



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 23, 2014 – 05:29 PM EDT

PDB ID : 4LX4
Title : Crystal Structure Determination of Pseudomonas stutzeri endoglucanase Cel5A using a Twinned Data Set
Authors : Dutoit, R.; Delsaute, M.; Berlemont, R.; Van Elder, D.; Galleni, M.; Bauvois, C.
Deposited on : 2013-07-29
Resolution : 1.56 Å(reported)

This is a full wwPDB validation 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>

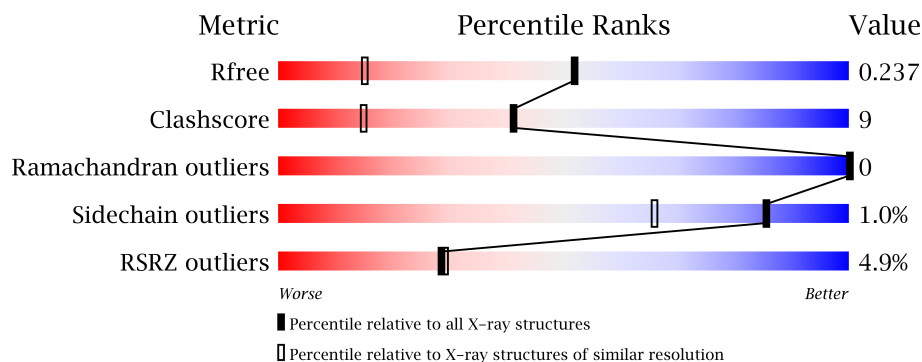
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : **FAILED**
Xtriage (Phenix) : dev-1439
EDS : stable23489
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) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 1.56 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	1117 (1.58-1.54)
Clashscore	79885	1249 (1.58-1.54)
Ramachandran outliers	78287	1212 (1.58-1.54)
Sidechain outliers	78261	1210 (1.58-1.54)
RSRZ outliers	66119	1117 (1.58-1.54)

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	330	
1	B	330	
1	C	330	
1	D	330	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	TRS	A	401	-	X

2 Entry composition i

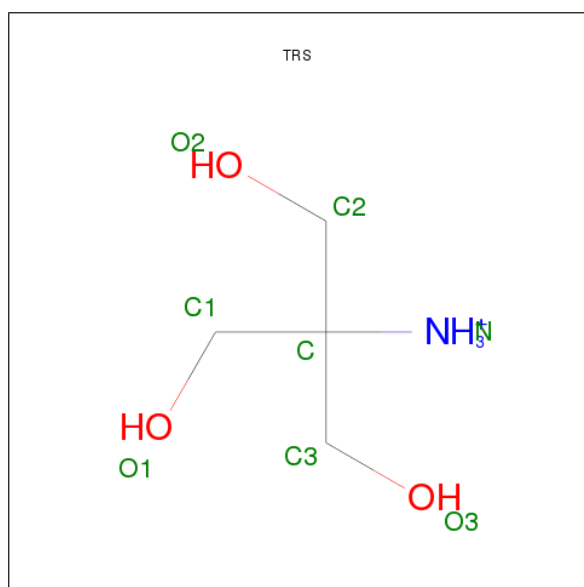
There are 3 unique types of molecules in this entry. The entry contains 21329 atoms, of which 9851 are hydrogens and 0 are deuterium.

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 Endoglucanase(Endo-1,4-beta-glucanase)protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	322	Total	C	H	N	O	S	0	0	0
			5019	1651	2444	448	467	9			
1	B	328	Total	C	H	N	O	S	0	0	0
			5113	1678	2494	456	476	9			
1	C	321	Total	C	H	N	O	S	0	0	0
			5022	1651	2451	447	464	9			
1	D	319	Total	C	H	N	O	S	0	0	0
			4964	1637	2414	440	464	9			

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
2	B	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
2	D	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

- Molecule 3 is water.

