Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:32 am BST

PDB ID	:	4ZN2
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 following versions of software and data (see references ⓘ) were used in the production of this report:

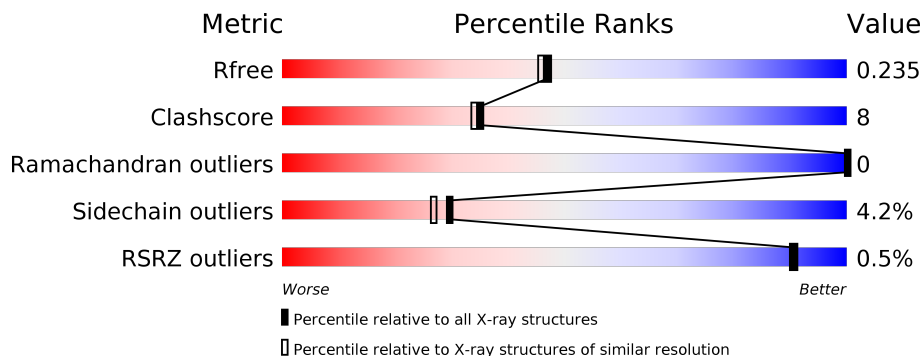|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.235
Clashscore		8
Ramachandran outliers		0
Sidechain outliers		4.2%
RSRZ outliers		0.5%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on 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 <=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	85% 13% ••
1	B	416	84% 14% ••
1	C	416	% 77% 22% •
1	D	416	% 79% 19% ••

2 Entry composition (i)

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 3377	C 2173	N 581	O 615	S 8	0	6	0
1	B	413	Total 3353	C 2159	N 575	O 611	S 8	0	3	0
1	C	413	Total 3377	C 2171	N 581	O 617	S 8	0	6	0
1	D	413	Total 3369	C 2171	N 579	O 611	S 8	0	4	0

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.

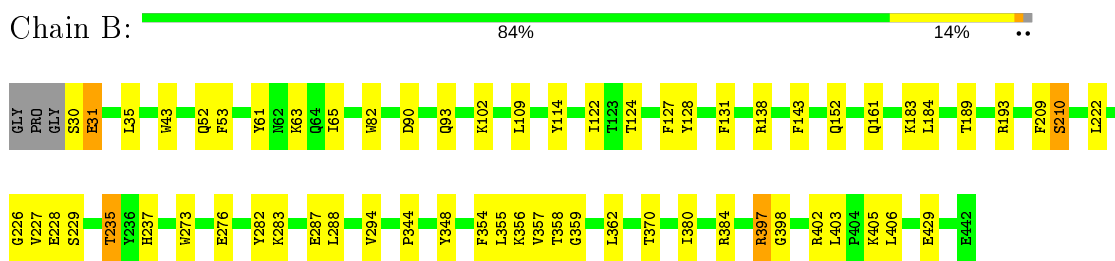| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	474	Total 474	O 474	0	0
2	B	464	Total 464	O 464	0	0
2	C	330	Total 330	O 330	0	0
2	D	358	Total 358	O 358	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA 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.
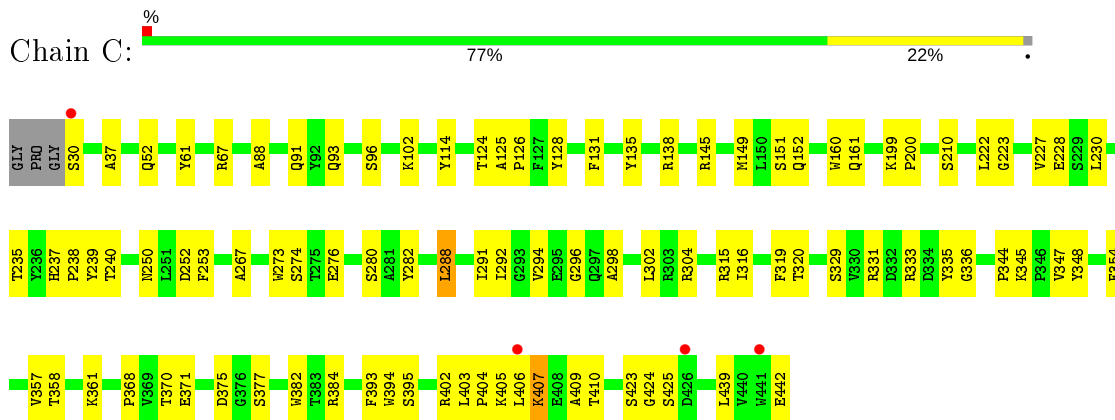
- Molecule 1: PslG

