



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:36 AM UTC

PDB ID : 3OTP / pdb_00003otp
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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

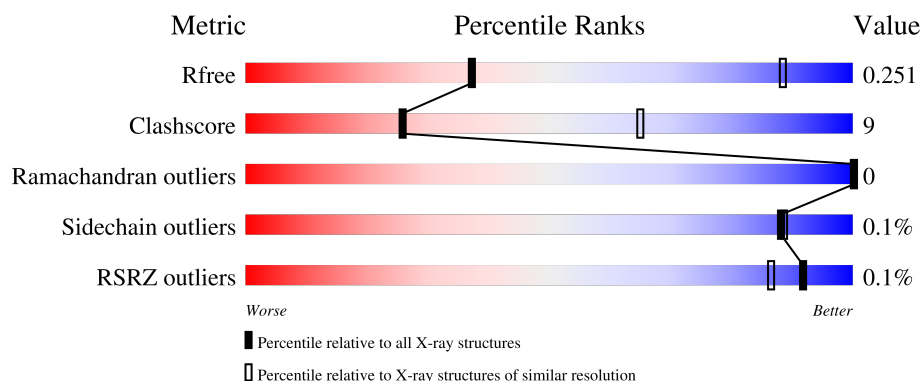
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
Ramachandran outliers	187476	1014 (3.90-3.62)
Sidechain outliers	187428	1009 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)

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 of 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	459	 65% 18% 17%
1	B	459	 68% 18% 15%
1	C	459	 66% 17% 17%
1	D	459	 69% 15% 15%
1	E	459	 69% 16% 15%

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Mol	Chain	Length	Quality of chain
1	F	459	64% 18% 18%
2	G	44	18% 5% 77%
2	H	44	11% 11% 77%
2	I	44	2% 30% 7% 64%
2	J	44	14% 9% 77%
2	K	44	2% 14% 9% 77%
2	L	44	16% 7% 77%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17037 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 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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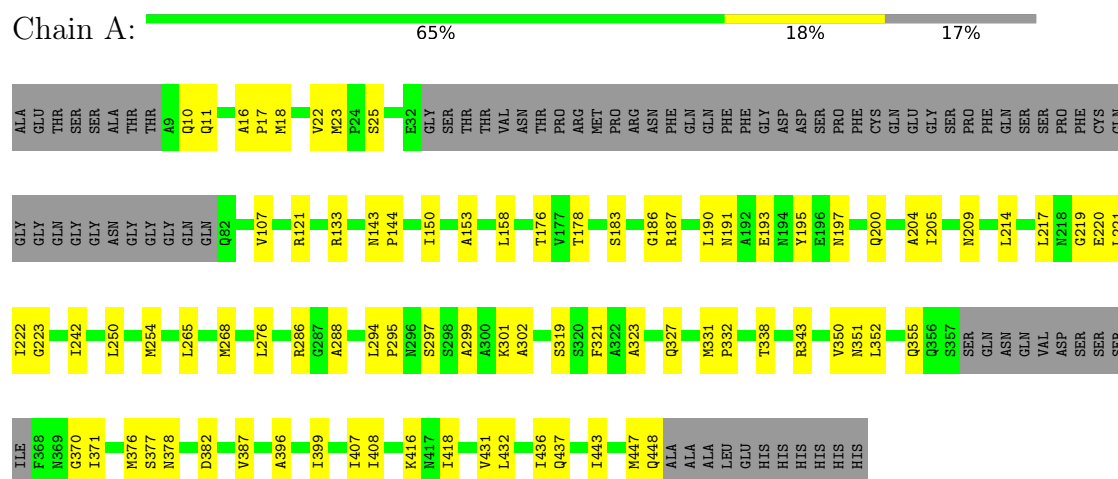
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Chain	Residue	Modelled	Actual	Comment	Reference
I	16	THR	-	expression tag	UNP B8YK79
I	17	GLY	-	expression tag	UNP B8YK79
I	30	SER	CYS	engineered mutation	UNP B8YK79
J	15	GLY	-	expression tag	UNP B8YK79
J	16	THR	-	expression tag	UNP B8YK79
J	17	GLY	-	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