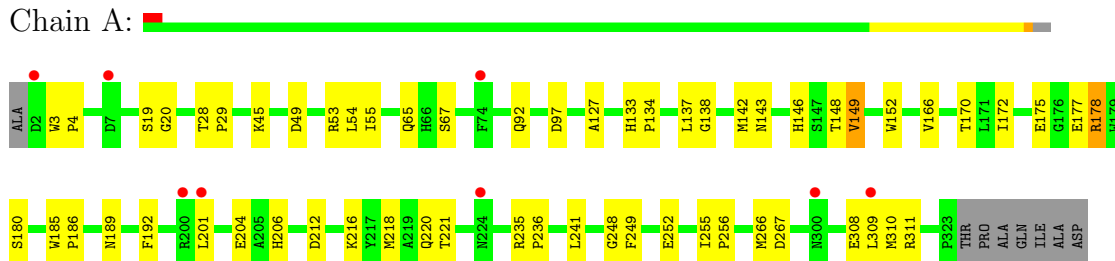
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	258	Total	O	0	0
			258	258		
3	B	312	Total	O	0	0
			312	312		
3	C	276	Total	O	0	0
			276	276		
3	D	285	Total	O	0	0
			285	285		

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 errors 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.

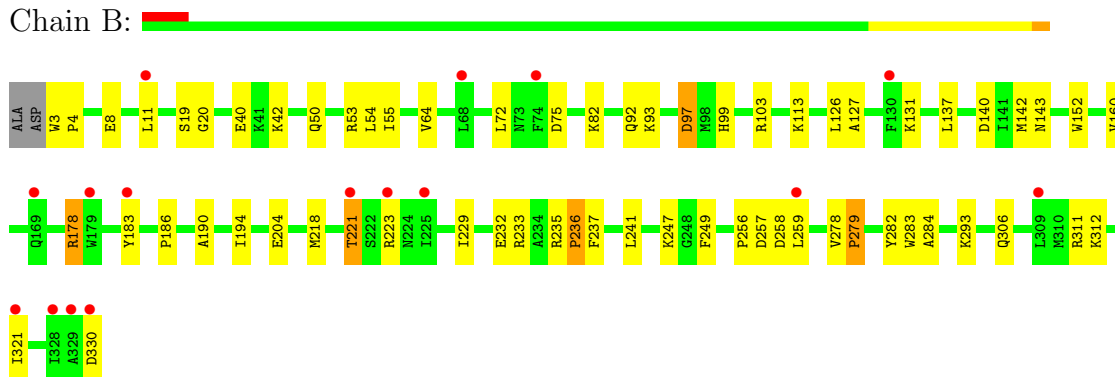
- Molecule 1: Endoglucanase(Endo-1,4-beta-glucanase)protein

Chain A:



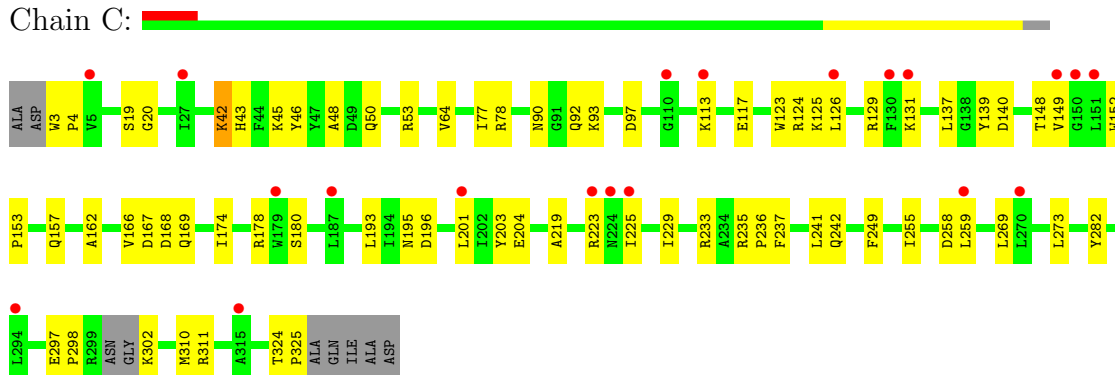
- Molecule 1: Endoglucanase(Endo-1,4-beta-glucanase)protein

