



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:32 AM UTC

PDB ID : 4ZN2 / pdb_00004zn2
Title : Glycosyl hydrolase from Pseudomonas aeruginosa
Authors : Su, T.; Liu, S.; Gu, L.
Deposited on : 2015-05-04
Resolution : 2.00 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

<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

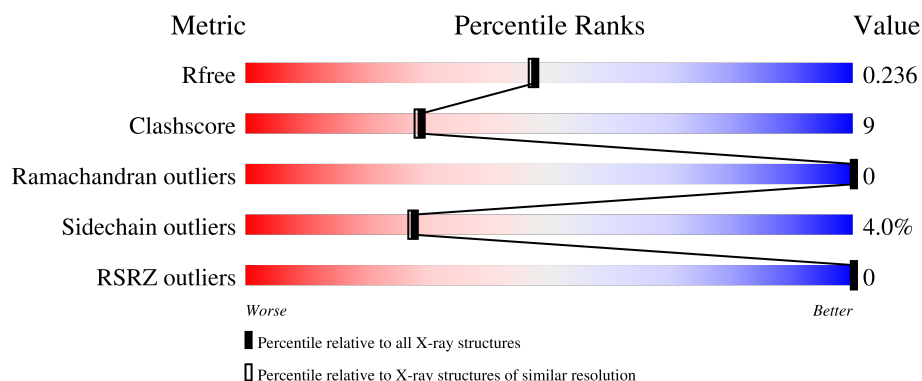
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	416	
1	B	416	
1	C	416	
1	D	416	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15102 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 PslG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	6	0
			3377	2173	581	615	8			
1	B	413	Total	C	N	O	S	0	3	0
			3353	2159	575	611	8			
1	C	413	Total	C	N	O	S	0	6	0
			3377	2171	581	617	8			
1	D	413	Total	C	N	O	S	0	4	0
			3369	2171	579	611	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	expression tag	UNP Q9I1N2
A	28	PRO	-	expression tag	UNP Q9I1N2
A	29	GLY	-	expression tag	UNP Q9I1N2
A	30	SER	-	expression tag	UNP Q9I1N2
B	27	GLY	-	expression tag	UNP Q9I1N2
B	28	PRO	-	expression tag	UNP Q9I1N2
B	29	GLY	-	expression tag	UNP Q9I1N2
B	30	SER	-	expression tag	UNP Q9I1N2
C	27	GLY	-	expression tag	UNP Q9I1N2
C	28	PRO	-	expression tag	UNP Q9I1N2
C	29	GLY	-	expression tag	UNP Q9I1N2
C	30	SER	-	expression tag	UNP Q9I1N2
D	27	GLY	-	expression tag	UNP Q9I1N2
D	28	PRO	-	expression tag	UNP Q9I1N2
D	29	GLY	-	expression tag	UNP Q9I1N2
D	30	SER	-	expression tag	UNP Q9I1N2

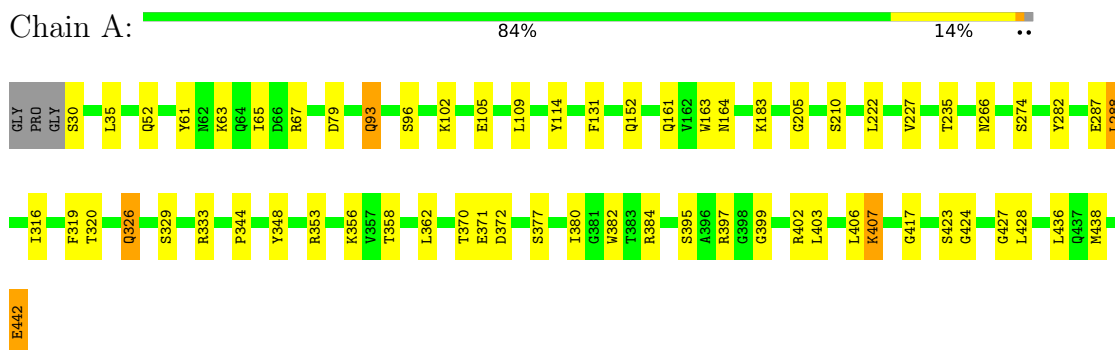
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	474	Total 474	O 474	0	0
2	B	464	Total 464	O 464	0	0
2	C	330	Total 330	O 330	0	0
2	D	358	Total 358	O 358	0	0

