



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 29, 2025 – 08:17 am BST

PDB ID : 9FI2 / pdb_00009fi2
Title : Bacteroides ovatus polysaccharide lyase family 38 (BoPL38) mutant N242A at pH 3.5
Authors : Tandrup, T.; Wilkens, C.
Deposited on : 2024-05-28
Resolution : 2.57 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	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

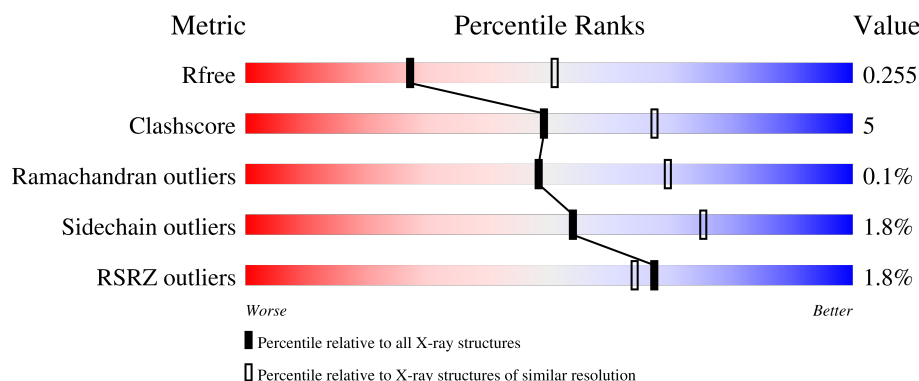
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (2.60-2.56)