Chain B:



- Molecule 1: Endoglucanase(Endo-1,4-beta-glucanase)protein

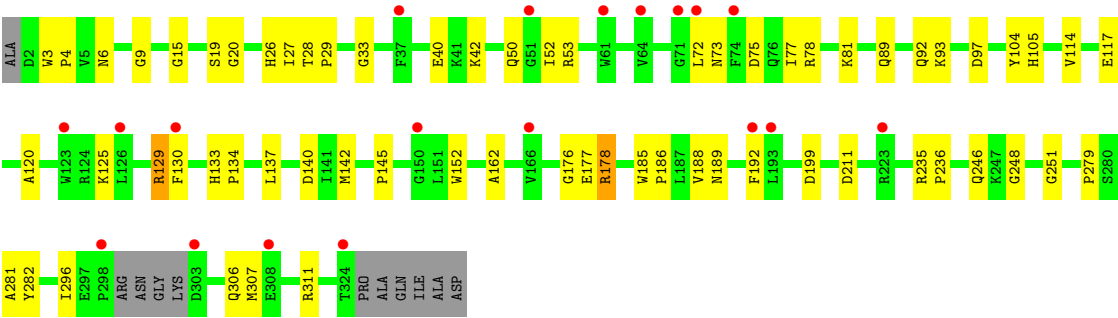
Chain C:



- Molecule 1: Endoglucanase(Endo-1,4-beta-glucanase)protein

Chain D:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.39Å 82.90Å 104.74Å 90.00° 92.08° 90.00°	Depositor
Resolution (Å)	48.28 – 1.56 48.28 – 1.56	Depositor EDS
% Data completeness (in resolution range)	91.6 (48.28-1.56) 82.3 (48.28-1.56)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.55Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.220 , 0.237 0.220 , 0.237	Depositor DCC
R_{free} test set	7882 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	12.4	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 21.2	EDS
Estimated twinning fraction	0.126 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.71$, $\langle L^2 \rangle = 0.60$	Xtriage
Outliers	1 of 157658 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21329	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: TRS

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	0.43	2/2655 (0.1%)	0.60	2/3607 (0.1%)
1	B	0.41	2/2700 (0.1%)	0.56	2/3668 (0.1%)
1	C	0.40	1/2651 (0.0%)	0.58	2/3601 (0.1%)
1	D	0.38	1/2629 (0.0%)	0.56	1/3573 (0.0%)
All	All	0.40	6/10635 (0.1%)	0.57	7/14449 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	279	PRO	N-CD	5.51	1.55	1.47
1	D	134	PRO	N-CD	5.36	1.55	1.47
1	C	153	PRO	N-CD	5.25	1.55	1.47
1	B	236	PRO	N-CD	5.16	1.55	1.47
1	A	256	PRO	N-CD	5.09	1.54	1.47
1	A	134	PRO	N-CD	5.03	1.54	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	255	ILE	C-N-CD	5.81	140.60	128.40
1	A	255	ILE	C-N-CD	5.76	140.50	128.40
1	A	133	HIS	C-N-CD	5.70	140.38	128.40
1	B	235	ARG	C-N-CD	5.64	140.24	128.40
1	C	152	TRP	C-N-CD	5.50	139.96	128.40
1	D	133	HIS	C-N-CD	5.46	139.86	128.40
1	B	278	VAL	C-N-CD	5.34	139.61	128.40

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	2575	2444	13	43	0
1	B	2619	2494	13	50	0
1	C	2571	2451	13	52	0
1	D	2550	2414	14	46	0
2	A	8	12	0	0	0
2	B	8	12	0	0	0
2	C	8	12	0	0	0
2	D	8	12	0	0	0
3	A	258	0	0	7	0
3	B	312	0	0	13	1
3	C	276	0	0	11	2
3	D	285	0	0	10	2
All	All	11478	9851	53	187	3

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.

