Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2023 – 06:19 pm GMT

PDB ID	:	8AUD
Title	:	Structure of peptidoglycan hydrolase Cg1735 from Corynebacterium glutamicum, orthorhombic crystal form
Authors	:	Gaday, Q.; Wehenkel, A.M.; Alzari, P.M.
Deposited on	:	2022-08-25
Resolution	:	4.50 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:

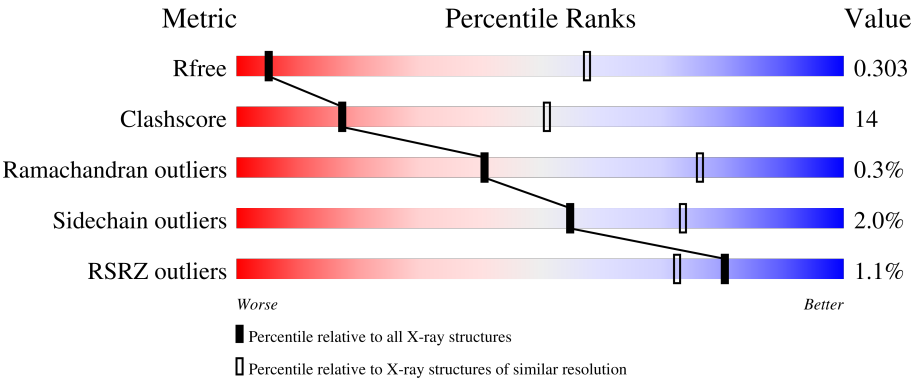
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.50 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}	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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 <=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	619	43% 13% 43%
1	B	619	% 40% 16% 44%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5142 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.

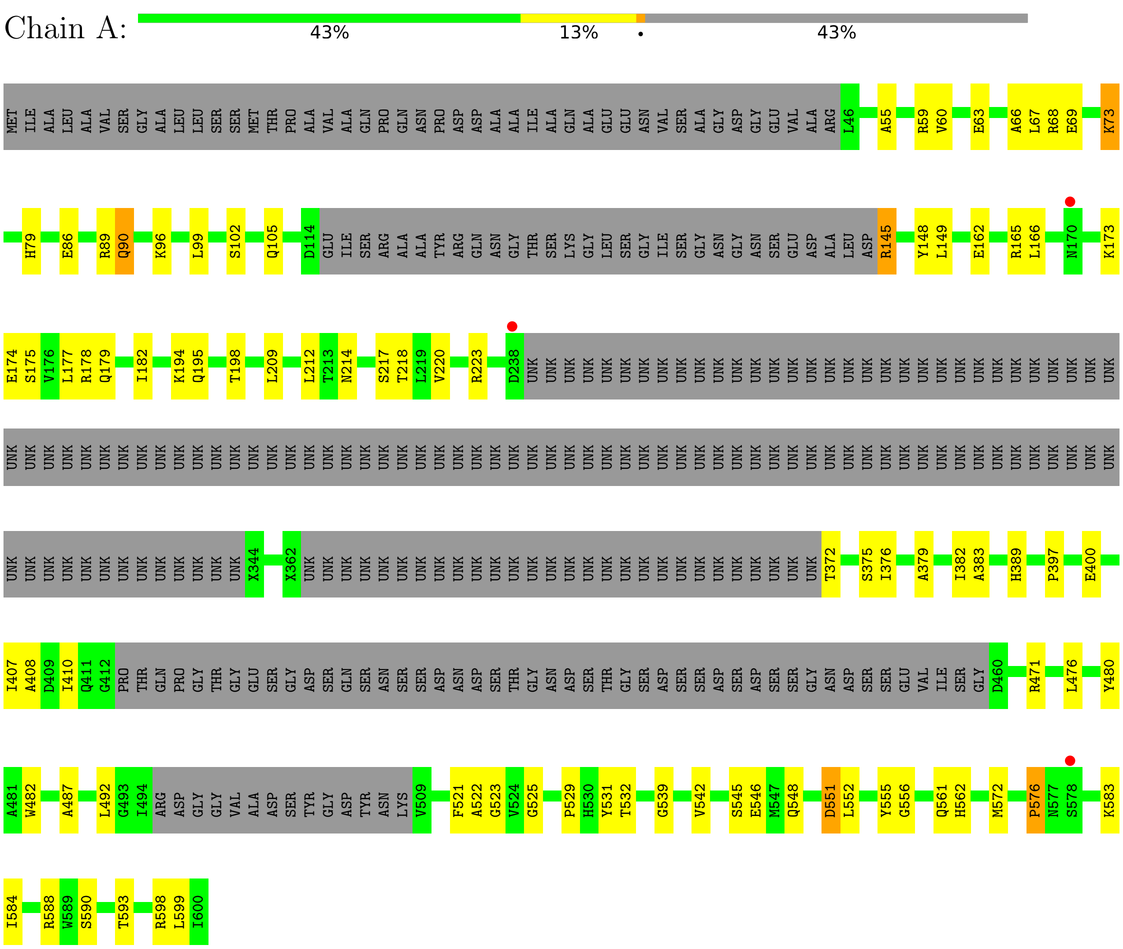
- Molecule 1 is a protein called Cell wall-associated hydrolases (Invasion-associated proteins).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2582	1574	470	532	6			
1	B	346	Total	C	N	O	S	0	0	0
			2560	1561	466	527	6			

