



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:33 PM GMT

PDB ID : 3ZSS
Title : APO FORM OF GLGE ISOFORM 1 FROM STREPTOMYCES COELICOLOR
Authors : Syson, K.; Stevenson, C.E.M.; Rejzek, M.; Fairhurst, S.A.; Nair, A.; Bruton, C.J.; Field, R.A.; Chater, K.F.; Lawson, D.M.; Bornemann, S.
Deposited on : 2011-06-30
Resolution : 1.80 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
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

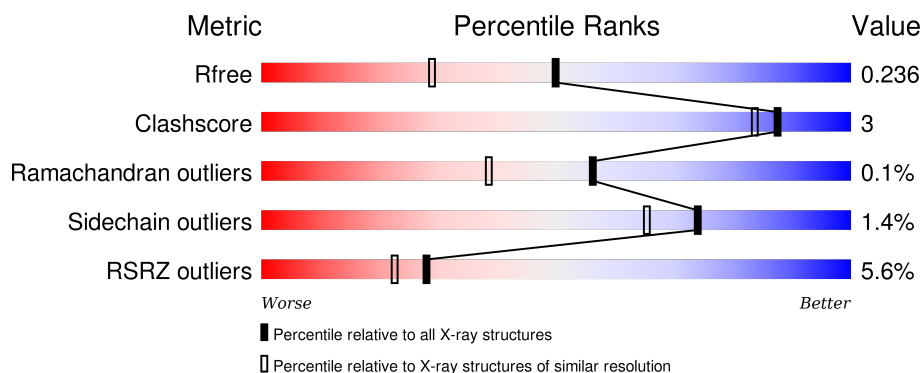
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	695	<div> <div></div> <div>86% 8% 7%</div> </div>
1	B	695	<div> <div>2%</div> <div>88% 5% 7%</div> </div>
1	C	695	<div> <div>7%</div> <div>85% 8% 7%</div> </div>
1	D	695	<div> <div>11%</div> <div>87% 6% 7%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20945 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 PUTATIVE GLUCANOHYDROLASE PEP1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	0	0
			5105	3228	922	945	10			
1	B	649	Total	C	N	O	S	0	0	0
			5101	3225	920	946	10			
1	C	649	Total	C	N	O	S	0	0	0
			5102	3228	921	943	10			
1	D	649	Total	C	N	O	S	0	0	0
			5097	3224	918	945	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q9L1K2
A	-18	GLY	-	EXPRESSION TAG	UNP Q9L1K2
A	-17	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	-16	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	-15	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-14	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-13	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-12	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-11	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-10	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-9	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	-8	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	-7	GLY	-	EXPRESSION TAG	UNP Q9L1K2
A	-6	LEU	-	EXPRESSION TAG	UNP Q9L1K2
A	-5	VAL	-	EXPRESSION TAG	UNP Q9L1K2
A	-4	PRO	-	EXPRESSION TAG	UNP Q9L1K2
A	-3	ARG	-	EXPRESSION TAG	UNP Q9L1K2
A	-2	GLY	-	EXPRESSION TAG	UNP Q9L1K2
A	-1	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	0	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-19	MET	-	EXPRESSION TAG	UNP Q9L1K2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP Q9L1K2
B	-17	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	-16	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	-15	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-14	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-13	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-12	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-11	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-10	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-9	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	-8	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	-7	GLY	-	EXPRESSION TAG	UNP Q9L1K2
B	-6	LEU	-	EXPRESSION TAG	UNP Q9L1K2
B	-5	VAL	-	EXPRESSION TAG	UNP Q9L1K2
B	-4	PRO	-	EXPRESSION TAG	UNP Q9L1K2
B	-3	ARG	-	EXPRESSION TAG	UNP Q9L1K2
B	-2	GLY	-	EXPRESSION TAG	UNP Q9L1K2
B	-1	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	0	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-19	MET	-	EXPRESSION TAG	UNP Q9L1K2
C	-18	GLY	-	EXPRESSION TAG	UNP Q9L1K2
C	-17	SER	-	EXPRESSION TAG	UNP Q9L1K2
C	-16	SER	-	EXPRESSION TAG	UNP Q9L1K2
C	-15	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-14	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-13	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-12	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-11	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-10	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-9	SER	-	EXPRESSION TAG	UNP Q9L1K2
C	-8	SER	-	EXPRESSION TAG	UNP Q9L1K2
C	-7	GLY	-	EXPRESSION TAG	UNP Q9L1K2
C	-6	LEU	-	EXPRESSION TAG	UNP Q9L1K2
C	-5	VAL	-	EXPRESSION TAG	UNP Q9L1K2
C	-4	PRO	-	EXPRESSION TAG	UNP Q9L1K2
C	-3	ARG	-	EXPRESSION TAG	UNP Q9L1K2
C	-2	GLY	-	EXPRESSION TAG	UNP Q9L1K2
C	-1	SER	-	EXPRESSION TAG	UNP Q9L1K2
C	0	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-19	MET	-	EXPRESSION TAG	UNP Q9L1K2
D	-18	GLY	-	EXPRESSION TAG	UNP Q9L1K2
D	-17	SER	-	EXPRESSION TAG	UNP Q9L1K2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP Q9L1K2
D	-15	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-14	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-13	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-12	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-11	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-10	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-9	SER	-	EXPRESSION TAG	UNP Q9L1K2
D	-8	SER	-	EXPRESSION TAG	UNP Q9L1K2
D	-7	GLY	-	EXPRESSION TAG	UNP Q9L1K2
D	-6	LEU	-	EXPRESSION TAG	UNP Q9L1K2
D	-5	VAL	-	EXPRESSION TAG	UNP Q9L1K2
D	-4	PRO	-	EXPRESSION TAG	UNP Q9L1K2
D	-3	ARG	-	EXPRESSION TAG	UNP Q9L1K2
D	-2	GLY	-	EXPRESSION TAG	UNP Q9L1K2
D	-1	SER	-	EXPRESSION TAG	UNP Q9L1K2
D	0	HIS	-	EXPRESSION TAG	UNP Q9L1K2