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GLY PRO GLY S30 E31 V34 L35 K36 A37 A40 W43 Q52 S57 R60 Y61 I65 D66 R67 R77 W82 S96 L109 Y114 I122 T123 T124 Y128 F131 R138 E141 R145 Q161 K175 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 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 A396 R397 R402 L403 L406 K407 P421 L422 S423 L428 E429 K433 S434 M438 W441 E442

4 Data and refinement statistics (i)

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
$<I/\sigma(I)>$ [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 , 0.235	Depositor DCC
R_{free} test set	7171 reflections (5.01%)	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)	0.32 , 25.6	EDS
L-test for twinning[2]	$<|L|> = 0.44, <L^2> = 0.27$	Xtriage
Estimated twinning fraction	0.159 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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	0.34	1/3474 (0.0%)	0.50	0/4732
1	B	0.33	0/3450	0.49	0/4701
1	C	0.34	1/3474 (0.0%)	0.47	0/4732
1	D	0.33	0/3467	0.50	0/4722
All	All	0.33	2/13865 (0.0%)	0.49	0/18887

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	442	GLU	C-OXT	-7.48	1.09	1.23
1	A	442	GLU	C-OXT	-6.42	1.11	1.23

There are no bond angle outliers.

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	45	0
1	B	3353	0	3290	47	0
1	C	3377	0	3307	61	0
1	D	3369	0	3309	66	0
2	A	474	0	0	7	0
2	B	464	0	0	9	0
2	C	330	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	358	0	0	13	0
All	All	15102	0	13220	218	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 8.

All (218) 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:C:361:LYS:NZ	2:C:501:HOH:O	2.08	0.86
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:294:VAL:HG22	2:B:743:HOH:O	2.01	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:D:34:VAL:HG22	1:D:379:SER:HB3	1.87	0.56
1:C:407:LYS:HG3	1:C:424:GLY:O	2.05	0.56
1:B:30:SER:C	1:B:31:GLU:HG3	2.25	0.56
1:D:379:SER:C	1:D:380:ILE:HG13	2.24	0.56
1:B:355:LEU:HA	1:B:358[A]:THR:HG22	1.86	0.56
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:102:LYS:HZ1	1:A:102:LYS:HB3	1.72	0.53
1:D:385:GLU:OE1	2:D:502:HOH:O	2.19	0.53
1:D:65[A]:ILE:HD12	1:D:109:LEU:HD11	1.91	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:HA	1:C:67[B]:ARG:HE	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
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:D:37:ALA:HB2	1:D:310:ALA:HA	1.94	0.49
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:353:ARG:HD3	1:A:417:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:359:GLY:HA3	2:D:536:HOH:O	2.12	0.48
1:D:35:LEU:HB2	1:D:380:ILE:HG12	1.95	0.48
1:C:273:TRP:HA	1:C:315:ARG:O	2.13	0.47
1:C:288:LEU:HA	1:C:288:LEU:HD12	1.66	0.47
1:A:326:GLN:HG3	1:A:326:GLN:O	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: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: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
1:B:43:TRP:NE1	1:B:358[A]:THR:HG21	2.31	0.45
1:C:292:ILE:HD12	1:C:296:GLY:C	2.37	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:A:371:GLU:OE1	1:A:402:ARG:NE	2.44	0.45
1:A:362:LEU:HD22	1:A:382:TRP:HB3	1.97	0.45
1:D:402:ARG:NH1	1:D:429:GLU:HB2	2.32	0.44
1:D:65[B]:ILE:HD13	1:D:109:LEU:HD11	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:370:THR:HG22	1:B:403:LEU:CD2	2.48	0.44
1:B:65[A]:ILE:HD12	1:B:109:LEU:CD1	2.45	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:B:402:ARG:C	1:B:403:LEU:HD23	2.38	0.44
1:A:183:LYS:HD2	1:A:183:LYS:HA	1.67	0.44
1:A:79:ASP:HB3	1:A:114:TYR:CZ	2.52	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:D:30:SER:C	1:D:31:GLU:HG3	2.38	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:HA	1:A:288:LEU:HD12	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:402:ARG:O	1:C:404:PRO:HD3	2.18	0.43
1:C:88:ALA:HB3	1:C:91:GLN:HB3	2.01	0.43
1:A:319:PHE:HA	1:A:320:THR:HA	1.86	0.43
1:A:96:SER:OG	1:B:127:PHE:CE2	2.71	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
1:C:377:SER:HA	1:C:395:SER:HB2	2.01	0.43
1:A:356:LYS:HB3	1:A:356:LYS:HE2	1.70	0.42
1:D:422:LEU:HD22	2:D:506:HOH:O	2.19	0.42
1:B:397:ARG:H	1:B:397:ARG:HD3	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:C:302[B]:LEU:HA	1:C:302[B]:LEU:HD13	1.90	0.42
1:D:280:SER:HB2	1:D:335:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:ARG:NH2	2:D:517:HOH:O	2.52	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:D:30:SER:C	1:D:31:GLU:CG	2.88	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:HA	1:C:405:LYS:HD3	1.81	0.41
1:D:82:TRP:CH2	1:D:122:ILE:HG21	2.56	0.41
1:D:57:SER:OG	1:D:60:ARG:HG3	2.20	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: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:B:235:THR:HB	1:B:273:TRP:HB2	2.04	0.40
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	345 (96%)	14 (4%)	32	30
1	B	356/354 (101%)	340 (96%)	16 (4%)	27	24
1	C	359/354 (101%)	342 (95%)	17 (5%)	26	22
1	D	357/354 (101%)	338 (95%)	19 (5%)	22	18
All	All	1431/1416 (101%)	1365 (95%)	66 (5%)	30	23