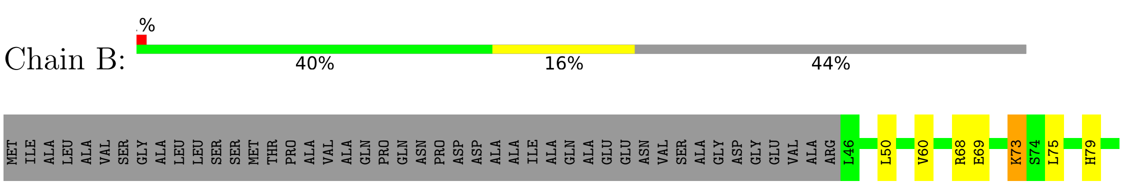
3 Residue-property plots ⓘ

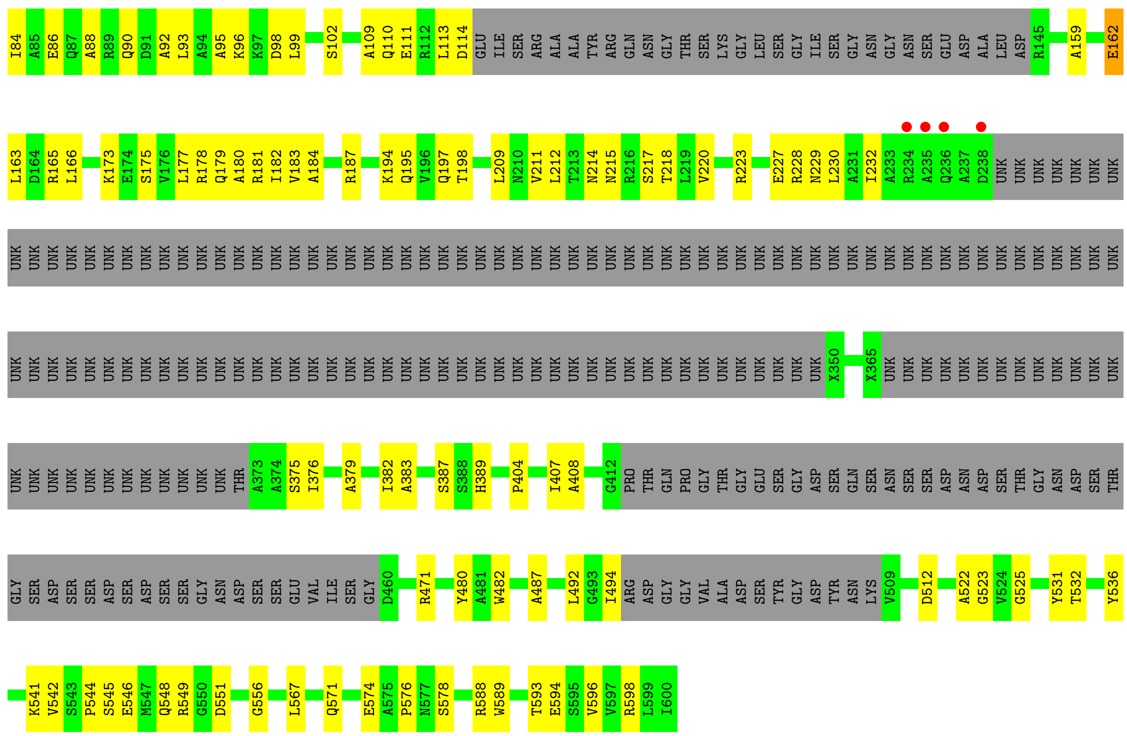
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cell wall-associated hydrolases (Invasion-associated proteins)