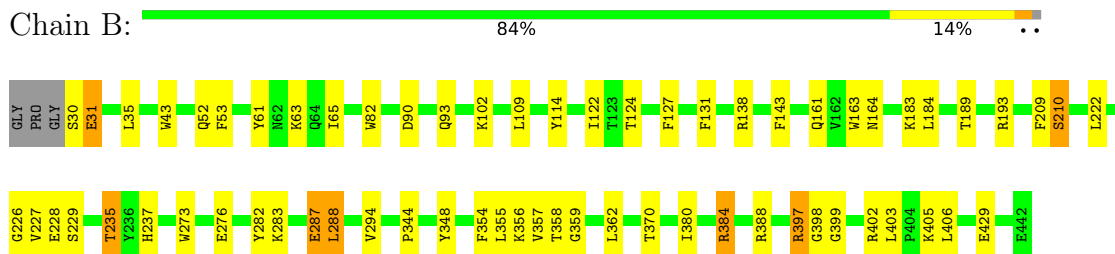
3 Residue-property plots

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.

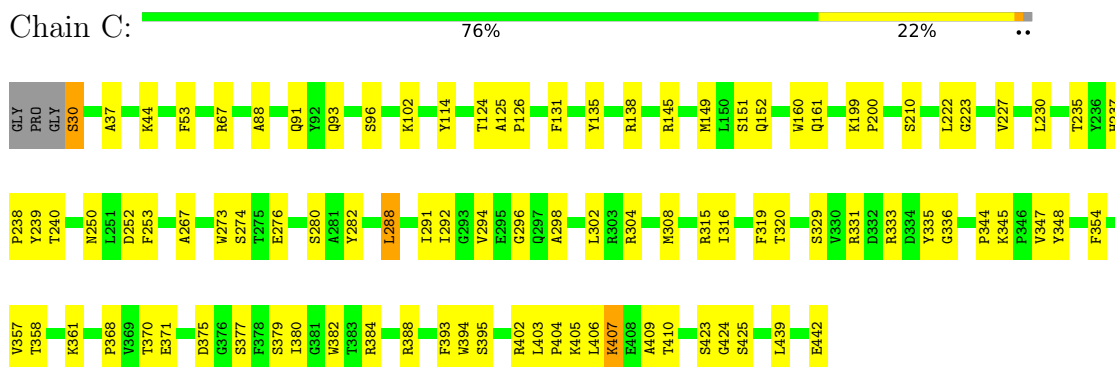
• Molecule 1: PslG



• Molecule 1: PslG



• Molecule 1: PslG



• Molecule 1: PslG



GLY	PRO	GLY	S30	E31	V34	L35	R36	A37	A40	W43	Q52	S57	R60	Y61	I65	D66	R67	R77	W82	S96	L109	Y114	I122	T123	T124	F131	R138	E141	R145	R146	M147	Q161	V162	W163	N164	K175	M194	V202				
S203	A204	G205	L222	G223	G226	V227	E228	S229	L230	T235	Y236	H237	P248	W249	W273	S274	T275	E276	S280	A281	Y282	E287	L288	V294	A298	D299	Y300	A310	Y335	G336	P344	V347	Y348	L349	R353	K356	V357	T358	G359	L362	R363	P364
T370	E371	D372	F378	S379	I380	G381	W382	E385	W391	L392	F393	W394	S395	R402	L403	P404	K405	L406	K407	P421	L422	S423	L428	E429	K433	S434	M438	E442														

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.56Å 88.21Å 222.39Å 90.00° 96.92° 90.00°	Depositor
Resolution (Å)	47.12 – 2.00 47.12 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.12-2.00) 98.1 (47.12-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.193 , 0.224 0.210 , 0.236	Depositor DCC
R_{free} test set	7171 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.159 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15102	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1066e-04.*

