124.85	118.30
1	E	72	ASP	CB-CG-OD1	6.67	124.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212[A]	ASP	CB-CG-OD2	6.62	124.25	118.30
1	B	212[B]	ASP	CB-CG-OD2	6.62	124.25	118.30
1	E	38	ASP	CB-CG-OD2	6.58	124.22	118.30
1	D	191	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	D	97	ASP	CB-CG-OD2	6.47	124.12	118.30
1	B	90	ASP	CB-CG-OD2	6.39	124.05	118.30
1	C	339	ASP	CB-CG-OD2	6.34	124.01	118.30
1	D	339	ASP	CB-CG-OD2	6.25	123.92	118.30
1	E	227	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	E	84	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	F	64	ASP	CB-CG-OD2	6.09	123.78	118.30
1	C	38	ASP	CB-CG-OD2	6.02	123.71	118.30
1	D	64	ASP	CB-CG-OD2	6.00	123.70	118.30
1	C	243	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	E	84	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	F	212	ASP	CB-CG-OD2	5.94	123.65	118.30
1	B	243	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	E	212	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	64	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	165	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	38	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	188[A]	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	A	188[B]	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	E	334	ASP	CB-CG-OD2	5.69	123.42	118.30
1	F	35	ASP	CB-CG-OD2	5.67	123.40	118.30
1	E	298	ASP	CB-CG-OD2	5.66	123.40	118.30
1	B	227[A]	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	227[B]	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	97	ASP	CB-CG-OD2	5.57	123.31	118.30
1	F	84	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	F	298	ASP	CB-CG-OD2	5.50	123.25	118.30
1	E	243	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	E	46[A]	ASP	CB-CG-OD2	5.48	123.23	118.30
1	E	46[B]	ASP	CB-CG-OD2	5.48	123.23	118.30
1	F	301	ASP	CB-CG-OD2	5.47	123.23	118.30
1	C	65[A]	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	65[B]	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	301	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	211	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	246	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	46	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	65[A]	ARG	NE-CZ-NH1	5.39	122.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65[B]	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	B	227[A]	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	B	227[B]	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	C	212[A]	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	212[B]	ASP	CB-CG-OD2	5.26	123.03	118.30
1	F	187	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	90	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	46	ASP	CB-CG-OD2	5.17	122.96	118.30
1	C	270	ASP	CB-CG-OD1	5.16	122.94	118.30
1	F	165	ASP	CB-CG-OD2	5.16	122.94	118.30
1	F	230	ASP	CB-CG-OD2	5.16	122.94	118.30