All (187) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:113:LYS:HB3	3:B:789:HOH:O	1.79	0.81
1:B:256:PRO:HG2	1:B:259:LEU:HG	1.63	0.80
1:A:172:ILE:HB	1:A:201:LEU:CD2	2.12	0.80
1:A:220:GLN:HB3	3:A:690:HOH:O	1.82	0.79
1:D:246:GLN:HA	3:D:742:HOH:O	1.81	0.79
1:A:172:ILE:HB	1:A:201:LEU:HD23	1.65	0.79
1:C:45:LYS:HA	3:C:728:HOH:O	1.83	0.77
1:B:183:TYR:HB2	1:B:233:ARG:HG2	1.69	0.75
1:C:53:ARG:HA	1:C:92:GLN:HG2	1.69	0.72
1:D:81:LYS:HG3	1:D:130:PHE:HE1	1.55	0.72
1:C:229:ILE:O	1:C:233:ARG:HG3	1.89	0.72
1:C:282:TYR:HB2	1:C:310:MET:HE1	1.73	0.71
1:C:282:TYR:CB	1:C:310:MET:HE1	2.20	0.71
1:B:293:LYS:HD3	3:B:658:HOH:O	1.92	0.70
1:B:40:GLU:HB3	3:B:803:HOH:O	1.91	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:177:GLU:HG3	1:D:178:ARG:H	1.58	0.68
1:C:282:TYR:HB2	1:C:310:MET:CE	2.23	0.68
1:A:266:MET:SD	1:A:309:LEU:HD23	2.34	0.67
1:C:258:ASP:O	1:C:259:LEU:HD23	1.95	0.67
1:A:267:ASP:CG	1:A:309:LEU:HD11	2.17	0.65
1:D:72:LEU:O	3:D:676:HOH:O	2.14	0.64
1:B:233:ARG:O	1:B:236:PRO:HD2	1.98	0.64
1:B:258:ASP:C	1:B:259:LEU:HD23	2.18	0.64
1:D:211:ASP:OD2	3:D:674:HOH:O	2.15	0.64
1:B:312:LYS:HE3	1:D:89:GLN:O	1.98	0.63
1:A:146:HIS:HA	1:A:177:GLU:OE2	1.99	0.63
1:C:3:TRP:CG	1:C:4:PRO:HD2	2.34	0.63
1:C:90:ASN:HB3	3:C:728:HOH:O	1.98	0.63
1:C:3:TRP:CD1	1:C:4:PRO:HD2	2.34	0.62
1:B:64:VAL:HG11	1:B:126:LEU:HD21	1.81	0.62
1:D:185:TRP:HB3	1:D:186:PRO:HD3	1.81	0.62
1:A:138:GLY:HA2	1:A:170:THR:CG2	2.31	0.61
1:A:185:TRP:HB3	1:A:186:PRO:HD3	1.82	0.61
1:B:64:VAL:HG12	1:B:72:LEU:HD22	1.81	0.61
1:C:50:GLN:O	1:C:311:ARG:NH1	2.35	0.60
1:B:259:LEU:N	1:B:259:LEU:HD23	2.16	0.59
1:B:321:ILE:HG12	3:B:718:HOH:O	2.03	0.59
1:D:75:ASP:HB3	3:D:692:HOH:O	2.03	0.58
1:D:125:LYS:O	1:D:129:ARG:HG3	2.03	0.58
1:D:251:GLY:O	1:D:281:ALA:HB3	2.04	0.58
1:A:53:ARG:HA	1:A:92:GLN:HG2	1.84	0.58
1:C:125:LYS:O	1:C:129:ARG:HG2	2.04	0.57
1:B:64:VAL:CG1	1:B:72:LEU:HD22	2.34	0.57
1:C:311:ARG:HH11	1:C:311:ARG:HG2	1.69	0.57
1:B:53:ARG:HA	1:B:92:GLN:HG2	1.87	0.57
1:C:148:THR:O	1:C:149:VAL:HG22	2.05	0.57
1:B:50:GLN:O	1:B:311:ARG:NH1	2.38	0.56
