



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:31 PM GMT

PDB ID : 3OTP
Title : Crystal structure of the DegP dodecamer with a model substrate
Authors : Kim, S.; Grant, R.A.; Sauer, R.T.
Deposited on : 2010-09-13
Resolution : 3.76 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

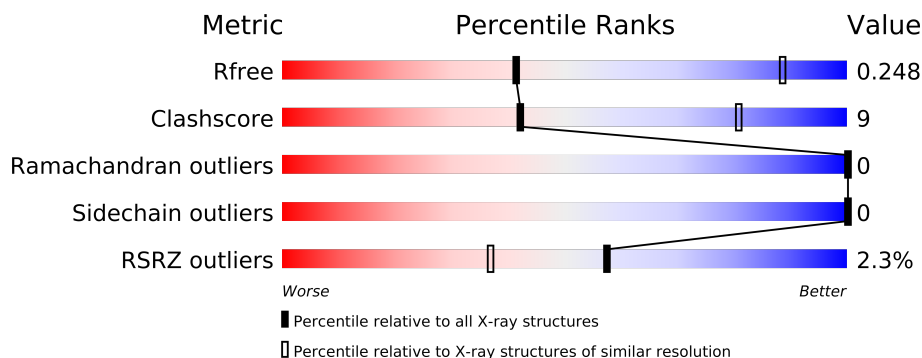
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.76 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}	66092	1134 (4.12-3.40)
Clashscore	79885	1067 (4.02-3.50)
Ramachandran outliers	78287	1017 (4.02-3.50)
Sidechain outliers	78261	1010 (4.02-3.50)
RSRZ outliers	66119	1135 (4.12-3.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	459	
1	B	459	
1	C	459	
1	D	459	
1	E	459	
1	F	459	
2	G	44	
2	H	44	
2	I	44	
2	J	44	
2	K	44	
2	L	44	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17037 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Protease do.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2736	1703	482	538	13			
1	B	392	Total	C	N	O	S	0	0	0
			2820	1752	495	560	13			
1	C	382	Total	C	N	O	S	0	0	0
			2743	1709	482	539	13			
1	D	388	Total	C	N	O	S	0	0	0
			2784	1731	488	553	12			
1	E	388	Total	C	N	O	S	0	0	0
			2795	1737	491	554	13			
1	F	378	Total	C	N	O	S	0	0	0
			2728	1700	480	535	13			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	210	ALA	SER	ENGINEERED MUTATION	UNP P0C0V0
A	449	ALA	-	EXPRESSION TAG	UNP P0C0V0
A	450	ALA	-	EXPRESSION TAG	UNP P0C0V0
A	451	ALA	-	EXPRESSION TAG	UNP P0C0V0
A	452	LEU	-	EXPRESSION TAG	UNP P0C0V0
A	453	GLU	-	EXPRESSION TAG	UNP P0C0V0
A	454	HIS	-	EXPRESSION TAG	UNP P0C0V0
A	455	HIS	-	EXPRESSION TAG	UNP P0C0V0
A	456	HIS	-	EXPRESSION TAG	UNP P0C0V0
A	457	HIS	-	EXPRESSION TAG	UNP P0C0V0
A	458	HIS	-	EXPRESSION TAG	UNP P0C0V0
A	459	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	210	ALA	SER	ENGINEERED MUTATION	UNP P0C0V0
B	449	ALA	-	EXPRESSION TAG	UNP P0C0V0
B	450	ALA	-	EXPRESSION TAG	UNP P0C0V0
B	451	ALA	-	EXPRESSION TAG	UNP P0C0V0
B	452	LEU	-	EXPRESSION TAG	UNP P0C0V0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	453	GLU	-	EXPRESSION TAG	UNP P0C0V0
