



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:57 am GMT

PDB ID : 1ODS
Title : CEPHALOSPORIN C DEACETYLASE FROM BACILLUS SUBTILIS
Authors : Vincent, F.; Charnock, S.J.; Verschueren, K.H.G.; Turkenburg, J.P.; Scott, D.J.; Offen, W.A.; Roberts, S.; Pell, G.; Gilbert, H.J.; Brannigan, J.A.; Davies, G.J.
Deposited on : 2003-02-20
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

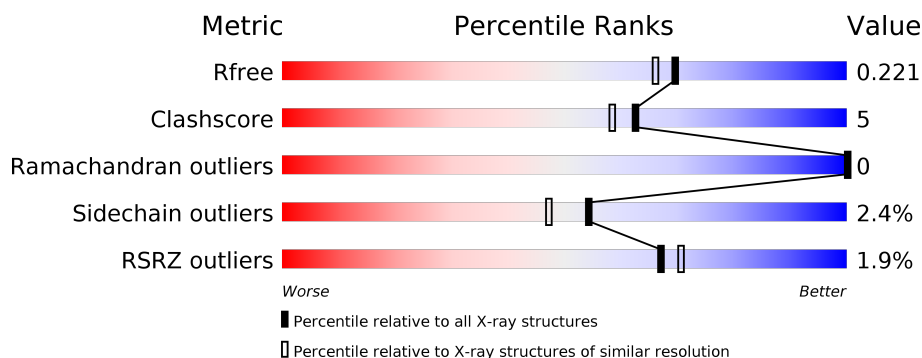
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



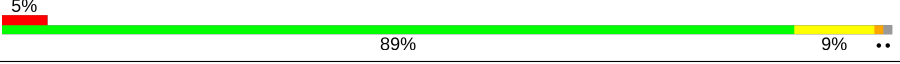

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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>90%</div> <div>9% ..</div> </div>
1	B	318	<div> <div>%</div> <div>86%</div> <div>13% ..</div> </div>
1	C	318	<div> <div>%</div> <div>87%</div> <div>11% ..</div> </div>
1	D	318	<div> <div>89%</div> <div>9% ..</div> </div>
1	E	318	<div> <div>4%</div> <div>86%</div> <div>12% ..</div> </div>
1	F	318	<div> <div>3%</div> <div>86%</div> <div>12% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	318	
1	H	318	

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	B	1318	-	-	-	X
2	CL	C	1318	-	-	-	X
2	CL	D	1318	-	-	-	X
2	CL	E	1318	-	-	-	X
2	CL	F	1318	-	-	-	X
2	CL	G	1318	-	-	-	X
2	CL	H	1318	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22366 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 CEPHALOSPORIN C DEACETYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	5	0
			2542	1645	413	478	6			
1	B	316	Total	C	N	O	S	0	4	0
			2539	1644	412	477	6			
1	C	316	Total	C	N	O	S	0	3	0
			2536	1641	412	477	6			
1	D	316	Total	C	N	O	S	0	5	0
			2543	1645	412	480	6			
1	E	316	Total	C	N	O	S	0	3	0
			2535	1641	413	475	6			
1	F	316	Total	C	N	O	S	0	2	0
			2531	1640	411	474	6			
1	G	316	Total	C	N	O	S	0	2	0
			2533	1638	411	478	6			
1	H	316	Total	C	N	O	S	0	5	0
			2542	1645	411	480	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	GLU	GLN	CONFLICT	UNP P94388
A	255	TYR	ASP	CONFLICT	UNP P94388
B	220	GLU	GLN	CONFLICT	UNP P94388
B	255	TYR	ASP	CONFLICT	UNP P94388
C	220	GLU	GLN	CONFLICT	UNP P94388
C	255	TYR	ASP	CONFLICT	UNP P94388
D	220	GLU	GLN	CONFLICT	UNP P94388
D	255	TYR	ASP	CONFLICT	UNP P94388
E	220	GLU	GLN	CONFLICT	UNP P94388
E	255	TYR	ASP	CONFLICT	UNP P94388
F	220	GLU	GLN	CONFLICT	UNP P94388
F	255	TYR	ASP	CONFLICT	UNP P94388
G	220	GLU	GLN	CONFLICT	UNP P94388