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	404	 83% 12% 5%
1	B	404	 82% 12% 6%
1	C	404	 81% 12% 6%
1	D	404	 79% 15% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12301 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 Alginate lyase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	1	0
			3069	1964	518	574	13			
1	B	381	Total	C	N	O	S	0	0	0
			3058	1957	517	571	13			
1	C	381	Total	C	N	O	S	0	0	0
			3058	1957	517	571	13			
1	D	381	Total	C	N	O	S	0	0	0
			3058	1957	517	571	13			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A5M5BWR5
A	2	GLY	-	expression tag	UNP A0A5M5BWR5
A	3	SER	-	expression tag	UNP A0A5M5BWR5
A	4	SER	-	expression tag	UNP A0A5M5BWR5
A	5	HIS	-	expression tag	UNP A0A5M5BWR5
A	6	HIS	-	expression tag	UNP A0A5M5BWR5
A	7	HIS	-	expression tag	UNP A0A5M5BWR5
A	8	HIS	-	expression tag	UNP A0A5M5BWR5
A	9	HIS	-	expression tag	UNP A0A5M5BWR5
A	10	HIS	-	expression tag	UNP A0A5M5BWR5
A	11	SER	-	expression tag	UNP A0A5M5BWR5
A	12	SER	-	expression tag	UNP A0A5M5BWR5
A	13	GLY	-	expression tag	UNP A0A5M5BWR5
A	14	LEU	-	expression tag	UNP A0A5M5BWR5
A	15	VAL	-	expression tag	UNP A0A5M5BWR5
A	16	PRO	-	expression tag	UNP A0A5M5BWR5
A	17	ARG	-	expression tag	UNP A0A5M5BWR5
A	18	GLY	-	expression tag	UNP A0A5M5BWR5
A	19	SER	-	expression tag	UNP A0A5M5BWR5
A	20	HIS	-	expression tag	UNP A0A5M5BWR5
A	21	MET	-	expression tag	UNP A0A5M5BWR5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	-	expression tag	UNP A0A5M5BWR5
A	23	SER	-	expression tag	UNP A0A5M5BWR5
B	1	MET	-	initiating methionine	UNP A0A5M5BWR5
B	2	GLY	-	expression tag	UNP A0A5M5BWR5
B	3	SER	-	expression tag	UNP A0A5M5BWR5
B	4	SER	-	expression tag	UNP A0A5M5BWR5
B	5	HIS	-	expression tag	UNP A0A5M5BWR5
B	6	HIS	-	expression tag	UNP A0A5M5BWR5
B	7	HIS	-	expression tag	UNP A0A5M5BWR5
B	8	HIS	-	expression tag	UNP A0A5M5BWR5
B	9	HIS	-	expression tag	UNP A0A5M5BWR5
B	10	HIS	-	expression tag	UNP A0A5M5BWR5
B	11	SER	-	expression tag	UNP A0A5M5BWR5
B	12	SER	-	expression tag	UNP A0A5M5BWR5
B	13	GLY	-	expression tag	UNP A0A5M5BWR5
B	14	LEU	-	expression tag	UNP A0A5M5BWR5
B	15	VAL	-	expression tag	UNP A0A5M5BWR5
B	16	PRO	-	expression tag	UNP A0A5M5BWR5
B	17	ARG	-	expression tag	UNP A0A5M5BWR5
B	18	GLY	-	expression tag	UNP A0A5M5BWR5
B	19	SER	-	expression tag	UNP A0A5M5BWR5
B	20	HIS	-	expression tag	UNP A0A5M5BWR5
B	21	MET	-	expression tag	UNP A0A5M5BWR5
B	22	ALA	-	expression tag	UNP A0A5M5BWR5
B	23	SER	-	expression tag	UNP A0A5M5BWR5
C	1	MET	-	initiating methionine	UNP A0A5M5BWR5
C	2	GLY	-	expression tag	UNP A0A5M5BWR5
C	3	SER	-	expression tag	UNP A0A5M5BWR5
C	4	SER	-	expression tag	UNP A0A5M5BWR5
C	5	HIS	-	expression tag	UNP A0A5M5BWR5
C	6	HIS	-	expression tag	UNP A0A5M5BWR5
C	7	HIS	-	expression tag	UNP A0A5M5BWR5
C	8	HIS	-	expression tag	UNP A0A5M5BWR5
C	9	HIS	-	expression tag	UNP A0A5M5BWR5
C	10	HIS	-	expression tag	UNP A0A5M5BWR5
C	11	SER	-	expression tag	UNP A0A5M5BWR5
C	12	SER	-	expression tag	UNP A0A5M5BWR5
C	13	GLY	-	expression tag	UNP A0A5M5BWR5
C	14	LEU	-	expression tag	UNP A0A5M5BWR5
C	15	VAL	-	expression tag	UNP A0A5M5BWR5
C	16	PRO	-	expression tag	UNP A0A5M5BWR5
C	17	ARG	-	expression tag	UNP A0A5M5BWR5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	GLY	-	expression tag	UNP A0A5M5BWR5
C	19	SER	-	expression tag	UNP A0A5M5BWR5
C	20	HIS	-	expression tag	UNP A0A5M5BWR5
C	21	MET	-	expression tag	UNP A0A5M5BWR5
C	22	ALA	-	expression tag	UNP A0A5M5BWR5
C	23	SER	-	expression tag	UNP A0A5M5BWR5
D	1	MET	-	initiating methionine	UNP A0A5M5BWR5
D	2	GLY	-	expression tag	UNP A0A5M5BWR5
D	3	SER	-	expression tag	UNP A0A5M5BWR5
D	4	SER	-	expression tag	UNP A0A5M5BWR5
D	5	HIS	-	expression tag	UNP A0A5M5BWR5
D	6	HIS	-	expression tag	UNP A0A5M5BWR5
D	7	HIS	-	expression tag	UNP A0A5M5BWR5
D	8	HIS	-	expression tag	UNP A0A5M5BWR5
D	9	HIS	-	expression tag	UNP A0A5M5BWR5
D	10	HIS	-	expression tag	UNP A0A5M5BWR5
D	11	SER	-	expression tag	UNP A0A5M5BWR5
D	12	SER	-	expression tag	UNP A0A5M5BWR5
D	13	GLY	-	expression tag	UNP A0A5M5BWR5
D	14	LEU	-	expression tag	UNP A0A5M5BWR5
D	15	VAL	-	expression tag	UNP A0A5M5BWR5
D	16	PRO	-	expression tag	UNP A0A5M5BWR5
D	17	ARG	-	expression tag	UNP A0A5M5BWR5
D	18	GLY	-	expression tag	UNP A0A5M5BWR5
D	19	SER	-	expression tag	UNP A0A5M5BWR5
D	20	HIS	-	expression tag	UNP A0A5M5BWR5
D	21	MET	-	expression tag	UNP A0A5M5BWR5
D	22	ALA	-	expression tag	UNP A0A5M5BWR5
D	23	SER	-	expression tag	UNP A0A5M5BWR5