1:C:195:ASN:HD22	1:D:33:GLY:HA2	1.70	0.56
1:C:229:ILE:HD13	3:C:650:HOH:O	2.06	0.56
1:C:123:TRP:CZ3	1:C:139:TYR:HB3	2.41	0.56
1:C:48:ALA:HB3	3:C:728:HOH:O	2.04	0.55
1:A:204:GLU:HG2	3:A:658:HOH:O	2.05	0.55
1:B:11:LEU:HD13	1:B:321:ILE:HD13	1.88	0.55
1:B:330:ASP:HB3	3:B:812:HOH:O	2.07	0.55
1:A:310:MET:HE3	3:A:700:HOH:O	2.05	0.55
1:A:54:LEU:O	1:A:55:ILE:HD13	2.09	0.53
1:D:311:ARG:HG2	1:D:311:ARG:HH11	1.74	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:29:PRO:HD3	3:A:575:HOH:O	2.08	0.52
1:B:232:GLU:O	1:B:236:PRO:HD3	2.09	0.52
1:D:145:PRO:HG2	1:D:176:GLY:O	2.08	0.52
1:D:26:HIS:CD2	1:D:27:ILE:HG13	2.45	0.52
1:D:73:ASN:O	1:D:77:ILE:HG12	2.10	0.52
1:A:28:THR:HA	1:A:29:PRO:C	2.29	0.52
1:B:311:ARG:HG2	1:B:311:ARG:HH11	1.75	0.52
1:B:40:GLU:HG3	1:B:42:LYS:HG2	1.91	0.52
1:A:142:MET:HB3	1:A:152:TRP:CH2	2.45	0.51
1:D:42:LYS:HE2	3:D:723:HOH:O	2.10	0.51
1:B:282:TYR:OH	1:B:306:GLN:HG2	2.11	0.51
1:C:225:ILE:O	3:C:692:HOH:O	2.19	0.51
1:B:237:PHE:O	1:B:241:LEU:HG	2.11	0.51
1:C:201:LEU:HD22	1:C:203:TYR:CE1	2.45	0.51
1:A:3:TRP:CG	1:A:4:PRO:HD2	2.46	0.51
1:A:189:ASN:HB3	1:A:192:PHE:HB2	1.91	0.51
1:C:113:LYS:HG3	3:C:686:HOH:O	2.10	0.51
1:A:216:LYS:HE2	1:A:218:MET:HE2	1.91	0.51
1:C:131:LYS:HE3	1:C:167:ASP:HA	1.92	0.50
1:C:42:LYS:HG3	1:C:43:HIS:N	2.25	0.50
1:D:248:GLY:O	1:D:279:PRO:HD2	2.11	0.50
1:B:53:ARG:HG3	3:B:601:HOH:O	2.10	0.50
1:B:160:VAL:HG21	1:B:194:ILE:HG21	1.93	0.50
1:D:189:ASN:HB3	1:D:192:PHE:HB2	1.94	0.50
1:C:124:ARG:NH1	3:C:662:HOH:O	2.44	0.50
1:A:177:GLU:HG3	1:A:178:ARG:N	2.26	0.50
1:A:189:ASN:HB3	1:A:192:PHE:CB	2.41	0.50
1:D:189:ASN:HB3	1:D:192:PHE:CB	2.42	0.49
1:B:247:LYS:HD3	1:B:321:ILE:HB	1.94	0.49
1:B:257:ASP:OD1	1:B:293:LYS:HD2	2.12	0.49
1:D:282:TYR:OH	1:D:306:GLN:HG2	2.12	0.49
1:C:46:TYR:O	1:C:50:GLN:HG2	2.13	0.49
1:C:168:ASP:OD1	1:C:169:GLN:HG2	2.13	0.48
1:A:311:ARG:CZ	1:A:311:ARG:HB2	2.43	0.48
1:A:186:PRO:HD2	3:A:743:HOH:O	2.13	0.48
1:D:28:THR:HA	1:D:29:PRO:C	2.34	0.48
1:D:3:TRP:CG	1:D:4:PRO:HD2	2.49	0.47
1:A:212:ASP:O	3:A:550:HOH:O	2.20	0.47