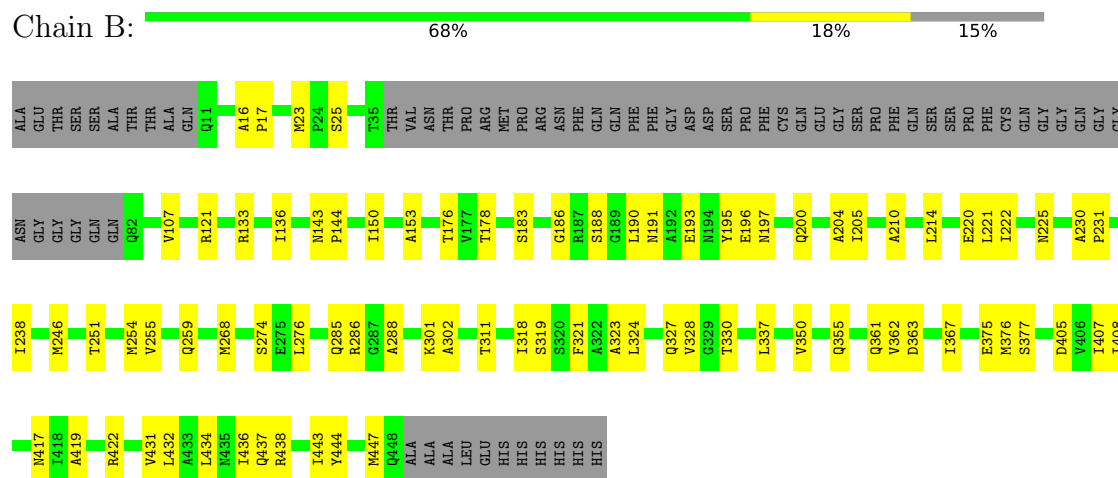
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