- Molecule 1: Cell wall-associated hydrolases (Invasion-associated proteins)




I84 A85 E86 Q87 A88 R89 Q90 D91 A92 L93 A94 A95 K96 K97 D98 L99 S102 A109 Q110 E111 R112 L113 D114 GLU ILE SER ARG ALA ALA TYR ARG GLN ASN GLY THR SER LYS GLY LEU SER GLY ILE SER GLY ASN GLY ASN SER GLU ASP ALA LEU ASP R145 A159 E162
L163 D164 R165 L166 K173 E174 S175 V176 L177 R178 Q179 A180 R181 I182 V183 A184 R187 K194 Q195 V196 Q197 T198 L209 N210 V211 L212 T213 N214 N215 R216 S217 T218 L219 V220 R223 E227 R228 N229 L230 A231 I232 A233 R234 A235 Q236 A237 D238 UNK UNK UNK UNK UNK UNK UNK
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UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK THR A373 A374 S375 I376 A379 I382 A383 S387 S388 H389 P404 I407 A408 G412 PRO THR GLN PRO GLY THR GLY GLU SER GLY ASP SER GLN SER ASN SER SER ASP ASN ASP SER THR GLY ASN ASP SER THR
GLY SER ASP SER SER ASP SER ASP SER SER GLY ASN ASP SER SER GLU VAL ILE SER GLY D460 R471 Y480 A481 W482 A487 L492 G493 I494 ARG ASP GLY GLY VAL ALA ASP SER TYR GLY ASP TYR ASN LYS V509 D512 A522 G523 V524 G525 Y531 T532 Y536
K541 V542 S543 P544 S545 E546 M547 Q548 R549 G550 D551 G556 L567 Q571 E574 A575 P576 N577 S578 R588 W589 T593 E594 S595 V596 V597 R598 L599 I600

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.57Å 123.08Å 209.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.54 – 4.50 61.54 – 4.50	Depositor EDS
% Data completeness (in resolution range)	74.8 (61.54-4.50) 74.8 (61.54-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.89 (at 4.46Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.278 , 0.307 0.283 , 0.303	Depositor DCC
R_{free} test set	585 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	94.3	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 104.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	5142	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.31	0/2512	0.67	2/3401 (0.1%)
1	B	0.31	0/2505	0.67	1/3391 (0.0%)
All	All	0.31	0/5017	0.67	3/6792 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	GLN	N-CA-CB	5.51	120.51	110.60
1	A	149	LEU	CA-CB-CG	-5.45	102.77	115.30
1	B	113	LEU	CA-CB-CG	5.29	127.46	115.30

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	2582	0	2444	66	0
1	B	2560	0	2434	74	0
All	All	5142	0	4878	138	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 14.