B	454	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	455	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	456	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	457	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	458	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	459	HIS	-	EXPRESSION TAG	UNP P0C0V0
C	210	ALA	SER	ENGINEERED MUTATION	UNP P0C0V0
C	449	ALA	-	EXPRESSION TAG	UNP P0C0V0
C	450	ALA	-	EXPRESSION TAG	UNP P0C0V0
C	451	ALA	-	EXPRESSION TAG	UNP P0C0V0
C	452	LEU	-	EXPRESSION TAG	UNP P0C0V0
C	453	GLU	-	EXPRESSION TAG	UNP P0C0V0
C	454	HIS	-	EXPRESSION TAG	UNP P0C0V0
C	455	HIS	-	EXPRESSION TAG	UNP P0C0V0
C	456	HIS	-	EXPRESSION TAG	UNP P0C0V0
C	457	HIS	-	EXPRESSION TAG	UNP P0C0V0
C	458	HIS	-	EXPRESSION TAG	UNP P0C0V0
C	459	HIS	-	EXPRESSION TAG	UNP P0C0V0
D	210	ALA	SER	ENGINEERED MUTATION	UNP P0C0V0
D	449	ALA	-	EXPRESSION TAG	UNP P0C0V0
D	450	ALA	-	EXPRESSION TAG	UNP P0C0V0
D	451	ALA	-	EXPRESSION TAG	UNP P0C0V0
D	452	LEU	-	EXPRESSION TAG	UNP P0C0V0
D	453	GLU	-	EXPRESSION TAG	UNP P0C0V0
D	454	HIS	-	EXPRESSION TAG	UNP P0C0V0
D	455	HIS	-	EXPRESSION TAG	UNP P0C0V0
D	456	HIS	-	EXPRESSION TAG	UNP P0C0V0
D	457	HIS	-	EXPRESSION TAG	UNP P0C0V0
D	458	HIS	-	EXPRESSION TAG	UNP P0C0V0
D	459	HIS	-	EXPRESSION TAG	UNP P0C0V0
E	210	ALA	SER	ENGINEERED MUTATION	UNP P0C0V0
E	449	ALA	-	EXPRESSION TAG	UNP P0C0V0
E	450	ALA	-	EXPRESSION TAG	UNP P0C0V0
E	451	ALA	-	EXPRESSION TAG	UNP P0C0V0
E	452	LEU	-	EXPRESSION TAG	UNP P0C0V0
E	453	GLU	-	EXPRESSION TAG	UNP P0C0V0
E	454	HIS	-	EXPRESSION TAG	UNP P0C0V0
E	455	HIS	-	EXPRESSION TAG	UNP P0C0V0
E	456	HIS	-	EXPRESSION TAG	UNP P0C0V0
E	457	HIS	-	EXPRESSION TAG	UNP P0C0V0
E	458	HIS	-	EXPRESSION TAG	UNP P0C0V0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	459	HIS	-	EXPRESSION TAG	UNP P0C0V0
F	210	ALA	SER	ENGINEERED MUTATION	UNP P0C0V0
F	449	ALA	-	EXPRESSION TAG	UNP P0C0V0
F	450	ALA	-	EXPRESSION TAG	UNP P0C0V0
F	451	ALA	-	EXPRESSION TAG	UNP P0C0V0
F	452	LEU	-	EXPRESSION TAG	UNP P0C0V0
F	453	GLU	-	EXPRESSION TAG	UNP P0C0V0
F	454	HIS	-	EXPRESSION TAG	UNP P0C0V0
F	455	HIS	-	EXPRESSION TAG	UNP P0C0V0
F	456	HIS	-	EXPRESSION TAG	UNP P0C0V0
F	457	HIS	-	EXPRESSION TAG	UNP P0C0V0
F	458	HIS	-	EXPRESSION TAG	UNP P0C0V0
F	459	HIS	-	EXPRESSION TAG	UNP P0C0V0