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	0.44	1/3474 (0.0%)	0.76	1/4732 (0.0%)
1	B	0.43	0/3450	0.75	1/4701 (0.0%)
1	C	0.41	1/3474 (0.0%)	0.73	1/4732 (0.0%)
1	D	0.41	0/3467	0.76	2/4722 (0.0%)
All	All	0.42	2/13865 (0.0%)	0.75	5/18887 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	442	GLU	C-OXT	-7.21	1.09	1.23
1	A	442	GLU	C-OXT	-6.20	1.11	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	GLY	N-CA-C	-7.50	102.25	112.52
1	B	399	GLY	N-CA-C	-6.01	103.64	111.52
1	D	162	VAL	N-CA-C	5.46	115.19	106.88
1	C	53	PHE	N-CA-C	5.18	117.67	111.71
1	D	336	GLY	N-CA-C	5.15	118.78	112.14

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	3377	0	3314	50	0
1	B	3353	0	3290	51	0
1	C	3377	0	3307	65	0
1	D	3369	0	3309	68	0
2	A	474	0	0	8	0
2	B	464	0	0	10	0
2	C	330	0	0	10	0
2	D	358	0	0	13	0
All	All	15102	0	13220	232	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.

All (232) 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:D:43:TRP:HE1	1:D:358:THR:HG21	1.34	0.92
1:D:433:LYS:NZ	2:D:501:HOH:O	2.10	0.85
1:B:114:TYR:HB3	1:B:161:GLN:HB3	1.59	0.84
1:A:65[A]:ILE:HD12	1:A:109:LEU:HD11	1.61	0.82
1:D:43:TRP:HE1	1:D:358:THR:CG2	1.94	0.80
1:A:63:LYS:HE2	2:A:553:HOH:O	1.81	0.79
1:A:407:LYS:HG3	1:A:424:GLY:O	1.84	0.78
1:C:294:VAL:HG22	2:C:537:HOH:O	1.83	0.77
1:B:358[A]:THR:HG23	1:B:359:GLY:O	1.85	0.76
1:C:114:TYR:HB3	1:C:161:GLN:HB3	1.66	0.76
1:D:124:THR:HG22	1:D:138:ARG:HG2	1.68	0.75
1:C:145:ARG:NH2	2:C:502:HOH:O	2.20	0.74
1:D:421:PRO:O	1:D:422:LEU:HD23	1.88	0.74
1:A:403:LEU:HD23	1:A:406:LEU:HD12	1.70	0.73
1:B:65[A]:ILE:HD12	1:B:109:LEU:HD11	1.70	0.73
1:B:358[A]:THR:OG1	1:B:362:LEU:HD11	1.88	0.73
1:C:354:PHE:O	1:C:358:THR:HG23	1.89	0.73
1:D:43:TRP:NE1	1:D:358:THR:HG21	2.02	0.72
1:D:61[A]:TYR:O	1:D:65[A]:ILE:HG12	1.90	0.72
1:B:183:LYS:NZ	2:B:502:HOH:O	2.23	0.71
1:D:300:TYR:HE1	2:D:514:HOH:O	1.72	0.71
1:B:397:ARG:N	1:B:397:ARG:HD3	2.06	0.71
1:B:397:ARG:HD2	2:B:846:HOH:O	1.92	0.69
1:C:223:GLY:HA2	2:C:512:HOH:O	1.93	0.69
1:B:90:ASP:OD2	2:B:501:HOH:O	2.11	0.68
1:D:61[B]:TYR:O	1:D:65[B]:ILE:HG13	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLU:HG2	2:A:509:HOH:O	1.96	0.65
1:A:114:TYR:HB3	1:A:161:GLN:HB3	1.77	0.65
1:D:287:GLU:O	1:D:288:LEU:HB2	1.96	0.65
1:A:102:LYS:NZ	1:A:102:LYS:HB3	2.10	0.65
1:A:424:GLY:O	2:A:501:HOH:O	2.15	0.65