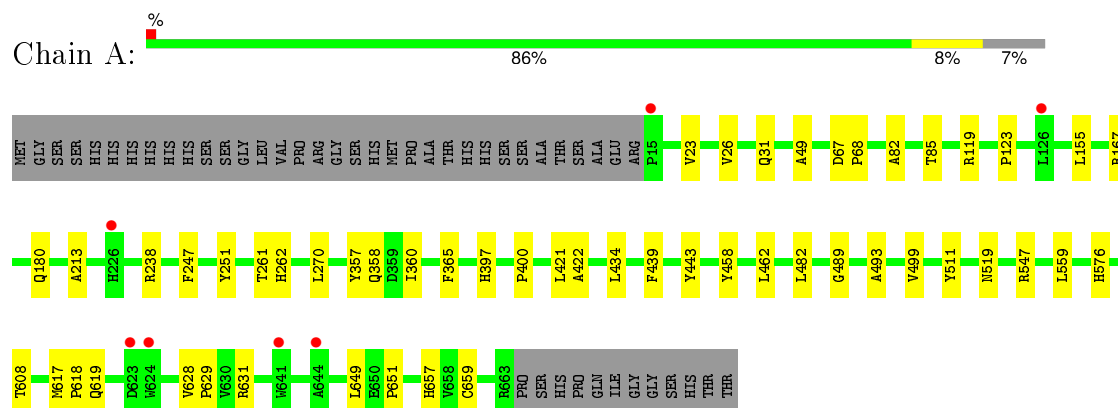
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	146	Total O 146 146	0	0
2	B	127	Total O 127 127	0	0
2	C	150	Total O 150 150	0	0
2	D	117	Total O 117 117	0	0

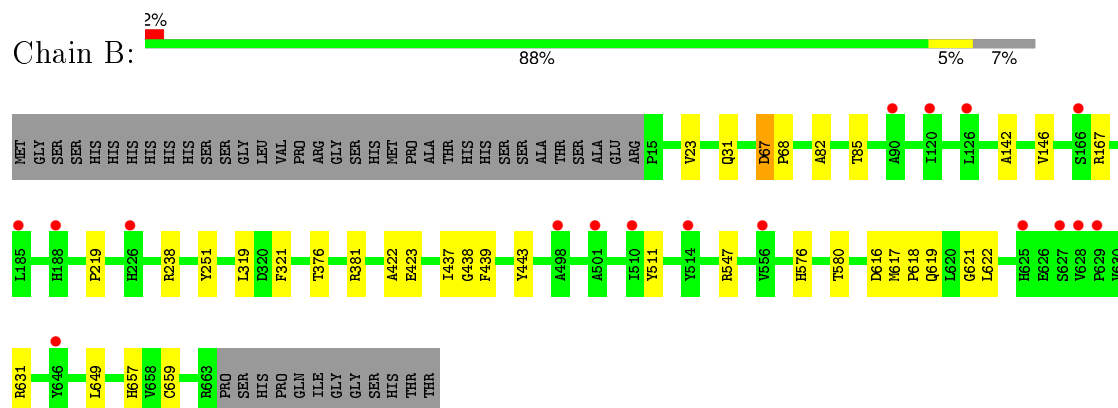
3 Residue-property plots [i](#)