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Chain	Residue	Modelled	Actual	Comment	Reference
G	255	TYR	ASP	CONFLICT	UNP P94388
H	220	GLU	GLN	CONFLICT	UNP P94388
H	255	TYR	ASP	CONFLICT	UNP P94388

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		
2	E	1	Total	Cl	0	0
			1	1		
2	H	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	310	Total	O	0	0
			310	310		
4	B	259	Total	O	0	0
			259	259		
4	C	275	Total	O	0	0
			275	275		
4	D	289	Total	O	0	0
			289	289		

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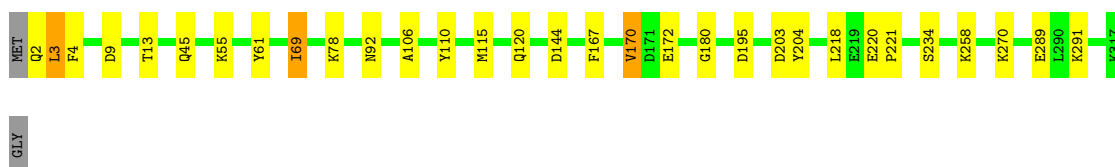
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	210	Total 210	O 210	0	0
4	F	242	Total 242	O 242	0	0
4	G	194	Total 194	O 194	0	0
4	H	276	Total 276	O 276	0	0

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 ($RSRZ > 2$). 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.

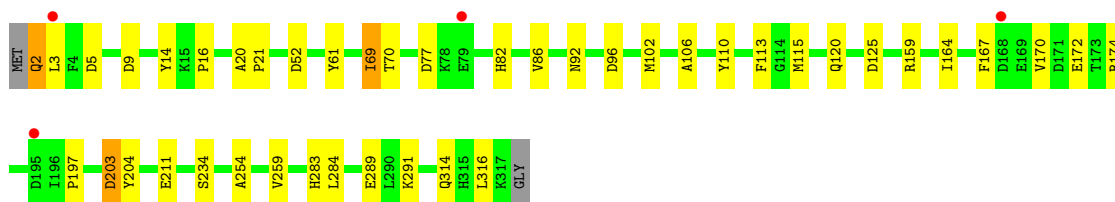
• Molecule 1: CEPHALOSPORIN C DEACETYLASE

Chain A: 




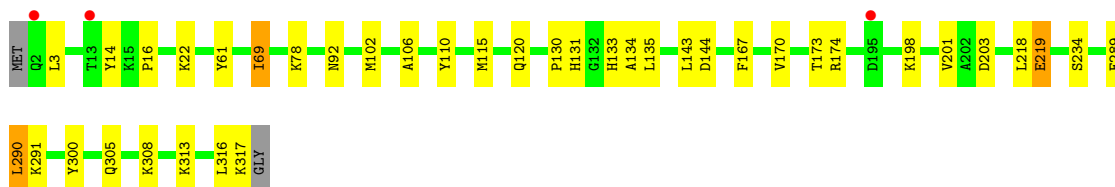
• Molecule 1: CEPHALOSPORIN C DEACETYLASE

Chain B: 



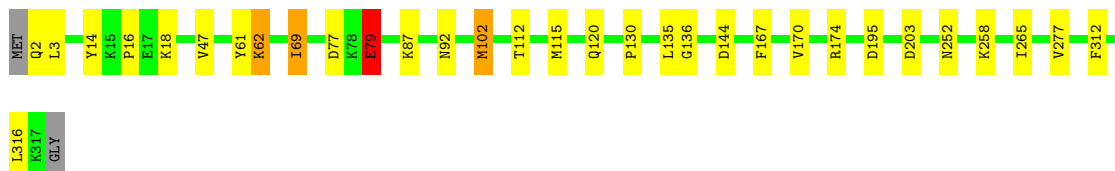
• Molecule 1: CEPHALOSPORIN C DEACETYLASE