All (138) 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:89:ARG:NH2	1:A:397:PRO:HB2	1.89	0.88
1:A:383:ALA:HB2	1:A:487:ALA:HB3	1.54	0.86
1:A:89:ARG:HD2	1:A:400:GLU:HA	1.55	0.86
1:A:66:ALA:HB2	1:A:561:GLN:HG2	1.64	0.77
1:B:60:VAL:HG13	1:B:212:LEU:HD12	1.68	0.76
1:A:89:ARG:HH11	1:A:400:GLU:HA	1.51	0.75
1:A:588:ARG:HH21	1:A:590:SER:HB2	1.57	0.69
1:B:175:SER:HA	1:B:178:ARG:HD2	1.75	0.69
1:A:60:VAL:HG13	1:A:212:LEU:HD12	1.74	0.68
1:B:387:SER:H	1:B:407:ILE:HD13	1.59	0.67
1:A:556:GLY:O	1:A:593:THR:HG22	1.96	0.65
1:B:383:ALA:HB2	1:B:487:ALA:HB3	1.77	0.65
1:B:211:VAL:O	1:B:215:ASN:ND2	2.26	0.64
1:A:102:SER:HB2	1:A:173:LYS:HD2	1.79	0.64
1:A:162:GLU:O	1:A:166:LEU:HG	1.99	0.62
1:B:102:SER:HB2	1:B:173:LYS:HD2	1.81	0.61
1:A:194:LYS:O	1:A:198:THR:HG23	2.00	0.61
1:A:175:SER:HA	1:A:178:ARG:HD2	1.83	0.60
1:A:542:VAL:HG21	1:A:598:ARG:NH1	2.17	0.59
1:B:73:LYS:HB2	1:B:531:TYR:CD1	2.37	0.59
1:B:99:LEU:HG	1:B:177:LEU:HD12	1.85	0.59
1:B:407:ILE:HD12	1:B:408:ALA:O	2.03	0.59
1:A:79:HIS:HD2	1:A:389:HIS:HD2	1.49	0.58
1:B:68:ARG:HH21	1:B:480:TYR:HE1	1.52	0.58
1:A:69:GLU:HG3	1:A:531:TYR:CD1	2.39	0.57
1:A:89:ARG:HD2	1:A:400:GLU:CA	2.32	0.57
1:B:548:GLN:HG2	1:B:598:ARG:HH21	1.69	0.56
1:B:549:ARG:NH1	1:B:567:LEU:O	2.36	0.56
1:A:105:GLN:HB3	1:A:166:LEU:HD13	1.87	0.56
1:A:179:GLN:HA	1:A:182:ILE:HG12	1.88	0.55
1:A:214:ASN:O	1:A:218:THR:HG23	2.06	0.55
1:B:214:ASN:O	1:B:218:THR:HG23	2.07	0.55
1:A:407:ILE:HD12	1:A:408:ALA:O	2.07	0.54
1:B:194:LYS:O	1:B:198:THR:HG23	2.08	0.54
1:B:536:TYR:CZ	1:B:541:LYS:HE2	2.43	0.54
1:B:86:GLU:O	1:B:90:GLN:HG3	2.09	0.53
1:B:379:ALA:HA	1:B:522:ALA:HB1	1.92	0.52
1:B:50:LEU:HD13	1:B:227:GLU:HG3	1.92	0.51
1:A:68:ARG:HH21	1:A:480:TYR:HE1	1.58	0.51
1:A:165:ARG:HE	1:A:166:LEU:CD2	2.23	0.51
1:A:220:VAL:HG23	1:A:223:ARG:HH21	1.76	0.51
1:B:546:GLU:N	1:B:546:GLU:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:HE	1:A:166:LEU:HD21	1.77	0.50
1:A:546:GLU:N	1:A:546:GLU:OE1	2.44	0.50
1:A:548:GLN:HG2	1:A:598:ARG:NH2	2.27	0.50
1:B:376:ILE:HA	1:B:471:ARG:HH12	1.77	0.50
1:A:551:ASP:OD1	1:A:598:ARG:NE	2.43	0.49
1:A:86:GLU:O	1:A:90:GLN:HG3	2.13	0.49
1:B:159:ALA:O	1:B:162:GLU:HG3	2.13	0.49
1:A:96:LYS:HA	1:A:177:LEU:HD11	1.95	0.49
1:A:68:ARG:HG3	1:A:209:LEU:HD21	1.95	0.48
1:A:59:ARG:HA	1:A:59:ARG:HD2	1.53	0.48
1:A:521:PHE:HE2	1:A:552:LEU:HD21	1.78	0.48
1:B:69:GLU:HG3	1:B:531:TYR:CD1	2.48	0.48
1:B:84:ILE:CG2	1:B:187:ARG:HD2	2.43	0.48
1:A:99:LEU:HD22	1:A:177:LEU:HD12	1.95	0.48