1:B:186:PRO:O	1:B:190:ALA:HB2	2.14	0.47
1:C:242:GLN:HG2	1:C:324:THR:O	2.14	0.47
1:D:117:GLU:HG3	3:D:660:HOH:O	2.15	0.47
1:D:78:ARG:NH2	3:D:692:HOH:O	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:42:LYS:NZ	3:D:636:HOH:O	2.47	0.47
1:B:8:GLU:HB2	3:B:686:HOH:O	2.15	0.47
1:C:311:ARG:NH1	1:C:311:ARG:HG2	2.29	0.47
1:B:293:LYS:CD	3:B:658:HOH:O	2.57	0.47
1:D:19:SER:HB2	1:D:20:GLY:CA	2.45	0.47
1:D:235:ARG:HB3	1:D:236:PRO:HD3	1.96	0.47
1:D:142:MET:HB3	1:D:152:TRP:CH2	2.50	0.47
1:D:3:TRP:CD1	1:D:4:PRO:HD2	2.50	0.47
1:C:97:ASP:HA	1:C:140:ASP:HB3	1.97	0.46
1:C:78:ARG:NH1	3:C:665:HOH:O	2.46	0.46
1:C:117:GLU:OE2	3:C:645:HOH:O	2.21	0.46
1:B:311:ARG:HG2	1:B:311:ARG:NH1	2.30	0.46
1:A:45:LYS:NZ	1:A:49:ASP:OD2	2.48	0.46
1:B:218:MET:HB2	1:B:221:THR:OG1	2.16	0.46
1:C:64:VAL:HG13	1:C:77:ILE:HD11	1.97	0.45
1:D:15:GLY:HA2	1:D:52:ILE:HG23	1.99	0.45
1:C:64:VAL:HG11	1:C:126:LEU:HD21	1.99	0.45
1:A:3:TRP:CD1	1:A:4:PRO:HD2	2.52	0.45
1:B:19:SER:HB2	1:B:20:GLY:CA	2.46	0.45
1:B:97:ASP:HA	1:B:140:ASP:HB3	1.99	0.45
1:C:131:LYS:HE3	1:C:166:VAL:O	2.17	0.45
1:C:219:ALA:O	1:C:223:ARG:HG3	2.17	0.45
1:B:99:HIS:HA	1:B:143:ASN:HB3	1.99	0.44
1:A:3:TRP:CZ3	1:A:137:LEU:HD21	2.53	0.44
1:A:175:GLU:HG2	3:A:658:HOH:O	2.17	0.44
1:A:206:HIS:CG	1:A:252:GLU:HB2	2.52	0.44
1:C:297:GLU:CD	1:C:298:PRO:HD2	2.38	0.44
1:C:124:ARG:HE	1:C:162:ALA:HB1	1.81	0.44
1:C:233:ARG:O	1:C:236:PRO:HD2	2.18	0.44
1:D:93:LYS:HB3	1:D:137:LEU:HB2	1.98	0.44
1:A:97:ASP:OD1	1:A:143:ASN:HB2	2.17	0.44
1:B:279:PRO:HD3	1:B:321:ILE:HG23	2.00	0.44
1:A:241:LEU:CD1	1:A:248:GLY:HA3	2.48	0.44
1:C:324:THR:HA	1:C:325:PRO:HD3	1.90	0.44
1:D:188:VAL:HG23	1:D:189:ASN:CG	2.39	0.43
1:A:148:THR:O	1:A:149:VAL:HG23	2.18	0.43
1:B:103:ARG:NE	3:B:689:HOH:O	2.43	0.43
1:A:308:GLU:HA	1:A:311:ARG:HE	1.83	0.43
1:D:97:ASP:HA	1:D:140:ASP:HB3	2.00	0.43
1:D:40:GLU:HG3	1:D:42:LYS:HG2	1.99	0.43
1:A:235:ARG:N	1:A:236:PRO:CD	2.82	0.43
1:D:177:GLU:HG3	1:D:178:ARG:N	2.30	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:178:ARG:HG3	3:B:800:HOH:O	2.19	0.42
1:A:241:LEU:HD13	1:A:248:GLY:HA3	2.01	0.42