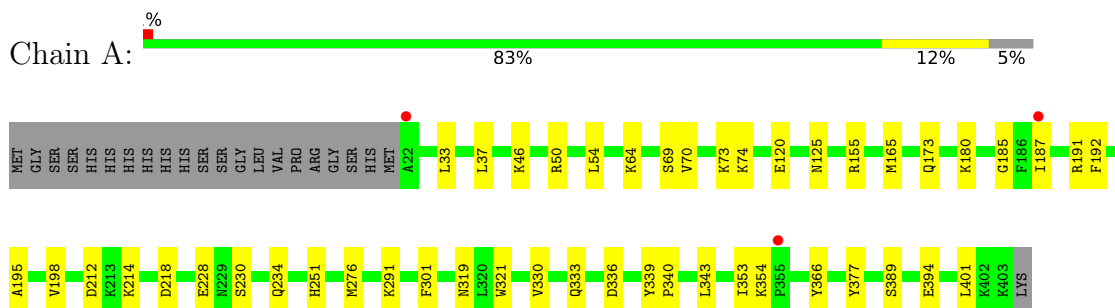
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	16	Total O 16 16	0	0
2	B	17	Total O 17 17	0	0
2	C	15	Total O 15 15	0	0
2	D	10	Total O 10 10	0	0

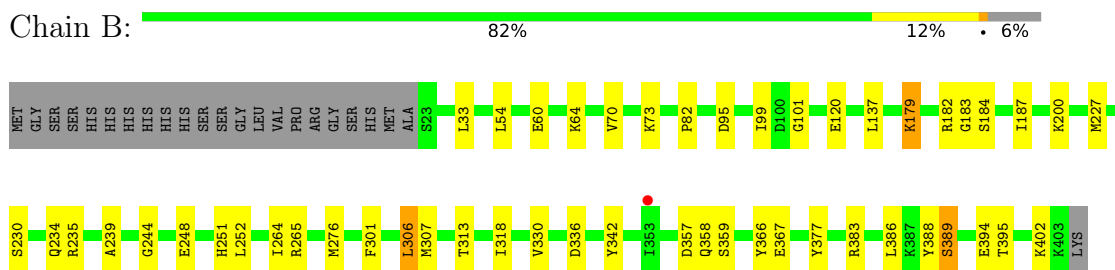
3 Residue-property plots [i](#)

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.

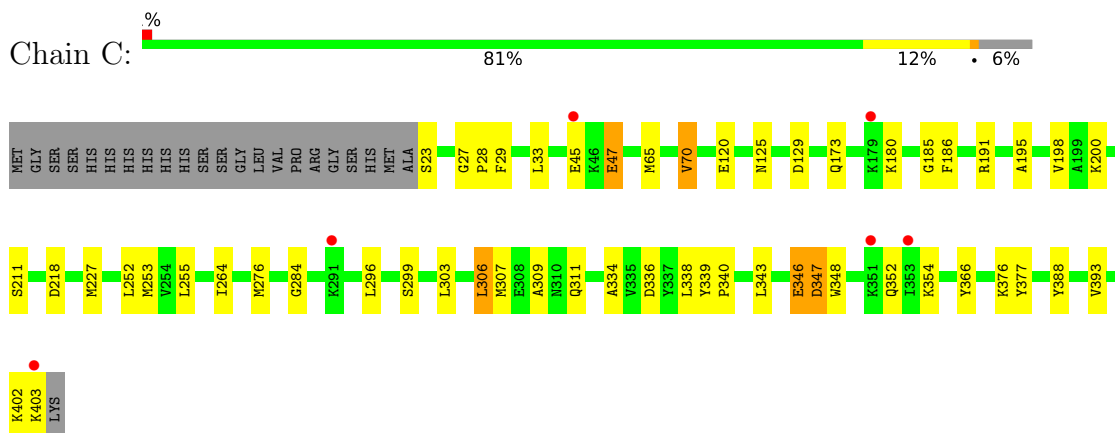
- Molecule 1: Alginate lyase family protein



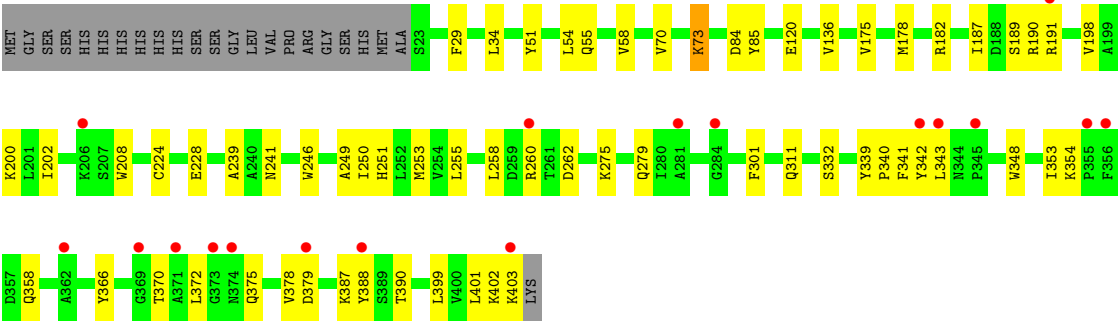
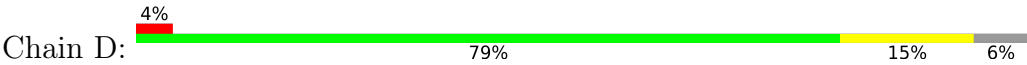
- Molecule 1: Alginate lyase family protein