1:B:79:HIS:CD2	1:B:389:HIS:HD2	2.31	0.48
1:A:96:LYS:HG3	1:A:177:LEU:HD21	1.96	0.48
1:B:90:GLN:HA	1:B:93:LEU:HD23	1.94	0.48
1:B:79:HIS:HD2	1:B:389:HIS:HD2	1.62	0.48
1:B:90:GLN:NE2	1:B:404:PRO:HD2	2.29	0.48
1:A:73:LYS:HB2	1:A:531:TYR:CE1	2.49	0.47
1:B:375:SER:O	1:B:523:GLY:HA2	2.13	0.47
1:A:68:ARG:HH11	1:A:209:LEU:HD22	1.80	0.47
1:A:217:SER:HA	1:A:220:VAL:HG12	1.97	0.47
1:B:69:GLU:HG3	1:B:531:TYR:HD1	1.80	0.47
1:A:548:GLN:HG2	1:A:598:ARG:HH21	1.80	0.47
1:B:88:ALA:HB1	1:B:184:ALA:HA	1.96	0.47
1:B:68:ARG:NH2	1:B:578:SER:HB2	2.29	0.47
1:A:476:LEU:HD21	1:A:584:ILE:HG13	1.96	0.46
1:A:69:GLU:HG2	1:A:532:THR:OG1	2.14	0.46
1:B:96:LYS:HG3	1:B:177:LEU:HD21	1.97	0.46
1:B:556:GLY:O	1:B:593:THR:HG22	2.15	0.46
1:B:111:GLU:O	1:B:114:ASP:HB2	2.16	0.46
1:B:545:SER:OG	1:B:546:GLU:OE1	2.28	0.46
1:B:229:ASN:HA	1:B:232:ILE:HD12	1.97	0.46
1:A:145:ARG:HA	1:A:148:TYR:CD2	2.51	0.46
1:B:68:ARG:HA	1:B:482:TRP:CZ2	2.52	0.45
1:B:541:LYS:HA	1:B:596:VAL:O	2.16	0.45
1:B:179:GLN:OE1	1:B:182:ILE:HD11	2.16	0.45
1:B:544:PRO:HD3	1:B:594:GLU:O	2.17	0.45
1:B:95:ALA:HB1	1:B:177:LEU:HA	1.98	0.45
1:B:567:LEU:HD22	1:B:571:GLN:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ARG:HD3	1:B:589:TRP:O	2.16	0.45
1:A:555:TYR:HB2	1:A:562:HIS:HB3	1.99	0.45
1:A:492:LEU:HD12	1:A:492:LEU:H	1.82	0.45
1:B:84:ILE:HG23	1:B:187:ARG:HD2	1.98	0.45
1:B:379:ALA:HB1	1:B:487:ALA:O	2.17	0.44
1:A:79:HIS:CD2	1:A:389:HIS:HD2	2.30	0.44
1:B:69:GLU:HG2	1:B:532:THR:OG1	2.16	0.44
1:A:63:GLU:O	1:A:67:LEU:HG	2.17	0.44
1:B:228:ARG:O	1:B:232:ILE:HG13	2.17	0.44
1:B:375:SER:HA	1:B:523:GLY:O	2.17	0.44
1:B:230:LEU:HD23	1:B:230:LEU:HA	1.90	0.44
1:A:69:GLU:HG3	1:A:531:TYR:HD1	1.81	0.44
1:A:376:ILE:HA	1:A:471:ARG:HH12	1.82	0.44
1:B:574:GLU:OE2	1:B:588:ARG:NH1	2.39	0.44
1:B:165:ARG:HE	1:B:166:LEU:HD23	1.83	0.44
1:A:73:LYS:HB2	1:A:531:TYR:CD1	2.53	0.43
1:A:572:MET:HE1	1:A:588:ARG:H	1.83	0.43
1:A:379:ALA:HA	1:A:522:ALA:HB1	1.99	0.43
1:A:576:PRO:HG3	1:A:583:LYS:NZ	2.33	0.43
1:B:220:VAL:HG23	1:B:223:ARG:HH21	1.83	0.43
1:A:79:HIS:HD2	1:A:389:HIS:CD2	2.34	0.43
1:B:542:VAL:HG21	1:B:598:ARG:NH1	2.33	0.43
1:A:174:GLU:O	1:A:178:ARG:HG3	2.18	0.43
1:B:75:LEU:HD11	1:B:494:ILE:CD1	2.49	0.43
1:B:109:ALA:HB1	1:B:163:LEU:HG	2.01	0.43
1:B:382:ILE:HD11	1:B:525:GLY:C	2.39	0.43
1:B:73:LYS:HB2	1:B:531:TYR:CG	2.53	0.43
1:A:73:LYS:HB2	1:A:531:TYR:CZ	2.53	0.43
1:B:194:LYS:HA	1:B:197:GLN:HB2	2.01	0.43
1:A:55:ALA:HB1	1:B:589:TRP:CG	2.54	0.42
