



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2025 – 06:11 PM JST

PDB ID : 9VDG / pdb_00009vdg
Title : Structure of a truncated loopB mutant from the human gut flora K. grimontii
Apg
Authors : Zhou, J.H.; Huang, J.Y.
Deposited on : 2025-06-08
Resolution : 2.67 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 Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

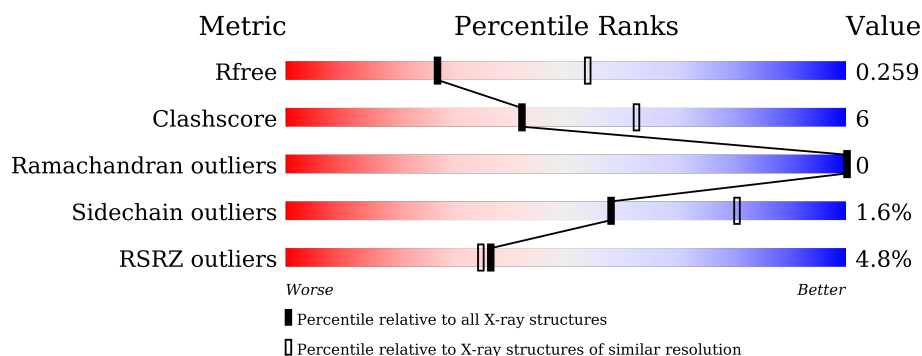
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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}	164625	4708 (2.70-2.66)
Clashscore	180529	5138 (2.70-2.66)
Ramachandran outliers	177936	5071 (2.70-2.66)
Sidechain outliers	177891	5071 (2.70-2.66)
RSRZ outliers	164620	4708 (2.70-2.66)

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	559	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>11%</div> <div>18%</div> </div> </div>
1	B	559	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>14%</div> <div>18%</div> </div> </div>
1	C	559	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>13%</div> <div>17%</div> </div> </div>
1	D	559	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>11%</div> <div>18%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14849 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 APG-truncated loopB.

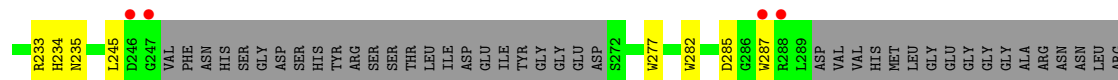
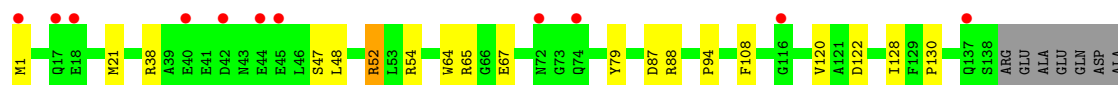
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3646	2350	640	642	14			
1	B	458	Total	C	N	O	S	0	0	0
			3616	2333	632	638	13			
1	C	463	Total	C	N	O	S	0	0	0
			3663	2361	641	647	14			
1	D	461	Total	C	N	O	S	0	0	0
			3612	2333	626	640	13			

- Molecule 2 is water.

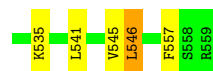
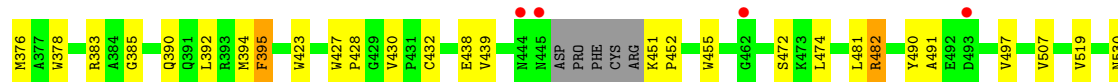
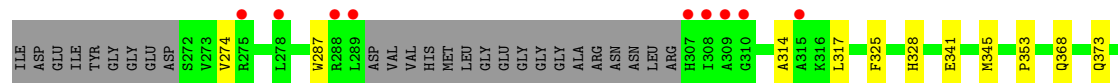
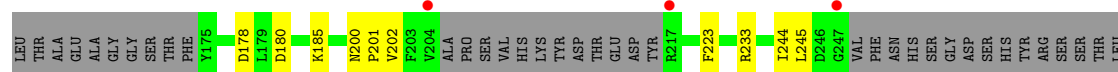
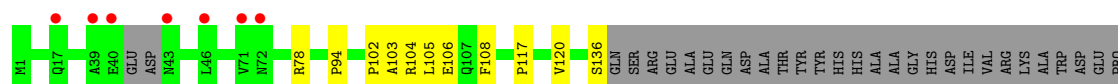
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	75	Total	O	0	0
			75	75		
2	B	76	Total	O	0	0
			76	76		
2	C	92	Total	O	0	0
			92	92		
2	D	69	Total	O	0	0
			69	69		