1:C:235:ARG:N	1:C:236:PRO:CD	2.81	0.42
1:C:269:LEU:O	1:C:273:LEU:HG	2.19	0.42
1:D:53:ARG:HA	1:D:92:GLN:HG2	2.01	0.42
1:A:127:ALA:HB3	1:A:166:VAL:HG21	2.01	0.42
1:C:174:ILE:HG13	1:C:201:LEU:HD21	2.01	0.42
1:B:142:MET:HB3	1:B:152:TRP:CH2	2.54	0.42
1:A:220:GLN:HG2	1:A:221:THR:HG23	2.02	0.42
1:D:105:HIS:HA	3:D:679:HOH:O	2.20	0.42
1:D:104:TYR:HB3	1:D:114:VAL:HG21	2.01	0.42
1:D:6:ASN:HB2	1:D:9:GLY:O	2.20	0.42
1:B:223:ARG:NH1	3:B:797:HOH:O	2.53	0.42
1:C:204:GLU:HA	1:C:249:PHE:O	2.20	0.42
1:C:78:ARG:NH2	3:C:765:HOH:O	2.52	0.42
1:B:3:TRP:CG	1:B:4:PRO:HD2	2.54	0.42
1:A:204:GLU:HA	1:A:249:PHE:O	2.20	0.42
1:B:283:TRP:HA	1:B:284:ALA:HB2	2.01	0.42
1:C:131:LYS:CE	1:C:167:ASP:HA	2.50	0.42
1:A:310:MET:HB3	1:A:310:MET:HE2	1.67	0.41
1:D:199:ASP:HA	3:D:538:HOH:O	2.20	0.41
1:D:296:ILE:HD11	1:D:307:MET:HA	2.03	0.41
1:A:266:MET:HG2	1:A:309:LEU:CD2	2.50	0.41
1:B:54:LEU:O	1:B:55:ILE:HD13	2.20	0.41
1:B:82:LYS:HD3	3:B:584:HOH:O	2.21	0.41
1:A:19:SER:HB2	1:A:20:GLY:CA	2.51	0.41
1:B:237:PHE:CZ	1:B:241:LEU:HD11	2.56	0.41
1:B:229:ILE:HA	1:B:229:ILE:HD12	1.94	0.41
1:C:193:LEU:HD21	1:D:33:GLY:HA3	2.03	0.41
1:C:157:GLN:HG2	1:D:40:GLU:OE2	2.21	0.41
1:B:127:ALA:O	1:B:131:LYS:HB2	2.21	0.41
1:C:237:PHE:CZ	1:C:241:LEU:HD11	2.56	0.41
1:D:50:GLN:HG3	1:D:307:MET:HE3	2.02	0.41
1:A:65:GLN:HG2	1:A:67:SER:O	2.20	0.41
1:B:204:GLU:HA	1:B:249:PHE:O	2.20	0.41
1:B:223:ARG:HB2	1:B:223:ARG:HE	1.70	0.41
1:D:125:LYS:O	1:D:129:ARG:CG	2.68	0.40
1:A:138:GLY:HA2	1:A:170:THR:HG22	2.03	0.40
1:B:75:ASP:OD2	3:B:725:HOH:O	2.22	0.40
1:C:196:ASP:CB	1:C:201:LEU:HD12	2.52	0.40
1:C:19:SER:HB2	1:C:20:GLY:CA	2.51	0.40
1:C:93:LYS:HB3	1:C:137:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:302:LYS:N	3:C:703:HOH:O	2.54	0.40
1:D:120:ALA:HB1	1:D:162:ALA:HB2	2.03	0.40
1:A:235:ARG:HB3	1:A:236:PRO:HD3	2.04	0.40
1:B:93:LYS:HB3	1:B:137:LEU:HB2	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:776:HOH:O	3:D:748:HOH:O[1_565]	2.03	0.17
3:C:765:HOH:O	3:D:780:HOH:O[1_565]	2.07	0.13
3:B:586:HOH:O	3:B:608:HOH:O[2_557]	2.19	0.01