1	E	97	ASP	CB-CG-OD2	5.15	122.94	118.30
1	F	140	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	212	ASP	CB-CG-OD2	5.13	122.92	118.30
1	F	84	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	A	265	ASP	CB-CG-OD1	5.11	122.90	118.30
1	D	265	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	312	ASP	CB-CG-OD2	5.08	122.87	118.30
1	E	187	ASP	CB-CG-OD2	5.08	122.87	118.30
1	E	137	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	97	ASP	CB-CG-OD2	5.06	122.85	118.30
1	F	46	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	312	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	97	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	191	ARG	CG-CD-NE	5.00	122.31	111.80

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	2589	0	2485	12	0
1	B	2592	0	2495	16	0
1	C	2576	0	2462	8	0
1	D	2548	0	2441	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2570	0	2462	17	0
1	F	2547	0	2438	16	0
2	A	1	0	0	6	0
2	B	1	0	0	4	0
2	C	1	0	0	5	0
2	D	1	0	0	6	0
2	E	1	0	0	5	0
2	F	1	0	0	5	0
3	A	447	0	0	8	0
3	B	356	0	0	7	0
3	C	371	0	0	7	0
3	D	277	0	0	7	0
3	E	291	0	0	8	0
3	F	168	0	0	4	0
All	All	17338	0	14783	105	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 (105) 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:B:165[A]:ASP:OD1	1:B:227[A]:ARG:CZ	1.69	1.39
1:B:165[A]:ASP:OD1	1:B:227[A]:ARG:NH2	1.58	1.34
1:B:336[A]:LYS:HE2	3:B:2344:HOH:O	1.41	1.17
1:B:194[A]:GLU:OE1	3:B:2200:HOH:O	1.72	1.06
2:C:1348:CL:CL	3:C:2179:HOH:O	2.23	0.91
1:D:77:THR:HG23	1:D:78:GLU:H	1.39	0.88
2:F:1347:CL:CL	3:F:2075:HOH:O	2.30	0.86
1:E:227:ARG:HG3	1:E:227:ARG:HH11	1.41	0.85
1:D:77:THR:HG22	3:D:2041:HOH:O	1.81	0.81
2:E:1348:CL:CL	3:E:2138:HOH:O	2.36	0.81
2:B:1348:CL:CL	3:B:2173:HOH:O	2.36	0.80
2:E:1348:CL:CL	3:E:2242:HOH:O	2.38	0.77
2:A:1348:CL:CL	3:A:2231:HOH:O	2.40	0.77
1:E:101:HIS:ND1	3:E:2095:HOH:O	2.20	0.75
1:C:31:ALA:HB1	3:C:2002:HOH:O	1.85	0.74
2:F:1347:CL:CL	3:F:2074:HOH:O	2.43	0.73
1:A:31:ALA:HB2	3:A:2001:HOH:O	1.89	0.72
2:D:1347:CL:CL	3:D:2065:HOH:O	2.43	0.72
2:D:1347:CL:CL	3:D:2246:HOH:O	2.44	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1348:CL:CL	3:A:2377:HOH:O	2.46	0.71
1:B:336[A]:LYS:CE	3:B:2344:HOH:O	2.11	0.71
2:A:1348:CL:CL	3:A:2230:HOH:O	2.47	0.70
1:E:31:ALA:HB1	3:E:2003:HOH:O	1.92	0.70
1:A:31:ALA:HB1	3:A:2003:HOH:O	1.91	0.69
2:D:1347:CL:CL	3:D:2066:HOH:O	2.49	0.68
2:F:1347:CL:CL	3:F:2150:HOH:O	2.49	0.68
2:B:1348:CL:CL	3:B:2093:HOH:O	2.49	0.67
2:A:1348:CL:CL	3:A:2132:HOH:O	2.50	0.67
1:F:293:SER:HB3	1:F:304:VAL:HB	1.77	0.66
2:C:1348:CL:CL	3:C:2178:HOH:O	2.50	0.66
1:E:291:HIS:NE2	2:E:1348:CL:CL	2.66	0.66
2:D:1347:CL:CL	3:D:2127:HOH:O	2.50	0.66
1:A:291:HIS:NE2	2:A:1348:CL:CL	2.66	0.65
1:C:212[A]:ASP:OD2	3:C:2233:HOH:O	2.12	0.65
2:D:1347:CL:CL	3:D:2247:HOH:O	2.50	0.64
2:E:1348:CL:CL	3:E:2139:HOH:O	2.52	0.63
1:B:334:ASP:OD2	1:B:336[B]:LYS:HE2	1.99	0.62
1:E:84:ARG:HD3	3:E:2028:HOH:O	2.00	0.62