- Molecule 1: APG-truncated loopB



- Molecule 1: APG-truncated loopB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.36Å 70.89Å 130.30Å 92.54° 100.14° 90.08°	Depositor
Resolution (Å)	48.62 – 2.67 48.62 – 2.67	Depositor EDS
% Data completeness (in resolution range)	90.9 (48.62-2.67) 90.8 (48.62-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.239 , 0.269 0.232 , 0.259	Depositor DCC
R_{free} test set	2787 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -h,k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14849	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.87% 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	0.26	0/3748	0.52	0/5101
1	B	0.30	0/3717	0.57	0/5062
1	C	0.28	0/3766	0.55	0/5125
1	D	0.26	0/3713	0.52	0/5060
All	All	0.28	0/14944	0.54	0/20348

There are no bond length outliers.

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	3646	0	3495	41	0
1	B	3616	0	3463	51	0
1	C	3663	0	3518	50	0
1	D	3612	0	3438	38	0
2	A	75	0	0	5	0
2	B	76	0	0	3	0
2	C	92	0	0	5	0
2	D	69	0	0	3	0
All	All	14849	0	13914	175	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 6.

All (175) 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:49:PRO:HB2	1:C:459:LEU:HD21	1.53	0.90
1:D:103:ALA:HB3	1:D:106:GLU:HG2	1.66	0.77
1:B:13:ILE:HG23	1:B:20:LEU:HD11	1.66	0.77
1:A:102:PRO:O	1:B:348:ARG:NH2	2.20	0.74
1:C:122:ASP:OD1	1:C:482:ARG:NH1	2.20	0.73
1:A:183:SER:OG	1:A:235:ASN:ND2	2.23	0.72
1:B:103:ALA:HB3	1:B:106:GLU:HG2	1.74	0.69
1:B:274:VAL:HG21	1:B:311:ILE:HG23	1.73	0.69
1:B:217:ARG:HH22	1:B:247:GLY:HA2	1.58	0.68
1:D:368:GLN:NE2	2:D:604:HOH:O	2.29	0.65
1:C:368:GLN:NE2	2:C:607:HOH:O	2.29	0.65
1:D:541:LEU:HD13	1:D:546:LEU:HD13	1.80	0.64
1:C:38:ARG:NH1	1:C:47:SER:OG	2.30	0.64
1:B:546:LEU:HG	1:B:548:LEU:HD21	1.80	0.64
1:A:505:GLN:NE2	2:A:601:HOH:O	2.22	0.62
1:A:49:PRO:CB	1:C:459:LEU:HD21	2.29	0.61
1:C:21:MET:HE3	1:C:65:ARG:HD3	1.82	0.61
1:A:120:VAL:HG12	1:A:430:VAL:HG11	1.83	0.60
1:D:373:GLN:HG3	1:D:491:ALA:O	2.02	0.59
1:A:348:ARG:NH2	1:B:102:PRO:O	2.36	0.58
1:A:202:VAL:HG21	1:A:245:LEU:HD22	1.85	0.58
1:A:180:ASP:OD2	1:A:231:ARG:NH2	2.35	0.58
1:D:274:VAL:HG13	1:D:287:TRP:CD1	2.39	0.58