Chain C: 

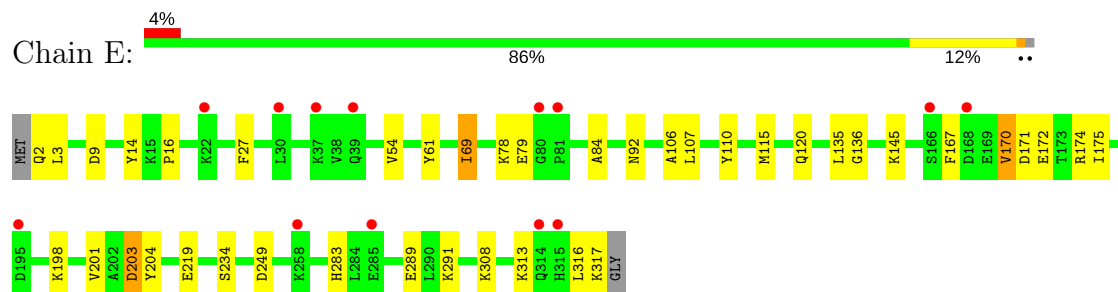


• Molecule 1: CEPHALOSPORIN C DEACETYLASE

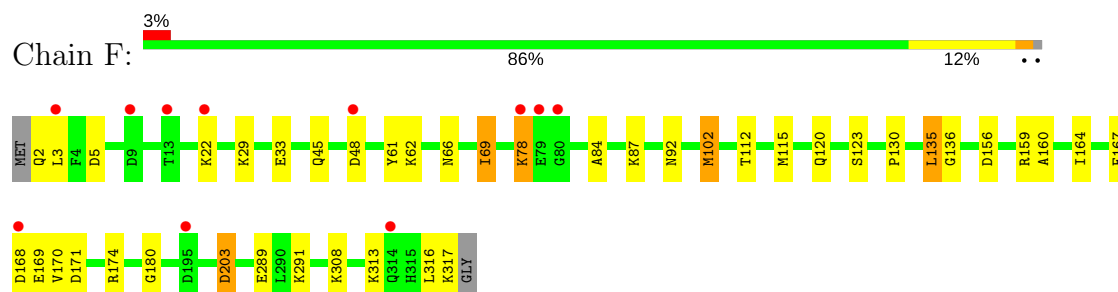
Chain D: 



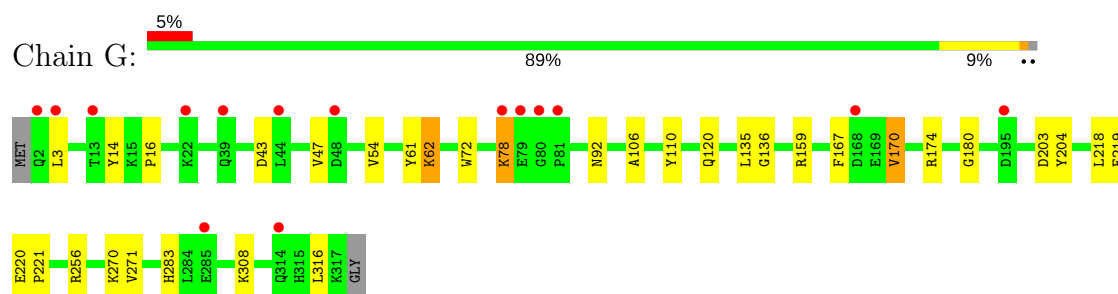
- Molecule 1: CEPHALOSPORIN C DEACETYLASE