1:D:102:LYS:HZ2	1:D:102:LYS:HB3	1.66	0.60
1:C:291:HIS:NE2	2:C:1348:CL:CL	2.72	0.60
1:A:145[A]:ILE:HD11	1:A:154:TRP:CZ3	2.37	0.60
1:E:227:ARG:HG3	1:E:227:ARG:NH1	2.16	0.59
1:D:77:THR:HG23	1:D:78:GLU:N	2.13	0.59
1:E:318:LEU:O	1:E:319:LYS:HD3	2.04	0.58
1:F:318:LEU:O	1:F:319:LYS:HD2	2.04	0.58
1:A:145[A]:ILE:HD11	1:A:154:TRP:CH2	2.39	0.58
1:D:102:LYS:NZ	1:D:102:LYS:HB3	2.19	0.57
1:F:136:TYR:O	1:F:137:ARG:HB3	2.05	0.57
1:F:40:VAL:HG12	1:F:51:PHE:HB2	1.88	0.55
2:E:1348:CL:CL	3:E:2197:HOH:O	2.55	0.55
2:A:1348:CL:CL	3:A:2376:HOH:O	2.55	0.55
1:D:291:HIS:NE2	2:D:1347:CL:CL	2.76	0.55
1:B:165[A]:ASP:CG	1:B:227[A]:ARG:NH2	2.53	0.54
1:C:30:GLY:O	1:C:31:ALA:HB2	2.08	0.54
1:F:33:GLN:OE1	1:F:319:LYS:NZ	2.39	0.54
2:F:1347:CL:CL	3:F:2151:HOH:O	2.56	0.54
1:B:165[A]:ASP:OD1	1:B:227[A]:ARG:NH1	2.33	0.52
1:F:219:GLN:HE21	1:F:239:GLY:HA2	1.74	0.52
1:A:30:GLY:O	1:A:31:ALA:HB2	2.09	0.52
2:C:1348:CL:CL	3:C:2309:HOH:O	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:HIS:HB2	1:C:332:GLN:HG3	1.92	0.52
1:E:241:CYS:O	1:E:243:ARG:HD3	2.09	0.51
1:B:291:HIS:NE2	2:B:1348:CL:CL	2.79	0.51
1:B:165[A]:ASP:OD2	1:B:227[A]:ARG:NH1	2.44	0.50
1:A:214:GLN:NE2	3:A:2293:HOH:O	2.31	0.50
1:E:283:ASN:HB2	1:E:284:LYS:NZ	2.27	0.49
1:B:165[A]:ASP:CG	1:B:227[A]:ARG:CZ	2.68	0.49
1:F:40:VAL:HG13	1:F:98:ILE:HG22	1.95	0.49
1:F:286:TRP:CZ3	1:F:309:GLU:HB2	2.47	0.48
1:B:219:GLN:HE21	1:B:239:GLY:HA2	1.79	0.48
1:D:88:SER:O	1:D:89:PHE:C	2.53	0.48
1:D:167:GLY:C	3:D:2139:HOH:O	2.52	0.47
1:A:240:LEU:HB3	1:A:243:ARG:HD3	1.98	0.46
1:C:31:ALA:HA	3:C:2368:HOH:O	2.16	0.46
1:A:30:GLY:O	1:A:31:ALA:CB	2.64	0.46
1:E:321[A]:LEU:HD22	1:E:337:GLU:CB	2.46	0.46
1:B:240:LEU:HB3	1:B:243:ARG:HD2	1.97	0.45
1:F:127:LYS:HG3	1:F:135:ASP:HB3	1.97	0.45
1:F:291:HIS:NE2	2:F:1347:CL:CL	2.86	0.45
1:D:33:GLN:HB2	1:D:317:LYS:HD2	1.99	0.45
1:E:31:ALA:HA	3:E:2286:HOH:O	2.16	0.44
1:E:62:SER:HB2	1:E:68:TRP:CE3	2.52	0.44
1:B:336[B]:LYS:HE3	3:B:2349:HOH:O	2.17	0.43
1:F:126:ASN:HB2	1:F:138:TRP:CE3	2.52	0.43
1:F:40:VAL:HG21	1:F:97:ASP:HA	2.00	0.43
1:E:219:GLN:HE21	1:E:239:GLY:HA2	1.83	0.43
1:A:145[A]:ILE:CD1	1:A:154:TRP:CZ3	3.01	0.43
2:C:1348:CL:CL	3:C:2092:HOH:O	2.59	0.43
2:B:1348:CL:CL	3:B:2095:HOH:O	2.59	0.42
1:F:211:ASP:OD2	1:F:213[A]:SER:HB2	2.19	0.42
1:A:219:GLN:HE21	1:A:239:GLY:HA2	1.85	0.42
1:B:347:LYS:HD3	1:B:347:LYS:HA	1.55	0.41
1:E:321[A]:LEU:HD22	1:E:337:GLU:HB2	2.02	0.41
1:D:331:PRO:O	1:D:332:GLN:NE2	2.53	0.41
1:B:305:LEU:HD12	1:B:305:LEU:C	2.41	0.41
1:E:244:LYS:HE2	1:E:314:TYR:CD1	2.56	0.41
1:C:30:GLY:O	1:C:31:ALA:CB	2.67	0.41
1:E:225:ILE:HA	1:E:233:TYR:O	2.20	0.41
1:D:320:ILE:C	1:D:321:LEU:HD23	2.41	0.41
1:F:243:ARG:O	1:F:243:ARG:HG3	2.21	0.41
1:F:289:LEU:HD12	1:F:289:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:LYS:HE3	1:F:338:LEU:O	2.21	0.40
1:A:172:SER:HA	1:A:181:LYS:O	2.21	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	324/318 (102%)	305 (94%)	17 (5%)	2 (1%)	30	17