1:C:130:PRO:HD2	1:C:201:PRO:HD2	1.87	0.57
1:C:348:ARG:NH2	1:D:102:PRO:O	2.37	0.57
1:C:345:MET:HA	1:C:395:PHE:HB3	1.86	0.57
1:D:202:VAL:HG21	1:D:245:LEU:HD22	1.86	0.57
1:C:230:LEU:HG	1:C:234:HIS:CE1	2.40	0.56
1:C:376:MET:HE1	1:C:423:TRP:HZ2	1.71	0.56
1:A:244:ILE:HG21	1:A:325:PHE:HE1	1.70	0.55
1:B:120:VAL:HG12	1:B:430:VAL:HG11	1.87	0.55
1:C:87:ASP:OD1	1:C:88:ARG:NH1	2.39	0.55
1:B:408:SER:OG	1:B:442:ASP:HB2	2.07	0.55
1:A:345:MET:HA	1:A:395:PHE:HB3	1.89	0.54
1:A:200:ASN:HD21	1:A:288:ARG:HH21	1.56	0.54
1:B:345:MET:HA	1:B:397:GLN:HE22	1.73	0.54
1:D:314:ALA:HA	1:D:317:LEU:HD12	1.89	0.54
1:A:407:LYS:HG3	1:A:417:LEU:HD22	1.91	0.53
1:B:8:PRO:HA	1:B:13:ILE:HD13	1.90	0.52
1:B:373:GLN:HG3	1:B:491:ALA:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:MET:HA	1:D:395:PHE:HB3	1.90	0.52
1:B:217:ARG:HD3	1:B:273:VAL:HG11	1.91	0.52
1:B:275:ARG:HE	1:B:318:GLU:HB2	1.73	0.52
1:B:346:ASN:ND2	2:B:607:HOH:O	2.42	0.52
1:C:233:ARG:NH2	1:C:285:ASP:OD2	2.41	0.52
1:A:412:LYS:HG2	2:A:643:HOH:O	2.09	0.52
1:B:413:ASP:HB3	1:B:416:ARG:HD2	1.92	0.52
1:C:413:ASP:HB3	1:C:416:ARG:HD2	1.92	0.52
1:A:105:LEU:O	1:A:385:GLY:HA2	2.10	0.52
1:D:383:ARG:HD2	1:D:427:TRP:CZ2	2.45	0.51
1:A:277:TRP:HB2	1:A:287:TRP:CZ2	2.46	0.51
1:B:353:PRO:HG3	1:B:378:TRP:CE2	2.45	0.51
1:C:490:TYR:HB3	1:C:497:VAL:HB	1.93	0.51
1:A:19:ARG:NH1	1:A:67:GLU:OE2	2.44	0.51
1:B:417:LEU:HB3	1:B:418:PRO:HD3	1.93	0.51
1:C:185:LYS:HE3	1:C:455:TRP:CZ3	2.46	0.51
1:C:202:VAL:HG21	1:C:245:LEU:HD22	1.92	0.50
1:B:481:LEU:HD21	1:B:507:VAL:HG11	1.93	0.50
1:D:104:ARG:NH2	2:D:605:HOH:O	2.31	0.50
1:B:103:ALA:HB3	1:B:106:GLU:CG	2.41	0.49
1:B:192:LEU:HD11	1:B:468:TYR:HB3	1.94	0.49
1:B:343:SER:OG	1:B:344:ALA:N	2.45	0.49
1:A:275:ARG:HG2	1:A:318:GLU:HB2	1.95	0.49
1:C:373:GLN:HG3	1:C:491:ALA:O	2.12	0.49
1:A:21:MET:HE3	1:A:65:ARG:HD3	1.93	0.49
1:C:120:VAL:HG12	1:C:430:VAL:HG11	1.94	0.49
1:D:103:ALA:HB3	1:D:106:GLU:CG	2.40	0.49
1:D:376:MET:HE1	1:D:423:TRP:HZ2	1.78	0.49
1:C:183:SER:OG	1:C:235:ASN:OD1	2.31	0.49
1:D:432:CYS:O	2:D:601:HOH:O	2.20	0.48
1:C:52:ARG:HG3	1:C:64:TRP:CZ2	2.48	0.48
1:B:217:ARG:HH22	1:B:247:GLY:CA	2.26	0.47
1:D:136:SER:HB3	1:D:180:ASP:HB2	1.96	0.47
1:B:38:ARG:NH1	1:B:47:SER:OG	2.48	0.47