1:B:92:ALA:HA	1:B:180:ALA:HB1	2.00	0.42
1:B:480:TYR:CE2	1:B:512:ASP:HA	2.55	0.42
1:B:542:VAL:HG21	1:B:598:ARG:HH12	1.84	0.42
1:A:89:ARG:HH22	1:A:397:PRO:HB2	1.76	0.42
1:B:180:ALA:O	1:B:183:VAL:HG12	2.20	0.42
1:B:492:LEU:H	1:B:492:LEU:HD12	1.84	0.42
1:B:68:ARG:HH22	1:B:578:SER:HB2	1.85	0.42
1:A:539:GLY:HA3	1:A:599:LEU:HD23	2.02	0.42
1:A:382:ILE:HD11	1:A:525:GLY:HA2	2.00	0.42
1:A:89:ARG:NH2	1:A:397:PRO:CB	2.73	0.42
1:B:387:SER:N	1:B:407:ILE:HD13	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:SER:O	1:A:523:GLY:HA2	2.20	0.41
1:B:177:LEU:HD22	1:B:181:ARG:HD2	2.03	0.41
1:B:217:SER:HA	1:B:220:VAL:HG12	2.00	0.41
1:A:68:ARG:HA	1:A:482:TRP:CZ2	2.56	0.41
1:A:372:THR:O	1:A:376:ILE:HG12	2.21	0.41
1:B:90:GLN:HA	1:B:93:LEU:CD2	2.51	0.41
1:B:68:ARG:HA	1:B:482:TRP:CE2	2.56	0.40
1:B:90:GLN:O	1:B:93:LEU:HG	2.22	0.40
1:B:162:GLU:O	1:B:166:LEU:HG	2.21	0.40
1:B:209:LEU:HD23	1:B:209:LEU:HA	1.90	0.40
1:A:68:ARG:NE	1:A:480:TYR:OH	2.54	0.40
1:A:410:ILE:HG22	1:A:529:PRO:HB3	2.01	0.40
1:B:175:SER:HA	1:B:178:ARG:CD	2.49	0.40
1:A:545:SER:OG	1:A:546:GLU:OE1	2.30	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	321/619 (52%)	314 (98%)	6 (2%)	1 (0%)	41 76
1	B	320/619 (52%)	313 (98%)	6 (2%)	1 (0%)	41 76
All	All	641/1238 (52%)	627 (98%)	12 (2%)	2 (0%)	41 76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	576	PRO
1	B	576	PRO

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	256/359 (71%)	252 (98%)	4 (2%)	62 79
1	B	255/359 (71%)	249 (98%)	6 (2%)	49 69
All	All	511/718 (71%)	501 (98%)	10 (2%)	55 73

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	145	ARG
1	A	195	GLN
1	A	551	ASP
1	B	73	LYS
1	B	98	ASP
1	B	110	GLN
1	B	162	GLU
1	B	195	GLN
1	B	551	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	HIS
1	B	79	HIS
1	B	389	HIS

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 monosaccharides 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

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, 95^{th} 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	331/619 (53%)	0.05	3 (0%)	84	77	40, 81, 134, 242	0
1	B	330/619 (53%)	-0.00	4 (1%)	79	70	43, 86, 145, 246	0
All	All	661/1238 (53%)	0.02	7 (1%)	80	72	40, 84, 138, 246	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	ASP	4.8
1	B	238	ASP	4.3
1	B	236	GLN	3.3
1	A	578	SER	3.2
1	B	235	ALA	2.9
1	B	234	ARG	2.4
1	A	170	ASN	2.1

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.