1	B	326/318 (102%)	311 (95%)	14 (4%)	1 (0%)	46	35
1	C	323/318 (102%)	305 (94%)	16 (5%)	2 (1%)	30	17
1	D	316/318 (99%)	300 (95%)	15 (5%)	1 (0%)	46	35
1	E	319/318 (100%)	304 (95%)	13 (4%)	2 (1%)	30	17
1	F	316/318 (99%)	300 (95%)	15 (5%)	1 (0%)	46	35
All	All	1924/1908 (101%)	1825 (95%)	90 (5%)	9 (0%)	34	21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	31	ALA
1	A	31	ALA
1	E	31	ALA
1	A	57	ILE
1	B	57	ILE
1	C	57	ILE
1	D	57	ILE
1	E	57	ILE
1	F	57	ILE

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	275/267 (103%)	264 (96%)	11 (4%)	38	26
1	B	277/267 (104%)	264 (95%)	13 (5%)	32	20
1	C	274/267 (103%)	271 (99%)	3 (1%)	80	79
1	D	268/267 (100%)	260 (97%)	8 (3%)	48	38
1	E	270/267 (101%)	261 (97%)	9 (3%)	45	34
1	F	268/267 (100%)	260 (97%)	8 (3%)	48	38
All	All	1632/1602 (102%)	1580 (97%)	52 (3%)	51	35

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	42	THR
1	A	84[A]	ARG
1	A	84[B]	ARG
1	A	145[A]	ILE
1	A	145[B]	ILE
1	A	188[A]	ASP
1	A	188[B]	ASP
1	A	191	ARG
1	A	243	ARG
1	A	249	TYR
1	B	63	LYS
1	B	77	THR
1	B	110	SER
1	B	137	ARG
1	B	165[A]	ASP
1	B	165[B]	ASP
1	B	194[A]	GLU
1	B	194[B]	GLU
1	B	227[A]	ARG
1	B	227[B]	ARG
1	B	249	TYR

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Mol	Chain	Res	Type
1	B	336[A]	LYS
1	B	336[B]	LYS
1	C	214[A]	GLN
1	C	214[B]	GLN
1	C	249	TYR
1	D	34	VAL
1	D	84	ARG
1	D	102	LYS
1	D	137	ARG
1	D	210	MET
1	D	243	ARG
1	D	246	ASP
1	D	249	TYR
1	E	84	ARG
1	E	110	SER
1	E	137	ARG
1	E	227	ARG
1	E	240	LEU
1	E	243	ARG
1	E	244	LYS
1	E	249	TYR
1	E	332	GLN
1	F	40	VAL
1	F	47	THR
1	F	84	ARG
1	F	137	ARG
1	F	240	LEU
1	F	249	TYR
1	F	292	ASN
1	F	293	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	219	GLN
1	A	258	GLN
1	B	214	GLN
1	B	219	GLN
1	C	332	GLN
1	D	214	GLN
1	D	219	GLN

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Mol	Chain	Res	Type
1	D	258	GLN
1	D	332	GLN
1	E	214	GLN
1	E	219	GLN
1	F	219	GLN
1	F	292	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

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	318/318 (100%)	0.33	4 (1%) 79 82	10, 14, 21, 42	0
1	B	317/318 (99%)	0.25	10 (3%) 51 54	10, 14, 20, 46	0
1	C	318/318 (100%)	0.23	10 (3%) 52 56	10, 14, 22, 37	0
1	D	316/318 (99%)	0.77	47 (14%) 3 3	8, 15, 22, 32	0
1	E	318/318 (100%)	0.43	25 (7%) 15 17	10, 14, 21, 41	0
1	F	316/318 (99%)	1.26	68 (21%) 1 1	9, 16, 20, 29	0
All	All	1903/1908 (99%)	0.54	164 (8%) 13 14	8, 15, 21, 46	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	31	ALA	7.4
1	F	46	ASP	5.4
1	F	114	PHE	5.3
1	F	311	ALA	5.2
1	F	346	LEU	5.1
1	E	231	TYR	4.9
1	D	311	ALA	4.9
1	F	31	ALA	4.8
1	D	346	LEU	4.8
1	E	132	ALA	4.7
1	F	327	GLY	4.5
1	D	45	GLY	4.4
1	F	314	TYR	4.4
1	D	246	ASP	4.3
1	D	242[A]	CYS	4.3
1	E	167	GLY	4.3
1	F	330	TRP	4.3
1	C	30	GLY	4.2
1	F	242	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	132	ALA	4.1
1	F	313	ASN	4.1
1	D	245	GLY	4.0