1:C:416:ARG:O	1:C:419:LEU:HB2	2.14	0.47
1:D:120:VAL:HG12	1:D:430:VAL:HG11	1.97	0.47
1:A:368:GLN:NE2	2:A:622:HOH:O	2.47	0.47
1:D:178:ASP:HB2	1:D:223:PHE:O	2.14	0.47
1:C:482:ARG:NH1	1:C:483:TYR:OH	2.48	0.47
1:D:105:LEU:O	1:D:385:GLY:HA2	2.15	0.47
1:D:392:LEU:HD22	1:D:482:ARG:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ASN:ND2	2:B:609:HOH:O	2.48	0.47
1:B:416:ARG:O	1:B:419:LEU:HB2	2.15	0.47
1:C:481:LEU:HD21	1:C:507:VAL:HG11	1.97	0.47
1:B:376:MET:HE1	1:B:423:TRP:CZ2	2.50	0.46
1:C:376:MET:HE1	1:C:423:TRP:CZ2	2.49	0.46
1:D:427:TRP:CD2	1:D:428:PRO:HD2	2.49	0.46
1:D:353:PRO:HG3	1:D:378:TRP:CE2	2.51	0.46
1:A:197:LEU:HB2	1:A:243:LEU:HD12	1.98	0.46
1:C:417:LEU:HB3	1:C:418:PRO:HD3	1.98	0.46
1:C:48:LEU:HD13	1:C:67:GLU:O	2.16	0.46
1:B:328:HIS:HE2	1:B:341:GLU:CD	2.22	0.46
1:A:180:ASP:CG	1:A:231:ARG:HH21	2.23	0.46
1:C:54:ARG:NH1	2:C:603:HOH:O	2.26	0.46
1:D:185:LYS:HE3	1:D:455:TRP:CE2	2.51	0.46
1:C:523:ASP:N	2:C:601:HOH:O	2.20	0.46
1:D:427:TRP:CG	1:D:428:PRO:HD2	2.51	0.46
1:A:353:PRO:HG3	1:A:378:TRP:CE2	2.51	0.45
1:B:345:MET:HA	1:B:395:PHE:HB3	1.98	0.45
1:D:328:HIS:NE2	1:D:341:GLU:OE2	2.31	0.45
1:A:312:THR:OG1	1:A:340:VAL:O	2.25	0.45
1:D:481:LEU:HD21	1:D:507:VAL:HG11	1.99	0.45
1:C:233:ARG:HG2	1:C:282:TRP:O	2.17	0.45
1:C:128:ILE:HG21	1:C:182:ILE:HD11	1.99	0.45
1:B:131:ASP:OD2	1:B:175:TYR:N	2.50	0.45
1:B:438:GLU:HG2	1:B:439:VAL:HG13	1.97	0.45
1:A:490:TYR:HB3	1:A:497:VAL:HB	1.98	0.45
1:C:346:ASN:ND2	2:C:632:HOH:O	2.50	0.45
1:B:540:ALA:HB3	1:B:547:THR:HB	1.99	0.45
1:A:413:ASP:HB3	1:A:416:ARG:HD2	2.00	0.45
1:C:233:ARG:NH2	2:C:633:HOH:O	2.50	0.45
1:B:527:LEU:HD22	1:B:532:TRP:CZ2	2.53	0.44
1:D:390:GLN:O	1:D:394:MET:HG2	2.17	0.44
1:C:380:ASP:OD1	1:C:383:ARG:NH1	2.45	0.44
1:B:380:ASP:OD1	1:B:383:ARG:NH1	2.51	0.44
1:B:530:ASN:ND2	1:B:559:ARG:O	2.50	0.44
1:A:288:ARG:HD2	1:A:288:ARG:C	2.43	0.44
1:D:200:ASN:HA	1:D:201:PRO:HA	1.87	0.44
1:B:419:LEU:HD11	1:B:551:ILE:C	2.42	0.44
1:B:426:SER:O	1:B:500:ARG:NH1	2.45	0.44
1:C:277:TRP:HB2	1:C:287:TRP:HZ2	1.83	0.44
1:B:229:LEU:HD21	1:B:245:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:PRO:HG3	1:C:108:PHE:CD1	2.53	0.43
1:D:490:TYR:HB3	1:D:497:VAL:HB	1.99	0.43