1:D:114:TYR:HB3	1:D:161:GLN:HB3	1.77	0.65
1:D:30:SER:O	1:D:31:GLU:HG3	1.96	0.64
1:C:30:SER:HB2	1:C:375:ASP:OD2	1.98	0.63
1:C:124:THR:HG22	1:C:138:ARG:HG2	1.81	0.63
1:A:102:LYS:NZ	2:A:504:HOH:O	2.30	0.63
1:B:35:LEU:HB2	1:B:380:ILE:HG12	1.80	0.63
1:B:124:THR:HG22	1:B:138:ARG:HG2	1.80	0.63
1:B:226:GLY:HA2	1:B:228:GLU:OE2	1.99	0.63
1:C:30:SER:CB	1:C:375:ASP:OD2	2.47	0.63
1:D:370:THR:HG22	1:D:403:LEU:HD22	1.81	0.63
1:D:370:THR:HG22	1:D:403:LEU:CD2	2.30	0.62
1:C:288:LEU:HB2	1:C:331:ARG:NH1	2.15	0.62
1:C:370:THR:HG22	1:C:403:LEU:CD2	2.29	0.62
1:D:344:PRO:HB3	1:D:348:TYR:CD1	2.35	0.61
1:C:149:MET:HA	2:C:729:HOH:O	2.00	0.61
1:D:379:SER:C	1:D:380:ILE:HG13	2.24	0.61
1:B:294:VAL:HG22	2:B:743:HOH:O	2.01	0.61
1:B:30:SER:C	1:B:31:GLU:HG3	2.25	0.61
1:B:287:GLU:O	1:B:288:LEU:HB2	2.01	0.60
1:C:370:THR:HG22	1:C:403:LEU:HD22	1.83	0.60
1:B:403:LEU:HD12	1:B:406:LEU:HD12	1.84	0.60
1:B:397:ARG:N	1:B:397:ARG:CD	2.65	0.59
1:D:226:GLY:HA2	1:D:228:GLU:OE2	2.03	0.59
1:C:407:LYS:CE	1:C:425:SER:O	2.50	0.59
1:B:398:GLY:HA3	2:B:570:HOH:O	2.01	0.58
1:D:175:LYS:HD3	2:D:589:HOH:O	2.02	0.58
1:D:237:HIS:CG	1:D:276:GLU:HB2	2.38	0.58
1:D:356[B]:LYS:HA	1:D:356[B]:LYS:HE2	1.86	0.58
1:A:65[B]:ILE:HG12	1:A:109:LEU:HD11	1.85	0.57
1:A:93[A]:GLN:HG2	2:A:699:HOH:O	2.03	0.57
1:B:102:LYS:HE3	2:B:705:HOH:O	2.05	0.57
1:D:391:TRP:HZ2	2:D:526:HOH:O	1.87	0.57
1:A:424:GLY:HA3	1:A:427:GLY:O	2.05	0.57
1:C:407:LYS:HG3	1:C:424:GLY:O	2.05	0.56
1:D:34:VAL:HG22	1:D:379:SER:HB3	1.87	0.56
1:B:355:LEU:HA	1:B:358[A]:THR:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:HIS:CG	1:C:276:GLU:HB2	2.41	0.56
1:C:410:THR:O	1:C:439:LEU:HD12	2.07	0.55
1:D:223:GLY:HA2	2:D:508:HOH:O	2.06	0.55
1:C:222:LEU:HD22	1:C:227:VAL:HG21	1.88	0.55
1:C:361:LYS:NZ	2:C:501:HOH:O	2.08	0.54
1:A:397:ARG:HG2	2:A:821:HOH:O	2.06	0.54
1:C:274:SER:HB3	1:C:316:ILE:HG22	1.89	0.54
1:B:355:LEU:O	1:B:358[A]:THR:HG22	2.07	0.54
1:D:371:GLU:O	1:D:372:ASP:HB2	2.07	0.54
1:D:248:PRO:HD2	1:D:249:TRP:CE3	2.43	0.53
1:B:63:LYS:HE2	2:B:512:HOH:O	2.08	0.53
1:D:163:TRP:CD1	1:D:164:ASN:H	2.27	0.53
1:A:102:LYS:HB3	1:A:102:LYS:HZ1	1.72	0.53
1:B:163:TRP:CD1	1:B:164:ASN:H	2.27	0.53
1:D:65[A]:ILE:HD12	1:D:109:LEU:HD11	1.91	0.53
1:D:385:GLU:OE1	2:D:502:HOH:O	2.19	0.53
1:C:357:VAL:O	1:C:384:ARG:HD2	2.09	0.53
1:D:356[B]:LYS:O	1:D:356[B]:LYS:NZ	2.30	0.53