1	D	284	LYS	4.0
1	F	328	GLU	4.0
1	F	284	LYS	3.9
1	E	327	GLY	3.8
1	F	134	PRO	3.8
1	D	103	GLY	3.8
1	E	230	ASP	3.8
1	F	135	ASP	3.8
1	B	134	PRO	3.8
1	C	114	PHE	3.7
1	F	187	ASP	3.7
1	F	70	TYR	3.7
1	C	88	SER	3.7
1	F	246	ASP	3.6
1	F	69	ARG	3.6
1	F	244	LYS	3.5
1	D	344	GLN	3.5
1	F	299	GLY	3.5
1	F	32	LYS	3.5
1	D	314	TYR	3.4
1	F	231	TYR	3.4
1	F	243	ARG	3.4
1	F	137	ARG	3.4
1	F	166	HIS	3.3
1	D	342	ILE	3.3
1	D	69	ARG	3.3
1	D	32	LYS	3.3
1	E	134	PRO	3.3
1	A	30	GLY	3.2
1	B	88	SER	3.2
1	D	286	TRP	3.2
1	D	336	LYS	3.1
1	E	229	GLY	3.1
1	D	298	ASP	3.1
1	F	342	ILE	3.1
1	E	329	GLY	3.1
1	F	63	LYS	3.1
1	F	103	GLY	3.1
1	C	132	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	241	CYS	3.1
1	D	46	ASP	3.1
1	F	278	LEU	3.0
1	D	244	LYS	3.0
1	D	137	ARG	3.0
1	D	48	TRP	3.0
1	F	340	SER	3.0
1	B	132	ALA	3.0
1	D	282	GLY	3.0
1	E	284	LYS	3.0
1	F	336	LYS	3.0
1	F	302	TYR	2.9
1	E	31	ALA	2.9
1	F	287	VAL	2.9
1	F	88	SER	2.9
1	E	298	ASP	2.9
1	F	136	TYR	2.9
1	D	132	ALA	2.9
1	E	30	GLY	2.8
1	D	114	PHE	2.8
1	F	167	GLY	2.8
1	F	334	ASP	2.8
1	F	66	VAL	2.8
1	F	104	LEU	2.8
1	E	187	ASP	2.8
1	F	47	THR	2.8
1	B	114	PHE	2.7
1	D	299	GLY	2.7
1	E	195	PRO	2.7
1	F	45	GLY	2.7
1	F	345	ARG	2.7
1	E	268	GLY	2.7
1	D	327	GLY	2.6
1	D	47	THR	2.6
1	C	87	PRO	2.6
1	F	245	GLY	2.6
1	F	48	TRP	2.5
1	E	46[A]	ASP	2.5
1	F	139	GLU	2.5
1	F	267	THR	2.5
1	D	135	ASP	2.5
1	E	299	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	330	TRP	2.4
1	D	130	ASN	2.4
1	D	167	GLY	2.4
1	D	313	ASN	2.4
1	F	130	ASN	2.4
1	A	107	LEU	2.4
1	D	312	ASP	2.4
1	D	66[A]	VAL	2.4
1	F	80	THR	2.4
1	C	313[A]	ASN	2.3
1	F	288	GLY	2.3
1	F	102	LYS	2.3
1	D	88	SER	2.3
1	F	282	GLY	2.3
1	D	300	LYS	2.3
1	C	246	ASP	2.3
1	A	162	ILE	2.3
1	B	137	ARG	2.3
1	F	162	ILE	2.3
1	B	77	THR	2.3
1	F	195	PRO	2.3
1	F	230	ASP	2.2
1	F	76	ALA	2.2
1	B	347	LYS	2.2
1	D	340	SER	2.2
1	D	243	ARG	2.2
1	F	329	GLY	2.2
1	F	312	ASP	2.2
1	F	298	ASP	2.2
1	E	325	TRP	2.2
1	F	68	TRP	2.2
1	E	114	PHE	2.2
1	A	109	TYR	2.2
1	D	285	ARG	2.2
1	D	34	VAL	2.2
1	E	135	ASP	2.1
1	F	64	ASP	2.1
1	F	286	TRP	2.1
1	F	332	GLN	2.1
1	C	134	PRO	2.1
1	D	324	HIS	2.1
1	D	247	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	267	THR	2.1
1	D	102	LYS	2.1
1	D	70	TYR	2.1
1	F	310	ALA	2.1
1	E	165	ASP	2.1
1	E	137	ARG	2.1
1	D	318	LEU	2.1
1	F	228	LYS	2.1
1	F	40	VAL	2.1
1	C	225	ILE	2.0
1	D	133	SER	2.0
1	F	341	TYR	2.0
1	D	248	THR	2.0
1	B	87	PRO	2.0
1	E	194	GLU	2.0
1	F	43	ARG	2.0
1	B	31	ALA	2.0
1	C	234	LEU	2.0
1	B	135	ASP	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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	CL	C	1348	1/1	0.99	0.17	8.30	28,28,28,28	0
2	CL	A	1348	1/1	0.99	0.18	7.77	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CL	E	1348	1/1	0.99	0.17	4.44	27,27,27,27	0
2	CL	B	1348	1/1	1.00	0.19	4.04	25,25,25,25	0
2	CL	D	1347	1/1	1.00	0.17	3.83	29,29,29,29	0
2	CL	F	1347	1/1	0.99	0.15	1.38	39,39,39,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.