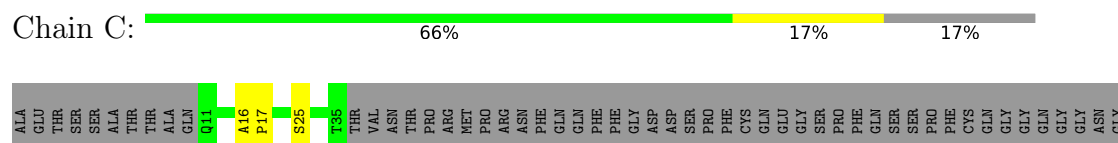
• Molecule 1: Protease do

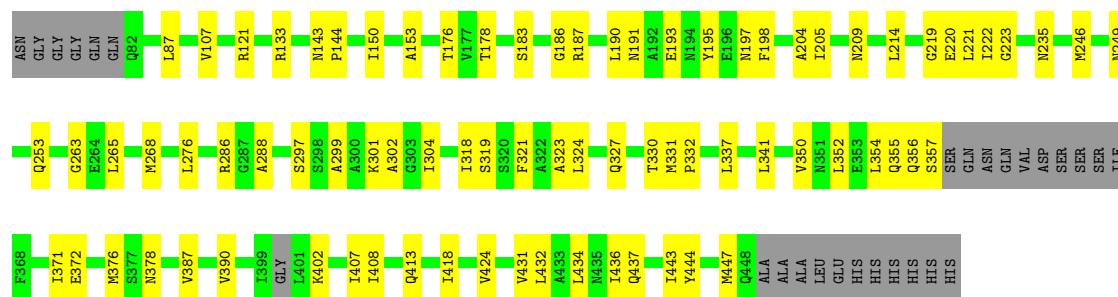


• Molecule 1: Protease do



• Molecule 1: Protease do





• Molecule 2: Lysozyme C



• Molecule 2: Lysozyme C



• Molecule 2: Lysozyme C



• Molecule 2: Lysozyme C



• Molecule 2: Lysozyme C



• Molecule 2: Lysozyme C



GLY	THR	GLY	ASP	ASN	TYR	ARG	GLY	TYR	SER	LEU	GLY	ASN	V28	V29	A32	LYS	PHE	GLU	SER	ASN	PHE	ASN	THR	GLN	ALA	THR	ASN	ARG	ASN	THR	ASP	GLY	SER	THR	ASP	TYR	G54	I55	I58
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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 14.99 – 3.76	Depositor EDS
% Data completeness (in resolution range)	88.2 (14.99-3.76) 86.8 (14.99-3.76)	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 1.6.4_486	Depositor
R, R_{free}	0.219 , 0.251 0.220 , 0.251	Depositor DCC
R_{free} test set	1391 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	113.8	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
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
F_o, F_c correlation	0.92	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.

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 [i](#)

5.1 Standard geometry [i](#)

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	0.31	0/2759	0.76	2/3735 (0.1%)
1	B	0.30	0/2845	0.74	2/3853 (0.1%)
1	C	0.31	0/2766	0.74	0/3742
1	D	0.29	0/2808	0.74	2/3804 (0.1%)
1	E	0.28	0/2819	0.75	0/3815
1	F	0.30	0/2750	0.74	1/3719 (0.0%)
2	G	0.18	0/64	0.60	0/83
2	H	0.22	0/64	0.60	0/83
2	I	0.26	0/99	0.70	0/131
2	J	0.20	0/64	0.55	0/83
2	K	0.22	0/64	0.65	0/83
2	L	0.24	0/64	0.59	0/83
All	All	0.30	0/17166	0.75	7/23214 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	MET	CA-C-N	-5.68	113.77	119.56
1	A	23	MET	C-N-CA	-5.68	113.77	119.56
1	B	23	MET	CA-C-N	-5.26	114.19	119.56
1	B	23	MET	C-N-CA	-5.26	114.19	119.56
1	F	198	PHE	N-CA-C	5.10	116.87	110.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2736	0	2768	57	0
1	B	2820	0	2849	57	0
1	C	2743	0	2793	62	0
1	D	2784	0	2807	54	0
1	E	2795	0	2831	53	0
1	F	2728	0	2778	59	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	6	0
2	L	66	0	68	4	0
All	All	17037	0	17257	324	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 9.

The worst 5 of 324 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: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 [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	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
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%)	299 (100%)	1 (0%)	86	84
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%)	288 (100%)	1 (0%)	86	84
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	1796 (100%)	2 (0%)	88	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	431	VAL
1	F	390	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	369	ASN
1	F	235	ASN
1	F	355	GLN
1	F	142	GLN
1	D	235	ASN

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 oligosaccharides 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	381/459 (83%)	-0.42	0 100 100	69, 117, 178, 215	0
1	B	392/459 (85%)	-0.41	0 100 100	69, 118, 185, 228	0
1	C	382/459 (83%)	-0.33	0 100 100	68, 116, 179, 215	0
1	D	388/459 (84%)	-0.40	0 100 100	70, 118, 186, 229	0
1	E	388/459 (84%)	-0.46	0 100 100	70, 119, 185, 228	0
1	F	378/459 (82%)	-0.36	0 100 100	70, 117, 179, 216	0
2	G	10/44 (22%)	-0.11	0 100 100	120, 148, 163, 166	0
2	H	10/44 (22%)	0.25	0 100 100	120, 148, 164, 166	0
2	I	16/44 (36%)	0.05	1 (6%) 26 21	119, 157, 182, 184	0
2	J	10/44 (22%)	-0.19	0 100 100	119, 148, 165, 167	0
2	K	10/44 (22%)	0.13	1 (10%) 12 14	119, 149, 164, 166	0
2	L	10/44 (22%)	-0.12	0 100 100	121, 149, 164, 167	0
All	All	2375/3018 (78%)	-0.39	2 (0%) 92 86	68, 119, 183, 229	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	32	ALA	2.6
2	I	32	ALA	2.4

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 oligosaccharides 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.