- Molecule 2 is a protein called Lysozyme C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	10	Total	C	N	O	0	0	0
			66	42	11	13			
2	H	10	Total	C	N	O	0	0	0
			66	42	11	13			
2	I	16	Total	C	N	O	0	0	0
			101	61	17	23			
2	J	10	Total	C	N	O	0	0	0
			66	42	11	13			
2	K	10	Total	C	N	O	0	0	0
			66	42	11	13			
2	L	10	Total	C	N	O	0	0	0
			66	42	11	13			

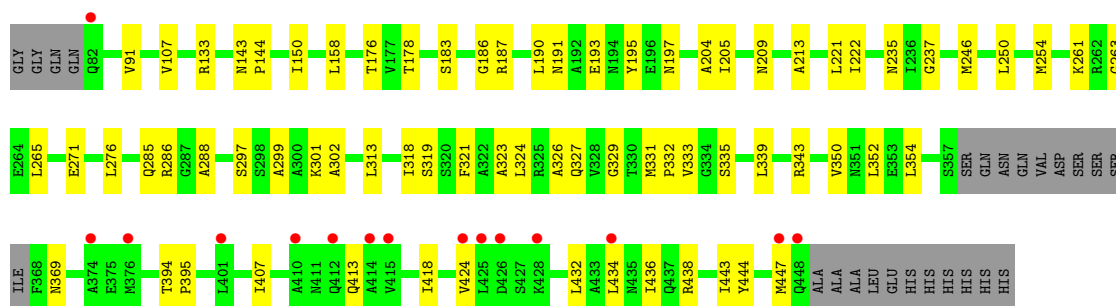
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	15	GLY	-	EXPRESSION TAG	UNP B8YK79
G	16	THR	-	EXPRESSION TAG	UNP B8YK79
G	17	GLY	-	EXPRESSION TAG	UNP B8YK79
G	30	SER	CYS	ENGINEERED MUTATION	UNP B8YK79
H	15	GLY	-	EXPRESSION TAG	UNP B8YK79
H	16	THR	-	EXPRESSION TAG	UNP B8YK79
H	17	GLY	-	EXPRESSION TAG	UNP B8YK79
H	30	SER	CYS	ENGINEERED MUTATION	UNP B8YK79
I	15	GLY	-	EXPRESSION TAG	UNP B8YK79

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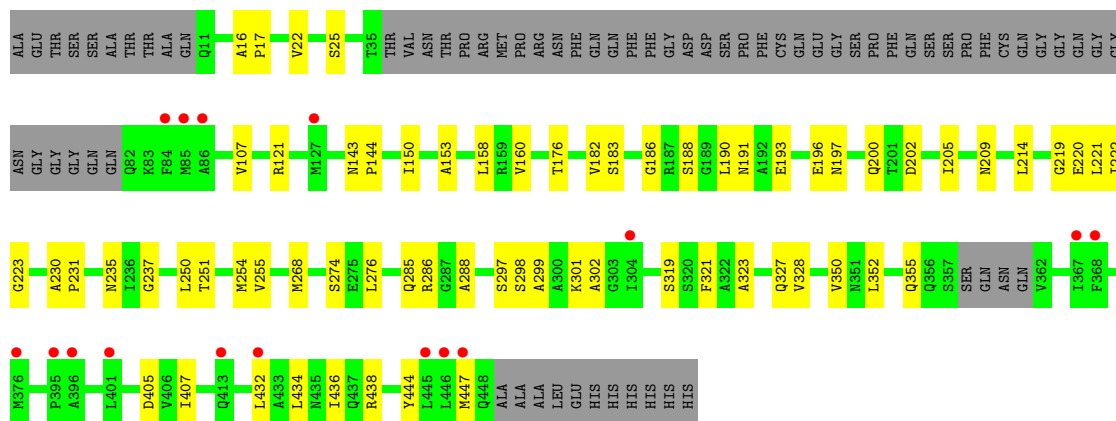
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Chain	Residue	Modelled	Actual	Comment	Reference
I	16	THR	-	EXPRESSION TAG	UNP B8YK79
I	17	GLY	-	EXPRESSION TAG	UNP B8YK79
I	30	SER	CYS	ENGINEERED MUTATION	UNP B8YK79
J	15	GLY	-	EXPRESSION TAG	UNP B8YK79
J	16	THR	-	EXPRESSION TAG	UNP B8YK79
J	17	GLY	-	EXPRESSION TAG	UNP B8YK79
J	30	SER	CYS	ENGINEERED MUTATION	UNP B8YK79
K	15	GLY	-	EXPRESSION TAG	UNP B8YK79
K	16	THR	-	EXPRESSION TAG	UNP B8YK79
K	17	GLY	-	EXPRESSION TAG	UNP B8YK79
K	30	SER	CYS	ENGINEERED MUTATION	UNP B8YK79
L	15	GLY	-	EXPRESSION TAG	UNP B8YK79
L	16	THR	-	EXPRESSION TAG	UNP B8YK79
L	17	GLY	-	EXPRESSION TAG	UNP B8YK79
L	30	SER	CYS	ENGINEERED MUTATION	UNP B8YK79