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	52	GLN
1	A	61	TYR
1	A	93[A]	GLN
1	A	93[B]	GLN
1	A	128	TYR
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

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Mol	Chain	Res	Type
1	B	93[A]	GLN
1	B	93[B]	GLN
1	B	128	TYR
1	B	131	PHE
1	B	152	GLN
1	B	210	SER
1	B	229	SER
1	B	235	THR
1	B	282	TYR
1	B	283	LYS
1	B	356	LYS
1	B	397	ARG
1	B	405	LYS
1	B	429	GLU
1	C	52	GLN
1	C	61	TYR
1	C	93[A]	GLN
1	C	93[B]	GLN
1	C	96[A]	SER
1	C	96[B]	SER
1	C	128	TYR
1	C	131	PHE
1	C	152	GLN
1	C	210	SER
1	C	228	GLU
1	C	235	THR
1	C	282	TYR
1	C	288	LEU
1	C	371	GLU
1	C	407	LYS
1	C	423	SER
1	D	30	SER
1	D	31	GLU
1	D	52	GLN
1	D	61[A]	TYR
1	D	61[B]	TYR
1	D	96	SER
1	D	128	TYR
1	D	131	PHE
1	D	175	LYS
1	D	282	TYR
1	D	294	VAL

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Mol	Chain	Res	Type
1	D	356[A]	LYS
1	D	356[B]	LYS
1	D	358	THR
1	D	402	ARG
1	D	407	LYS
1	D	423	SER
1	D	429	GLU
1	D	442	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	152	GLN
1	A	261	ASN
1	A	389	ASN
1	A	437	GLN
1	B	52	GLN
1	B	99	GLN
1	B	152	GLN
1	B	256	HIS
1	B	259	GLN
1	B	261	ASN
1	B	389	ASN
1	B	437	GLN
1	C	52	GLN
1	C	91	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	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 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(Å²)	Q<0.9
1	A	413/416 (99%)	-0.43	1 (0%)	95	94	15, 21, 35, 45	0
1	B	413/416 (99%)	-0.39	0	100	100	15, 23, 36, 47	0
1	C	413/416 (99%)	-0.14	4 (0%)	82	81	18, 29, 45, 52	0
1	D	413/416 (99%)	-0.23	4 (0%)	82	81	16, 26, 44, 53	0
All	All	1652/1664 (99%)	-0.30	9 (0%)	91	90	15, 25, 41, 53	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	30	SER	4.5
1	D	397	ARG	3.7
1	C	406	LEU	3.4
1	D	441	TRP	3.2
1	A	30	SER	3.2
1	C	441	TRP	2.9
1	D	442	GLU	2.5
1	C	426	ASP	2.5
1	D	406	LEU	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 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.