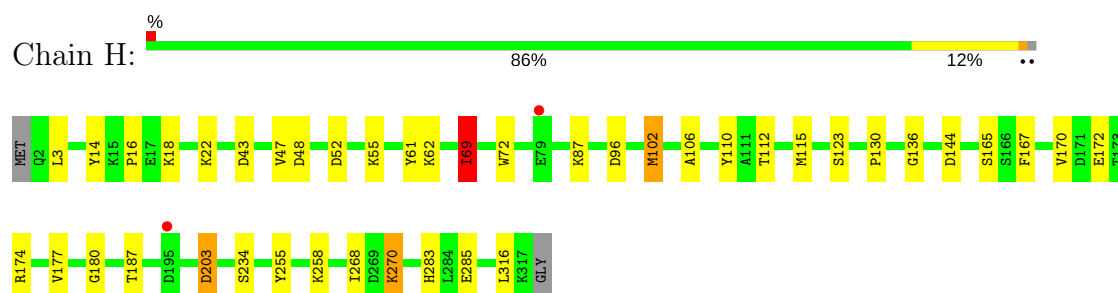
- Molecule 1: CEPHALOSPORIN C DEACETYLASE



- Molecule 1: CEPHALOSPORIN C DEACETYLASE



- Molecule 1: CEPHALOSPORIN C DEACETYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	315.21Å 315.21Å 68.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 1.90 14.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (100.00-1.90) 99.9 (14.99-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.152 , 0.186 0.197 , 0.221	Depositor DCC
R_{free} test set	10040 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22366	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: MG, 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	0.54	0/2638	0.78	3/3584 (0.1%)
1	B	0.56	1/2630 (0.0%)	0.79	7/3573 (0.2%)
1	C	0.52	0/2622	0.76	3/3562 (0.1%)
1	D	0.55	0/2639	0.79	4/3584 (0.1%)
1	E	0.46	0/2621	0.73	4/3561 (0.1%)
1	F	0.51	0/2612	0.76	5/3549 (0.1%)
1	G	0.45	0/2614	0.74	1/3551 (0.0%)
1	H	0.51	0/2638	0.78	9/3584 (0.3%)
All	All	0.51	1/21014 (0.0%)	0.77	36/28548 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	MET	SD-CE	-5.23	1.48	1.77

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	H	69[A]	ILE	CG1-CB-CG2	7.51	127.93	111.40
1	H	69[B]	ILE	CG1-CB-CG2	7.51	127.93	111.40
1	H	144	ASP	CB-CG-OD1	6.76	124.39	118.30
1	E	171	ASP	CB-CG-OD2	6.59	124.23	118.30
1	B	5	ASP	CB-CG-OD2	6.38	124.04	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	2542	0	2486	23	0
1	B	2539	0	2481	28	0
1	C	2536	0	2474	20	0
1	D	2543	0	2481	24	0
1	E	2535	0	2479	26	0
1	F	2531	0	2475	32	0
1	G	2533	0	2465	25	0
1	H	2542	0	2479	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	1	0
2	D	1	0	0	1	0
2	E	1	0	0	0	0
2	F	1	0	0	1	0
2	G	1	0	0	0	0
2	H	1	0	0	1	0
3	A	2	0	0	0	0
4	A	310	0	0	7	1
4	B	259	0	0	3	1
4	C	275	0	0	1	0
4	D	289	0	0	2	0
4	E	210	0	0	2	0
4	F	242	0	0	3	0
4	G	194	0	0	3	0
4	H	276	0	0	1	0
All	All	22366	0	19820	200	1

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 5.