1:C:149:MET:HG2	2:C:729:HOH:O	2.09	0.52
1:D:222:LEU:HD22	1:D:227:VAL:HG21	1.92	0.52
1:A:35:LEU:HB2	1:A:380:ILE:HG12	1.92	0.52
1:C:407:LYS:HE2	1:C:425:SER:O	2.10	0.52
1:C:407:LYS:HE3	1:C:425:SER:O	2.09	0.52
1:A:65[A]:ILE:HD12	1:A:109:LEU:CD1	2.36	0.52
1:C:67[B]:ARG:HE	1:C:67[B]:ARG:HA	1.75	0.52
1:A:370:THR:HG22	1:A:403:LEU:CD1	2.41	0.51
1:B:43:TRP:HE1	1:B:358[A]:THR:HG21	1.75	0.51
1:B:61:TYR:O	1:B:65[A]:ILE:HG12	2.10	0.51
1:D:358:THR:HG22	1:D:359:GLY:O	2.11	0.51
1:B:354:PHE:O	1:B:358[B]:THR:HG23	2.11	0.51
1:C:30:SER:HB3	1:C:375:ASP:OD2	2.11	0.50
1:B:237:HIS:CG	1:B:276:GLU:HB2	2.47	0.50
1:C:344:PRO:HB3	1:C:348:TYR:CD1	2.46	0.50
1:C:250:ASN:OD1	1:C:252:ASP:HB3	2.11	0.50
1:A:424:GLY:N	1:A:428:LEU:HD23	2.27	0.50
1:C:368:PRO:O	1:C:370:THR:HG23	2.12	0.50
1:D:379:SER:HB2	2:D:526:HOH:O	2.10	0.50
1:C:227:VAL:HG13	1:C:230:LEU:HD12	1.94	0.50
1:C:298:ALA:HA	1:C:347:VAL:HG23	1.93	0.50
1:B:82:TRP:CH2	1:B:122:ILE:HG21	2.47	0.49
1:C:67[B]:ARG:HA	1:C:67[B]:ARG:NE	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:NZ	1:A:102:LYS:CB	2.75	0.49
1:C:238:PRO:HB2	1:C:253:PHE:HE1	1.77	0.49
1:D:395:SER:O	1:D:434:SER:HA	2.12	0.49
1:D:349:LEU:O	1:D:353:ARG:HG3	2.12	0.49
1:C:292:ILE:HD12	1:C:296:GLY:C	2.37	0.49
1:B:402:ARG:C	1:B:403:LEU:HD23	2.38	0.49
1:D:37:ALA:HB2	1:D:310:ALA:HA	1.94	0.49
1:D:30:SER:C	1:D:31:GLU:HG3	2.38	0.48
1:D:379:SER:CB	2:D:526:HOH:O	2.59	0.48
1:A:358:THR:O	1:A:384:ARG:HG2	2.13	0.48
1:A:344:PRO:HB3	1:A:348:TYR:CD1	2.48	0.48
1:A:163:TRP:CD1	1:A:164:ASN:H	2.31	0.48
1:A:353:ARG:HD3	1:A:417:GLY:HA2	1.95	0.48
1:B:53:PHE:CZ	1:B:65[A]:ILE:HD11	2.49	0.48
1:A:61:TYR:O	1:A:65[A]:ILE:HG12	2.14	0.48
1:C:37:ALA:HB2	1:C:382:TRP:CH2	2.49	0.48
1:B:222:LEU:HD22	1:B:227:VAL:HG21	1.96	0.48
1:D:35:LEU:HB2	1:D:380:ILE:HG12	1.95	0.48
1:D:359:GLY:HA3	2:D:536:HOH:O	2.12	0.48
1:A:424:GLY:C	2:A:501:HOH:O	2.57	0.47
1:C:273:TRP:HA	1:C:315:ARG:O	2.13	0.47
1:C:288:LEU:HD12	1:C:288:LEU:HA	1.66	0.47
1:A:326:GLN:O	1:A:326:GLN:HG3	2.14	0.47
1:B:143:PHE:CD1	1:B:184:LEU:HD11	2.49	0.47
1:C:409:ALA:HB1	1:C:439:LEU:HD11	1.96	0.47
1:D:372:ASP:O	2:D:503:HOH:O	2.20	0.47
1:C:288:LEU:HB2	1:C:331:ARG:HH12	1.78	0.47
1:C:291:ILE:N	1:C:291:ILE:HD13	2.29	0.47
1:A:205:GLY:HA2	1:A:235:THR:HG23	1.96	0.47
1:D:422:LEU:HB3	1:D:428:LEU:HD22	1.96	0.47