1:A:237:GLN:NE2	2:A:613:HOH:O	2.37	0.43
1:C:312:THR:O	1:C:316:LYS:HG2	2.18	0.43
1:B:95:GLN:NE2	1:B:106:GLU:OE1	2.51	0.43
1:C:326:GLY:HA3	1:C:341:GLU:OE2	2.18	0.43
1:A:506:ARG:HB2	1:A:558:SER:HB3	1.99	0.43
1:C:277:TRP:HB2	1:C:287:TRP:CZ2	2.54	0.43
1:B:395:PHE:O	1:B:397:GLN:NE2	2.51	0.43
1:B:490:TYR:HB3	1:B:497:VAL:HB	2.01	0.43
1:A:122:ASP:CG	1:A:483:TYR:HH	2.25	0.43
1:A:546:LEU:HD23	1:A:546:LEU:HA	1.91	0.43
2:A:622:HOH:O	1:B:100:PHE:HA	2.17	0.43
1:B:202:VAL:HG21	1:B:245:LEU:HD22	2.01	0.43
1:A:390:GLN:O	1:A:394:MET:HG2	2.19	0.43
1:B:244:ILE:HG21	1:B:325:PHE:HE1	1.84	0.43
1:B:376:MET:HE1	1:B:423:TRP:HZ2	1.84	0.43
1:A:417:LEU:HB3	1:A:418:PRO:HD3	2.01	0.42
1:D:94:PRO:HG3	1:D:108:PHE:CD1	2.54	0.42
1:D:438:GLU:HG2	1:D:439:VAL:HG13	2.00	0.42
1:C:355:TRP:HH2	1:C:403:THR:HB	1.84	0.42
1:D:535:LYS:HG3	1:D:557:PHE:CD1	2.54	0.42
1:B:232:LEU:HD12	1:B:232:LEU:HA	1.75	0.42
1:C:38:ARG:O	1:C:79:TYR:HA	2.19	0.42
1:D:244:ILE:HG21	1:D:325:PHE:HE1	1.85	0.42
1:A:187:PRO:O	1:A:191:GLN:HG3	2.19	0.42
1:A:226:ASP:HB3	1:A:282:TRP:HH2	1.85	0.42
1:C:459:LEU:HA	1:C:459:LEU:HD23	1.83	0.42
1:C:380:ASP:HA	1:C:383:ARG:HD3	2.02	0.42
1:C:52:ARG:HG3	1:C:64:TRP:CE2	2.54	0.41
1:B:217:ARG:HH11	1:B:273:VAL:HG11	1.85	0.41
1:D:117:PRO:HB2	1:D:120:VAL:HG23	2.02	0.41
1:A:128:ILE:HG21	1:A:182:ILE:HD11	2.02	0.41
1:B:329:PHE:HZ	1:B:402:ASP:HB2	1.85	0.41
1:A:85:TRP:HZ3	1:A:90:LEU:HB2	1.84	0.41
1:C:438:GLU:HG2	1:C:439:VAL:HG13	2.01	0.41
1:C:535:LYS:HG3	1:C:557:PHE:CD1	2.55	0.41
1:C:347:TYR:HA	1:C:351:THR:HB	2.02	0.41
1:C:427:TRP:CD2	1:C:428:PRO:HD2	2.55	0.41
1:B:383:ARG:HG3	2:B:650:HOH:O	2.20	0.41
1:D:233:ARG:HA	1:D:233:ARG:HD2	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:HIS:HE2	1:D:341:GLU:CD	2.22	0.41
1:B:520:VAL:HA	1:B:544:GLY:O	2.21	0.41
1:C:474:LEU:HD23	1:C:474:LEU:HA	1.93	0.40
1:D:376:MET:HE1	1:D:423:TRP:CZ2	2.56	0.40
1:C:179:LEU:HG	1:C:223:PHE:HB3	2.04	0.40
1:D:474:LEU:HA	1:D:474:LEU:HD23	1.84	0.40
1:A:117:PRO:HB2	1:A:120:VAL:HG23	2.03	0.40
1:A:200:ASN:ND2	1:A:288:ARG:HH21	2.18	0.40
1:A:312:THR:O	1:A:316:LYS:HD2	2.22	0.40
1:A:481:LEU:HD23	1:A:481:LEU:HA	1.91	0.40
1:B:407:LYS:HG3	1:B:417:LEU:HD22	2.04	0.40
1:D:451:LYS:HA	1:D:452:PRO:HD3	1.96	0.40