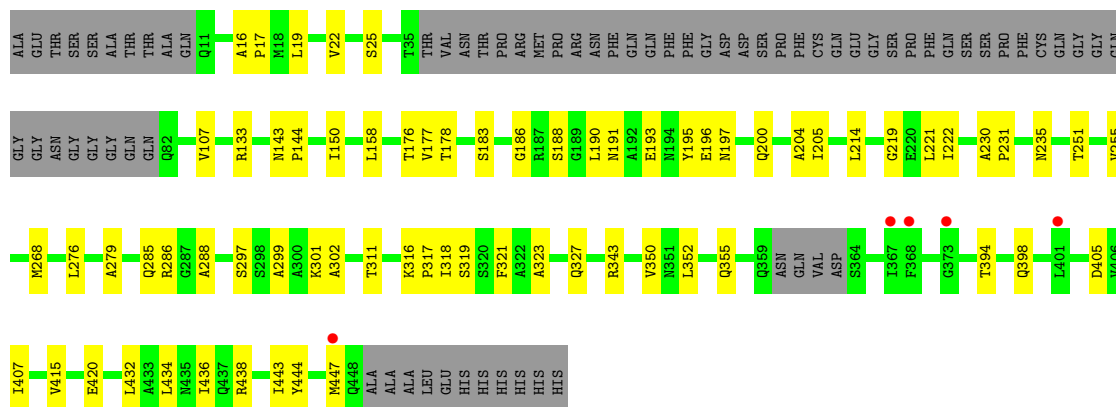
• Molecule 1: Protease do

Chain D:



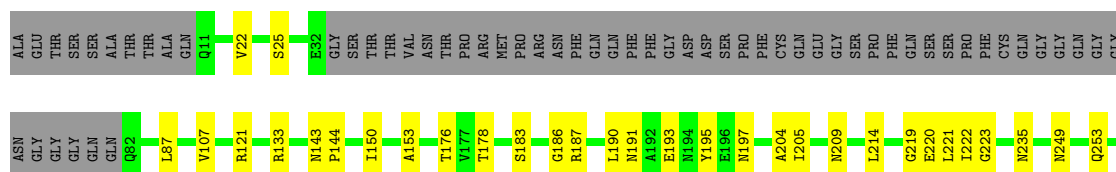
• Molecule 1: Protease do

Chain E:



• Molecule 1: Protease do

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.43Å 122.76Å 138.74Å 90.00° 117.98° 90.00°	Depositor
Resolution (Å)	14.99 – 3.76 54.88 – 3.76	Depositor EDS
% Data completeness (in resolution range)	88.2 (14.99-3.76) 88.3 (54.88-3.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4-486)	Depositor
R, R_{free}	0.219 , 0.251 0.215 , 0.248	Depositor DCC
R_{free} test set	1391 reflections (4.83%)	DCC
Wilson B-factor (Å ²)	113.8	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 72.9	EDS
Estimated twinning fraction	0.029 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.034 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 28826 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17037	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.24	0/2759	0.42	0/3735
1	B	0.23	0/2845	0.41	0/3853
1	C	0.24	0/2766	0.42	0/3742
1	D	0.24	0/2808	0.41	0/3804
1	E	0.23	0/2819	0.41	0/3815
1	F	0.24	0/2750	0.41	0/3719
2	G	0.21	0/64	0.37	0/83
2	H	0.19	0/64	0.36	0/83
2	I	0.21	0/99	0.47	0/131
2	J	0.20	0/64	0.35	0/83
2	K	0.21	0/64	0.38	0/83
2	L	0.18	0/64	0.36	0/83
All	All	0.24	0/17166	0.41	0/23214