1:A:274:SER:HB3	1:A:316:ILE:HG22	1.96	0.47
1:D:378:PHE:O	1:D:393:PHE:HA	2.15	0.46
1:A:152:GLN:NE2	1:D:194:MET:HE1	2.29	0.46
1:C:393:PHE:O	1:C:394:TRP:HB3	2.14	0.46
1:D:294:VAL:HG22	2:D:641:HOH:O	2.14	0.46
1:A:287:GLU:O	1:A:288:LEU:HB2	2.14	0.46
1:B:357:VAL:O	1:B:384:ARG:HD2	2.16	0.46
1:D:30:SER:C	1:D:31:GLU:CG	2.88	0.46
1:D:202:VAL:HG12	1:D:203:SER:O	2.16	0.46
1:D:235:THR:HA	1:D:273:TRP:O	2.16	0.46
1:C:227:VAL:N	2:C:512:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:TRP:NE1	1:B:358[A]:THR:HG21	2.31	0.45
1:A:362:LEU:HB3	1:A:382:TRP:CE3	2.52	0.45
1:D:298:ALA:HA	1:D:347:VAL:HG23	1.98	0.45
1:B:53:PHE:CD1	1:B:61:TYR:HB2	2.52	0.45
1:C:308:MET:HE2	1:C:316:ILE:HG21	1.99	0.45
1:A:362:LEU:HD22	1:A:382:TRP:HB3	1.97	0.45
1:A:371:GLU:OE1	1:A:402:ARG:NE	2.44	0.45
1:D:65[B]:ILE:HD13	1:D:109:LEU:HD11	1.98	0.44
1:D:402:ARG:NH1	1:D:429:GLU:HB2	2.32	0.44
1:B:114:TYR:CB	1:B:161:GLN:HB3	2.38	0.44
1:B:183:LYS:HD3	2:B:783:HOH:O	2.17	0.44
1:C:329:SER:O	1:C:333:ARG:HG3	2.16	0.44
1:D:205:GLY:HA2	1:D:235:THR:HG23	2.00	0.44
1:D:391:TRP:O	1:D:438:MET:HA	2.16	0.44
1:A:370:THR:HG22	1:A:403:LEU:HD11	1.98	0.44
1:A:424:GLY:N	1:A:428:LEU:CD2	2.80	0.44
1:B:183:LYS:CD	2:B:783:HOH:O	2.65	0.44
1:D:37:ALA:CB	1:D:382:TRP:CH2	3.01	0.44
1:B:65[A]:ILE:HD12	1:B:109:LEU:CD1	2.45	0.44
1:B:370:THR:HG22	1:B:403:LEU:CD2	2.48	0.44
1:C:199:LYS:HA	1:C:200:PRO:HD3	1.82	0.44
1:D:141:GLU:O	1:D:145:ARG:HG3	2.18	0.44
1:A:371:GLU:O	1:A:372:ASP:HB2	2.17	0.44
1:A:79:ASP:HB3	1:A:114:TYR:CZ	2.52	0.44
1:A:183:LYS:HD2	1:A:183:LYS:HA	1.67	0.44
1:D:222:LEU:O	1:D:227:VAL:HG23	2.17	0.44
1:C:336:GLY:O	1:C:345:LYS:HD3	2.17	0.44
1:C:125:ALA:HA	1:C:126:PRO:HD3	1.87	0.43
1:A:114:TYR:CB	1:A:161:GLN:HB3	2.44	0.43
1:A:288:LEU:HD12	1:A:288:LEU:HA	1.81	0.43
1:D:77:ARG:NE	1:D:275:THR:HB	2.33	0.43
1:C:114:TYR:CB	1:C:161:GLN:HB3	2.43	0.43
1:C:102:LYS:HE3	2:C:786:HOH:O	2.19	0.43
1:A:67[A]:ARG:HA	1:A:67[A]:ARG:NE	2.34	0.43
1:C:240:THR:OG1	1:C:304:ARG:NH2	2.51	0.43
1:C:88:ALA:HB3	1:C:91:GLN:HB3	2.01	0.43
1:C:402:ARG:O	1:C:404:PRO:HD3	2.18	0.43
1:A:96:SER:OG	1:B:127:PHE:CE2	2.71	0.43
1:A:319:PHE:HA	1:A:320:THR:HA	1.86	0.43
1:B:398:GLY:CA	2:B:570:HOH:O	2.65	0.43
1:A:266:ASN:ND2	2:A:511:HOH:O	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:SER:HA	1:C:395:SER:HB2	2.01	0.43
1:A:356:LYS:HE2	1:A:356:LYS:HB3	1.70	0.42