The worst 5 of 200 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:69:ILE:HB	4:A:2183:HOH:O	1.60	1.01
1:H:102:MET:HE2	1:H:112:THR:HG22	1.38	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:LYS:HE2	4:F:2076:HOH:O	1.63	0.98
1:E:174:ARG:HD2	1:E:316:LEU:O	1.66	0.94
1:D:174:ARG:HD2	1:D:316:LEU:O	1.70	0.90

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2169:HOH:O	4:B:2147:HOH:O[2_655]	2.01	0.19

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	319/318 (100%)	306 (96%)	13 (4%)	0	100	100
1	B	318/318 (100%)	306 (96%)	12 (4%)	0	100	100
1	C	317/318 (100%)	305 (96%)	12 (4%)	0	100	100
1	D	319/318 (100%)	306 (96%)	13 (4%)	0	100	100
1	E	317/318 (100%)	302 (95%)	15 (5%)	0	100	100
1	F	316/318 (99%)	301 (95%)	15 (5%)	0	100	100
1	G	316/318 (99%)	299 (95%)	17 (5%)	0	100	100
1	H	319/318 (100%)	305 (96%)	14 (4%)	0	100	100
All	All	2541/2544 (100%)	2430 (96%)	111 (4%)	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	271/267 (102%)	265 (98%)	6 (2%)	57	51
1	B	270/267 (101%)	264 (98%)	6 (2%)	57	51
1	C	269/267 (101%)	261 (97%)	8 (3%)	46	37
1	D	271/267 (102%)	264 (97%)	7 (3%)	51	43
1	E	269/267 (101%)	262 (97%)	7 (3%)	51	43
1	F	268/267 (100%)	259 (97%)	9 (3%)	42	32
1	G	268/267 (100%)	262 (98%)	6 (2%)	57	51
1	H	271/267 (102%)	264 (97%)	7 (3%)	51	43
All	All	2157/2136 (101%)	2101 (97%)	56 (3%)	54	43

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	79	GLU
1	E	172	GLU
1	H	69[A]	ILE
1	D	102	MET
1	E	69	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	12	GLN
1	E	314	GLN
1	H	120	GLN
1	E	182	GLN
1	F	10	GLN

5.3.3 RNA ⓘ

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 10 ligands modelled in this entry, 10 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, 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	316/318 (99%)	-0.07	0 100 100	5, 9, 14, 19	5 (1%)
1	B	316/318 (99%)	0.02	4 (1%) 77 80	5, 9, 14, 21	9 (2%)
1	C	316/318 (99%)	-0.03	3 (0%) 84 86	5, 9, 14, 21	6 (1%)
1	D	316/318 (99%)	-0.08	0 100 100	6, 9, 14, 19	7 (2%)
1	E	316/318 (99%)	0.24	13 (4%) 38 42	4, 10, 14, 19	7 (2%)
1	F	316/318 (99%)	0.09	11 (3%) 44 48	6, 10, 14, 20	5 (1%)
1	G	316/318 (99%)	0.22	15 (4%) 32 36	4, 10, 14, 24	3 (0%)
1	H	316/318 (99%)	-0.10	2 (0%) 89 90	5, 10, 15, 20	5 (1%)
All	All	2528/2544 (99%)	0.04	48 (1%) 67 70	4, 9, 14, 24	47 (1%)

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	285	GLU	4.0
1	G	80	GLY	3.9
1	E	195	ASP	3.8
1	E	30	LEU	3.7
1	F	195	ASP	3.5

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 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	E	1318	1/1	0.99	0.15	7.25	24,24,24,24	0
2	CL	C	1318	1/1	0.99	0.16	6.80	19,19,19,19	0
2	CL	F	1318	1/1	0.99	0.19	4.77	18,18,18,18	0
2	CL	B	1318	1/1	0.99	0.18	3.76	16,16,16,16	0
2	CL	D	1318	1/1	0.99	0.19	3.70	18,18,18,18	0
2	CL	G	1318	1/1	0.99	0.15	2.81	24,24,24,24	0
2	CL	H	1318	1/1	0.99	0.14	2.27	17,17,17,17	0
2	CL	A	1318	1/1	1.00	0.14	1.30	16,16,16,16	0
3	MG	A	1319	1/1	0.93	0.05	-1.66	31,31,31,31	0
3	MG	A	1320	1/1	0.98	0.07	-1.99	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.