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2736	0	2768	57	0
1	B	2820	0	2849	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2743	0	2793	59	0
1	D	2784	0	2807	52	0
1	E	2795	0	2831	50	0
1	F	2728	0	2778	57	0
2	G	66	0	68	2	0
2	H	66	0	68	6	0
2	I	101	0	91	5	0
2	J	66	0	68	5	0
2	K	66	0	68	5	0
2	L	66	0	68	4	0
All	All	17037	0	17257	308	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 308 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:361:GLN:HB3	1:B:377:SER:HB3	1.45	0.96
1:E:190:LEU:HD22	2:K:29:VAL:HG21	1.53	0.89
1:C:190:LEU:HD22	2:I:29:VAL:HG21	1.56	0.86
1:D:190:LEU:HD22	2:J:29:VAL:HG21	1.61	0.82
1:F:190:LEU:HD22	2:L:29:VAL:HG21	1.63	0.80

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	375/459 (82%)	365 (97%)	10 (3%)	0	100	100
1	B	388/459 (84%)	378 (97%)	10 (3%)	0	100	100
1	C	376/459 (82%)	362 (96%)	14 (4%)	0	100	100
1	D	382/459 (83%)	373 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	382/459 (83%)	370 (97%)	12 (3%)	0	100	100
1	F	370/459 (81%)	362 (98%)	8 (2%)	0	100	100
2	G	6/44 (14%)	6 (100%)	0	0	100	100
2	H	6/44 (14%)	6 (100%)	0	0	100	100
2	I	12/44 (27%)	11 (92%)	1 (8%)	0	100	100
2	J	6/44 (14%)	6 (100%)	0	0	100	100
2	K	6/44 (14%)	6 (100%)	0	0	100	100
2	L	6/44 (14%)	6 (100%)	0	0	100	100
All	All	2315/3018 (77%)	2251 (97%)	64 (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	287/364 (79%)	287 (100%)	0	100	100
1	B	300/364 (82%)	300 (100%)	0	100	100
1	C	290/364 (80%)	290 (100%)	0	100	100
1	D	295/364 (81%)	295 (100%)	0	100	100
1	E	298/364 (82%)	298 (100%)	0	100	100
1	F	289/364 (79%)	289 (100%)	0	100	100
2	G	6/35 (17%)	6 (100%)	0	100	100
2	H	6/35 (17%)	6 (100%)	0	100	100
2	I	9/35 (26%)	9 (100%)	0	100	100
2	J	6/35 (17%)	6 (100%)	0	100	100
2	K	6/35 (17%)	6 (100%)	0	100	100
2	L	6/35 (17%)	6 (100%)	0	100	100
All	All	1798/2394 (75%)	1798 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	369	ASN
1	C	235	ASN
1	E	235	ASN
1	B	355	GLN
1	D	235	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

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	381/459 (83%)	0.25	3 (0%) 83 64	69, 117, 178, 215	0
1	B	392/459 (85%)	0.15	4 (1%) 79 58	69, 118, 185, 228	0
1	C	382/459 (83%)	0.39	15 (3%) 37 25	68, 116, 179, 215	0
1	D	388/459 (84%)	0.43	16 (4%) 35 23	70, 118, 186, 229	0
1	E	388/459 (84%)	0.21	5 (1%) 74 51	70, 119, 185, 228	0
1	F	378/459 (82%)	0.24	6 (1%) 68 46	70, 117, 179, 216	0
2	G	10/44 (22%)	0.96	0 100 100	120, 148, 163, 166	0
2	H	10/44 (22%)	0.53	0 100 100	120, 148, 164, 166	0
2	I	16/44 (36%)	1.06	5 (31%) 1 2	119, 157, 182, 184	0
2	J	10/44 (22%)	0.77	1 (10%) 8 8	119, 148, 165, 167	0
2	K	10/44 (22%)	0.73	0 100 100	119, 149, 164, 166	0
2	L	10/44 (22%)	0.62	0 100 100	121, 149, 164, 167	0
All	All	2375/3018 (78%)	0.29	55 (2%) 57 37	68, 119, 183, 229	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	370	GLY	5.1
1	D	85	MET	4.4
1	C	82	GLN	4.4
1	D	368	PHE	4.1
1	D	446	LEU	3.9

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.