1:C:379:SER:C	1:C:380:ILE:HG13	2.43	0.42
1:D:422:LEU:HD22	2:D:506:HOH:O	2.19	0.42
1:B:397:ARG:HD3	1:B:397:ARG:H	1.79	0.42
1:C:358:THR:O	1:C:384:ARG:HG3	2.20	0.42
1:D:161:GLN:HA	1:D:202:VAL:O	2.19	0.42
1:B:189:THR:O	1:B:193:ARG:HG3	2.19	0.42
1:C:126:PRO:HD3	1:C:135:TYR:CE2	2.54	0.42
1:C:239:TYR:HB3	2:C:805:HOH:O	2.18	0.42
1:D:227:VAL:HG13	1:D:230:LEU:HD12	2.01	0.42
1:A:222:LEU:HD22	1:A:227:VAL:HG21	2.01	0.42
1:B:344:PRO:HB3	1:B:348:TYR:CD1	2.54	0.42
1:A:436:LEU:HD23	1:A:436:LEU:C	2.44	0.42
1:C:152:GLN:NE2	1:C:152:GLN:C	2.78	0.42
1:C:302[B]:LEU:HD13	1:C:302[B]:LEU:HA	1.90	0.42
1:D:280:SER:HB2	1:D:335:TYR:CE2	2.54	0.42
1:D:363:ARG:NH2	2:D:517:HOH:O	2.52	0.41
1:A:358:THR:HG23	1:A:438:MET:HE1	2.01	0.41
1:B:228:GLU:H	1:B:228:GLU:CD	2.28	0.41
1:C:267:ALA:N	2:C:514:HOH:O	2.54	0.41
1:D:40:ALA:HA	1:D:364:PRO:HD3	2.01	0.41
1:B:43:TRP:HE1	1:B:358[A]:THR:CG2	2.33	0.41
1:C:151:SER:HA	1:C:160:TRP:CZ2	2.55	0.41
1:D:362:LEU:HB3	1:D:382:TRP:CE3	2.55	0.41
1:D:385:GLU:OE1	1:D:385:GLU:HA	2.20	0.41
1:B:209:PHE:O	1:B:210:SER:CB	2.68	0.41
1:B:370:THR:HG22	1:B:403:LEU:HD22	2.02	0.41
1:C:280:SER:HB2	1:C:335:TYR:CE2	2.55	0.41
1:B:35:LEU:N	1:B:35:LEU:HD12	2.36	0.41
1:C:403:LEU:HD12	1:C:406:LEU:HD12	2.03	0.41
1:C:405:LYS:HD3	1:C:405:LYS:HA	1.81	0.41
1:D:57:SER:OG	1:D:60:ARG:HG3	2.20	0.41
1:D:82:TRP:CH2	1:D:122:ILE:HG21	2.56	0.41
1:A:329:SER:O	1:A:333:ARG:HG3	2.20	0.41
1:A:377:SER:HA	1:A:395:SER:HB2	2.02	0.41
1:B:30:SER:C	1:B:31:GLU:CG	2.94	0.40
1:C:319:PHE:HA	1:C:320:THR:HA	1.75	0.40
1:D:67[A]:ARG:CZ	1:D:344:PRO:HD3	2.52	0.40
1:C:348:TYR:CD1	1:C:348:TYR:C	2.99	0.40
1:B:235:THR:HB	1:B:273:TRP:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:HIS:CD2	1:D:276:GLU:HB2	2.56	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	417/416 (100%)	403 (97%)	14 (3%)	0	100	100
1	B	414/416 (100%)	400 (97%)	14 (3%)	0	100	100
1	C	417/416 (100%)	406 (97%)	11 (3%)	0	100	100
1	D	415/416 (100%)	397 (96%)	18 (4%)	0	100	100
All	All	1663/1664 (100%)	1606 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	359/354 (101%)	347 (97%)	12 (3%)	33	34
1	B	356/354 (101%)	338 (95%)	18 (5%)	21	19
1	C	359/354 (101%)	344 (96%)	15 (4%)	26	25
1	D	357/354 (101%)	340 (95%)	17 (5%)	23	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1431/1416 (101%)	1369 (96%)	62 (4%)	28	25