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.

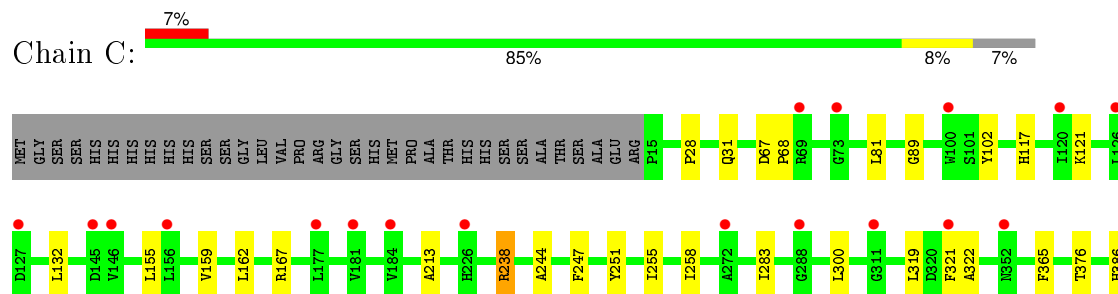
• Molecule 1: PUTATIVE GLUCANOHYDROLASE PEP1A

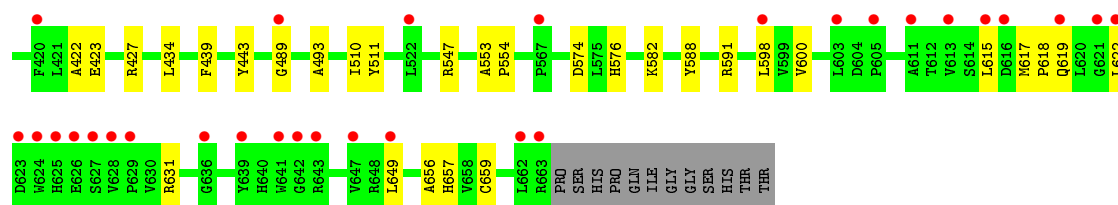


• Molecule 1: PUTATIVE GLUCANOHYDROLASE PEP1A

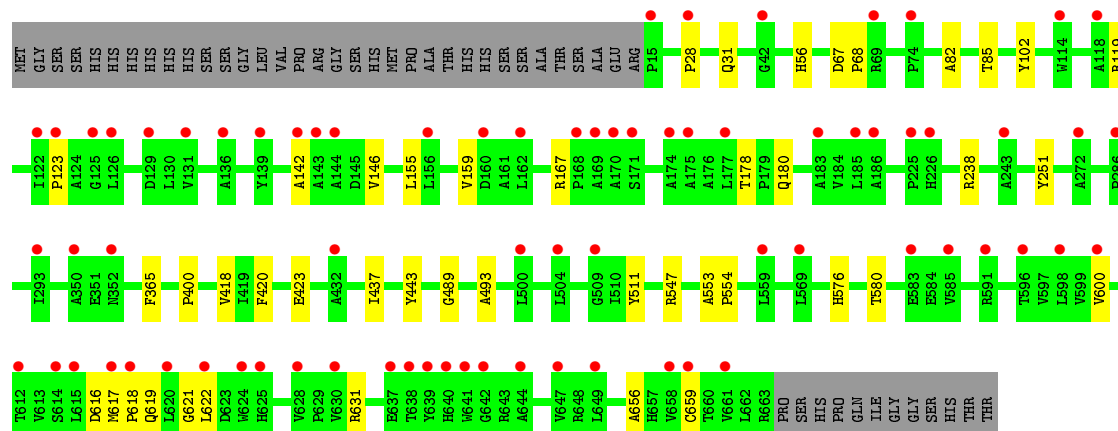
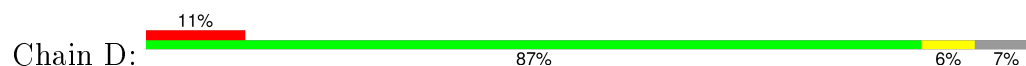