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	320/330 (97%)	317 (99%)	3 (1%)	0	100	100
1	B	326/330 (99%)	321 (98%)	5 (2%)	0	100	100
1	C	317/330 (96%)	311 (98%)	6 (2%)	0	100	100
1	D	315/330 (96%)	312 (99%)	3 (1%)	0	100	100
All	All	1278/1320 (97%)	1261 (99%)	17 (1%)	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	261/267 (98%)	258 (99%)	3 (1%)	84	63
1	B	266/267 (100%)	263 (99%)	3 (1%)	84	63
1	C	262/267 (98%)	259 (99%)	3 (1%)	84	63
1	D	259/267 (97%)	257 (99%)	2 (1%)	89	74
All	All	1048/1068 (98%)	1037 (99%)	11 (1%)	85	66

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	VAL
1	A	178	ARG
1	A	180	SER
1	B	97	ASP
1	B	178	ARG
1	B	221	THR
1	C	42	LYS
1	C	178	ARG
1	C	180	SER
1	D	129	ARG
1	D	178	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

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	322/330 (97%)	0.68	8 (2%) 54 59	6, 11, 18, 25	0
1	B	328/330 (99%)	0.80	16 (4%) 28 29	6, 11, 18, 24	0
1	C	321/330 (97%)	0.87	20 (6%) 20 21	6, 12, 20, 26	0
1	D	319/330 (96%)	0.87	19 (5%) 21 22	5, 12, 19, 28	0
All	All	1290/1320 (97%)	0.81	63 (4%) 28 29	5, 11, 19, 28	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	LEU	5.6
1	B	329	ALA	5.2
1	D	74	PHE	4.2
1	C	225	ILE	3.8
1	B	328	ILE	3.8
1	D	72	LEU	3.6
1	C	201	LEU	3.2
1	A	201	LEU	3.0
1	C	151	LEU	3.0
1	D	71	GLY	2.9
1	C	179	TRP	2.9
1	C	224	ASN	2.9
1	B	179	TRP	2.8
1	C	150	GLY	2.8
1	B	74	PHE	2.7
1	C	315	ALA	2.7
1	C	5	VAL	2.7
1	B	223	ARG	2.6
1	D	298	PRO	2.6
1	D	64	VAL	2.6
1	B	11	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	324	THR	2.6
1	C	126	LEU	2.5
1	B	169	GLN	2.5
1	A	7	ASP	2.5
1	C	187	LEU	2.5
1	B	330	ASP	2.4
1	D	130	PHE	2.4
1	C	259	LEU	2.4
1	D	166	VAL	2.4
1	D	51	GLY	2.3
1	C	113	LYS	2.3
1	C	270	LEU	2.3
1	D	193	LEU	2.3
1	A	74	PHE	2.3
1	A	2	ASP	2.3
1	C	131	LYS	2.3
1	A	200	ARG	2.2
1	D	37	PHE	2.2
1	D	223	ARG	2.2
1	B	68	LEU	2.2
1	A	224	ASN	2.2
1	D	150	GLY	2.2
1	D	61	TRP	2.2
1	A	300	ASN	2.2
1	C	27	ILE	2.2
1	D	308	GLU	2.1
1	D	123	TRP	2.1
1	D	303	ASP	2.1
1	B	183	TYR	2.1
1	D	126	LEU	2.1
1	C	149	VAL	2.1
1	B	130	PHE	2.1
1	B	309	LEU	2.1
1	C	294	LEU	2.1
1	B	221	THR	2.1
1	B	225	ILE	2.1
1	B	321	ILE	2.1
1	C	223	ARG	2.1
1	A	309	LEU	2.1
1	C	110	GLY	2.0
1	D	192	PHE	2.0
1	C	130	PHE	2.0

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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	TRS	A	401	8/8	0.21	9.29	8,16,24,29	0
2	TRS	C	401	8/8	0.14	0.89	8,12,15,19	0
2	TRS	B	401	8/8	0.14	0.77	8,12,16,18	0
2	TRS	D	401	8/8	0.12	0.04	9,12,15,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.