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	52	GLN
1	A	93[A]	GLN
1	A	93[B]	GLN
1	A	131	PHE
1	A	210	SER
1	A	282	TYR
1	A	288	LEU
1	A	326	GLN
1	A	407	LYS
1	A	423	SER
1	A	442	GLU
1	B	31	GLU
1	B	52	GLN
1	B	93[A]	GLN
1	B	93[B]	GLN
1	B	131	PHE
1	B	210	SER
1	B	229	SER
1	B	235	THR
1	B	282	TYR
1	B	283	LYS
1	B	287	GLU
1	B	288	LEU
1	B	356	LYS
1	B	384	ARG
1	B	388	ARG
1	B	397	ARG
1	B	405	LYS
1	B	429	GLU
1	C	30	SER
1	C	44	LYS
1	C	93[A]	GLN
1	C	93[B]	GLN
1	C	96[A]	SER
1	C	96[B]	SER
1	C	131	PHE

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Mol	Chain	Res	Type
1	C	210	SER
1	C	235	THR
1	C	282	TYR
1	C	288	LEU
1	C	371	GLU
1	C	388	ARG
1	C	407	LYS
1	C	423	SER
1	D	30	SER
1	D	31	GLU
1	D	52	GLN
1	D	96	SER
1	D	131	PHE
1	D	147	MET
1	D	175	LYS
1	D	282	TYR
1	D	294	VAL
1	D	356[A]	LYS
1	D	356[B]	LYS
1	D	358	THR
1	D	405	LYS
1	D	407	LYS
1	D	423	SER
1	D	429	GLU
1	D	442	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	91	GLN
1	A	186	GLN
1	A	224	HIS
1	A	326	GLN
1	A	389	ASN
1	A	437	GLN
1	B	52	GLN
1	B	152	GLN
1	B	224	HIS
1	B	256	HIS
1	B	259	GLN
1	B	261	ASN

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Mol	Chain	Res	Type
1	B	389	ASN
1	B	437	GLN
1	C	152	GLN
1	C	256	HIS
1	C	261	ASN
1	C	389	ASN
1	C	437	GLN
1	D	52	GLN
1	D	91	GLN
1	D	99	GLN
1	D	256	HIS
1	D	261	ASN
1	D	389	ASN
1	D	437	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 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	413/416 (99%)	-1.47	0 100 100	10, 21, 35, 45	6 (1%)
1	B	413/416 (99%)	-1.44	0 100 100	10, 23, 36, 47	3 (0%)
1	C	413/416 (99%)	-1.28	0 100 100	13, 29, 45, 52	6 (1%)
1	D	413/416 (99%)	-1.33	0 100 100	10, 26, 44, 53	4 (0%)
All	All	1652/1664 (99%)	-1.38	0 100 100	10, 25, 41, 53	19 (1%)

There are no RSRZ outliers to report.

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.