There are no symmetry-related clashes.

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	447/559 (80%)	427 (96%)	20 (4%)	0	100	100
1	B	444/559 (79%)	427 (96%)	17 (4%)	0	100	100
1	C	451/559 (81%)	430 (95%)	21 (5%)	0	100	100
1	D	447/559 (80%)	428 (96%)	19 (4%)	0	100	100
All	All	1789/2236 (80%)	1712 (96%)	77 (4%)	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	368/469 (78%)	362 (98%)	6 (2%)	58	80
1	B	365/469 (78%)	361 (99%)	4 (1%)	70	86
1	C	371/469 (79%)	365 (98%)	6 (2%)	58	80
1	D	361/469 (77%)	353 (98%)	8 (2%)	47	73
All	All	1465/1876 (78%)	1441 (98%)	24 (2%)	58	80

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	316	LYS
1	A	395	PHE
1	A	518	GLU
1	A	519	VAL
1	A	545	VAL
1	B	13	ILE
1	B	78	ARG
1	B	96	GLU
1	B	519	VAL
1	C	1	MET
1	C	52	ARG
1	C	368	GLN
1	C	430	VAL
1	C	519	VAL
1	C	545	VAL
1	D	78	ARG
1	D	395	PHE
1	D	472	SER
1	D	482	ARG
1	D	519	VAL
1	D	530	ASN
1	D	545	VAL
1	D	546	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	A	200	ASN
1	A	234	HIS
1	A	235	ASN
1	A	381	ASN
1	A	397	GLN
1	A	530	ASN
1	B	16	GLN
1	B	89	GLN
1	B	95	GLN
1	B	381	ASN
1	B	397	GLN
1	C	55	GLN
1	C	107	GLN
1	C	381	ASN
1	C	479	GLN
1	C	487	GLN
1	D	89	GLN
1	D	107	GLN
1	D	381	ASN
1	D	397	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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, 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	461/559 (82%)	0.33	24 (5%) 34 32	14, 26, 43, 64	0
1	B	458/559 (81%)	0.39	17 (3%) 45 44	14, 24, 46, 57	0
1	C	463/559 (82%)	0.38	24 (5%) 34 32	13, 23, 46, 66	0
1	D	461/559 (82%)	0.39	23 (4%) 35 33	15, 27, 46, 68	0
All	All	1843/2236 (82%)	0.37	88 (4%) 36 35	13, 25, 46, 68	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	ILE	4.7
1	D	307	HIS	4.0
1	A	43	ASN	3.9
1	A	204	VAL	3.8
1	C	17	GLN	3.8
1	A	289	LEU	3.8
1	B	247	GLY	3.7
1	A	17	GLN	3.7
1	C	137	GLN	3.4
1	A	217	ARG	3.4
1	D	46	LEU	3.3
1	A	307	HIS	3.2
1	D	289	LEU	3.2
1	B	365	TYR	3.2
1	B	308	ILE	3.1
1	A	327	GLU	3.1
1	D	43	ASN	3.1
1	C	74	GLN	3.1
1	C	40	GLU	3.0
1	A	72	ASN	3.0
1	C	247	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	452	PRO	3.0
1	D	278	LEU	3.0
1	C	288	ARG	3.0
1	D	72	ASN	3.0
1	A	310	GLY	3.0
1	B	44	GLU	2.9
1	B	17	GLN	2.9
1	C	307	HIS	2.9
1	B	444	ASN	2.7
1	A	247	GLY	2.7
1	D	217	ARG	2.7
1	D	40	GLU	2.7
1	D	17	GLN	2.7
1	C	287	TRP	2.7
1	A	309	ALA	2.6
1	D	309	ALA	2.6
1	B	443	GLY	2.6
1	D	308	ILE	2.6
1	B	451	LYS	2.6
1	D	39	ALA	2.6
1	C	542	HIS	2.6
1	C	200	ASN	2.5
1	A	40	GLU	2.5
1	C	246	ASP	2.5
1	C	116	GLY	2.5
1	D	444	ASN	2.4
1	D	71	VAL	2.4
1	B	72	ASN	2.4
1	C	530	ASN	2.4
1	C	522	GLU	2.4
1	D	288	ARG	2.4
1	A	1	MET	2.4
1	D	310	GLY	2.4
1	B	289	LEU	2.4
1	D	493	ASP	2.4
1	A	492	GLU	2.3
1	C	44	GLU	2.3
1	A	451	LYS	2.3
1	C	1	MET	2.3
1	D	275	ARG	2.3
1	B	273	VAL	2.3
1	C	72	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	287	TRP	2.3
1	A	444	ASN	2.3
1	A	543	ASP	2.3
1	B	521	ILE	2.3
1	C	18	GLU	2.2
1	C	42	ASP	2.2
1	A	401	HIS	2.2
1	A	443	GLY	2.2
1	B	272	SER	2.2
1	C	202	VAL	2.2
1	A	46	LEU	2.2
1	D	315	ALA	2.2
1	C	335	TRP	2.1
1	D	445	ASN	2.1
1	B	54	ARG	2.1
1	D	247	GLY	2.1
1	A	368	GLN	2.1
1	A	493	ASP	2.1
1	D	462	GLY	2.1
1	C	45	GLU	2.1
1	C	544	GLY	2.1
1	B	459	LEU	2.0
1	A	480	ALA	2.0
1	B	404	ALA	2.0
1	D	204	VAL	2.0

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.