• Molecule 1: PUTATIVE GLUCANOHYDROLASE PEP1A





• Molecule 1: PUTATIVE GLUCANOHYDROLASE PEP1A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.09Å 112.98Å 314.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	314.44 – 1.80 50.57 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.6 (314.44-1.80) 94.8 (50.57-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.6.0101	Depositor
R, R_{free}	0.231 , 0.249 0.226 , 0.236	Depositor DCC
R_{free} test set	17673 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.8	EDS
Estimated twinning fraction	0.528 for H,K,L 0.472 for K,H,-L 0.446 for k,h,-l	Xtriage
Reported twinning fraction	0.528 for H,K,L 0.472 for K,H,-L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Outliers	0 of 351738 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	20945	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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

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	0.66	0/5257	0.73	1/7195 (0.0%)
1	B	0.61	0/5252	0.70	1/7187 (0.0%)
1	C	0.64	0/5254	0.71	1/7191 (0.0%)
1	D	0.61	0/5249	0.71	0/7185
All	All	0.63	0/21012	0.71	3/28758 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	LEU	CB-CG-CD2	5.44	120.25	111.00
1	C	510	ILE	CG1-CB-CG2	5.03	122.46	111.40
1	B	67	ASP	CB-CG-OD1	5.02	122.82	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	5105	0	4917	28	0
1	B	5101	0	4912	18	0
1	C	5102	0	4912	34	0
1	D	5097	0	4896	23	0
2	A	146	0	0	0	0
2	B	127	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	150	0	0	6	0
2	D	117	0	0	1	0
All	All	20945	0	19637	103	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.

The worst 5 of 103 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:628:VAL:HG13	1:A:629:PRO:HD2	1.60	0.82
1:D:178:THR:HB	1:D:180:GLN:HE21	1.54	0.73
1:D:178:THR:HB	1:D:180:GLN:NE2	2.04	0.72
1:B:82:ALA:HB3	1:B:85:THR:HG21	1.77	0.66
1:B:437:ILE:HD12	1:B:437:ILE:C	2.18	0.64

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	647/695 (93%)	634 (98%)	13 (2%)	0	100	100
1	B	647/695 (93%)	637 (98%)	9 (1%)	1 (0%)	52	35
1	C	647/695 (93%)	635 (98%)	12 (2%)	0	100	100
1	D	647/695 (93%)	632 (98%)	14 (2%)	1 (0%)	52	35
All	All	2588/2780 (93%)	2538 (98%)	48 (2%)	2 (0%)	56	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	616	ASP
1	B	616	ASP

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	530/575 (92%)	523 (99%)	7 (1%)	76	68
1	B	529/575 (92%)	521 (98%)	8 (2%)	72	62
1	C	528/575 (92%)	521 (99%)	7 (1%)	76	68
1	D	527/575 (92%)	520 (99%)	7 (1%)	76	68
All	All	2114/2300 (92%)	2085 (99%)	29 (1%)	74	65

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	547	ARG
1	C	167	ARG
1	D	511	TYR
1	B	580	THR
1	C	238	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	436	GLN
1	C	397	HIS
1	D	262	HIS
1	B	397	HIS
1	D	180	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](#)

There are no ligands in this entry.

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	649/695 (93%)	0.55	7 (1%) 82 80	15, 23, 36, 50	0
1	B	649/695 (93%)	0.64	17 (2%) 59 54	17, 24, 37, 47	0
1	C	649/695 (93%)	0.76	48 (7%) 17 14	16, 24, 34, 46	0
1	D	649/695 (93%)	0.94	74 (11%) 7 5	16, 24, 38, 44	0
All	All	2596/2780 (93%)	0.72	146 (5%) 28 22	15, 24, 37, 50	0

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	641	TRP	7.0
1	C	126	LEU	6.5
1	D	644	ALA	6.0
1	D	628	VAL	5.7
1	C	662	LEU	5.5

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.