- Molecule 1: Alginate lyase family protein



- Molecule 1: Alginate lyase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	198.57Å 89.15Å 147.48Å 90.00° 120.45° 90.00°	Depositor
Resolution (Å)	49.16 – 2.57 49.16 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.16-2.57) 99.1 (49.16-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.208 , 0.255 0.208 , 0.255	Depositor DCC
R_{free} test set	3610 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12301	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.56% 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	0.41	0/3150	0.57	0/4268
1	B	0.41	0/3136	0.57	0/4249
1	C	0.38	0/3136	0.56	0/4249
1	D	0.38	0/3136	0.54	0/4249
All	All	0.40	0/12558	0.56	0/17015

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	3069	0	3042	31	0
1	B	3058	0	3031	30	0
1	C	3058	0	3031	31	0
1	D	3058	0	3031	37	0
2	A	16	0	0	0	0
2	B	17	0	0	0	0
2	C	15	0	0	2	0
2	D	10	0	0	0	0
All	All	12301	0	12135	129	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 5.

All (129) 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:342:TYR:O	1:D:358:GLN:NE2	2.18	0.76
1:A:70:VAL:HG23	1:A:120:GLU:HG2	1.71	0.72
1:C:218:ASP:CG	2:C:501:HOH:O	2.32	0.71
1:C:125:ASN:HD22	1:C:191:ARG:HD3	1.53	0.71
1:C:218:ASP:OD2	2:C:501:HOH:O	2.11	0.68
1:B:276:MET:SD	1:B:306:LEU:HD13	2.35	0.67
1:A:340:PRO:HA	1:A:343:LEU:HD12	1.79	0.65
1:D:239:ALA:HB1	1:D:241:ASN:ND2	2.12	0.65
1:A:336:ASP:OD1	1:A:377:TYR:OH	2.14	0.64
1:D:366:TYR:HD1	1:D:401:LEU:HD21	1.61	0.64
1:A:339:TYR:CE2	1:A:343:LEU:HD11	2.35	0.61
1:B:336:ASP:OD1	1:B:377:TYR:OH	2.17	0.61
1:D:190:ARG:HD2	1:D:246:TRP:CZ3	2.37	0.60
1:B:60:GLU:HG3	1:B:64:LYS:HE3	1.83	0.60
1:B:342:TYR:O	1:B:358:GLN:NE2	2.30	0.59
1:B:54:LEU:HD21	1:B:389:SER:HA	1.86	0.58
1:B:388:TYR:HA	1:B:402:LYS:HB3	1.84	0.58
1:B:33:LEU:HD11	1:B:366:TYR:CE1	2.40	0.57
1:D:187:ILE:HD11	1:D:301:PHE:CZ	2.39	0.57
1:A:187:ILE:HD11	1:A:301:PHE:CE2	2.40	0.56
1:C:388:TYR:HA	1:C:402:LYS:HB3	1.86	0.56
1:A:330:VAL:HG23	1:A:333:GLN:HG3	1.86	0.56
1:A:187:ILE:HD11	1:A:301:PHE:HE2	1.70	0.56
1:D:187:ILE:HD11	1:D:301:PHE:CE2	2.40	0.56
1:C:186:PHE:CZ	1:C:227:MET:HE3	2.42	0.55
1:A:319:ASN:C	1:A:319:ASN:HD22	2.15	0.55
1:C:28:PRO:HB3	1:C:253:MET:HG2	1.88	0.54
1:C:252:LEU:HD22	1:C:264:ILE:HG23	1.89	0.54
1:D:258:LEU:HD13	1:D:260:ARG:HH21	1.72	0.54
1:C:129:ASP:HA	1:C:393:VAL:HG21	1.89	0.53
1:D:51:TYR:CD1	1:D:399:LEU:HD13	2.43	0.53
1:C:347:ASP:N	1:C:347:ASP:OD1	2.42	0.53
1:B:182:ARG:HG3	1:B:184:SER:H	1.73	0.52
1:C:299:SER:HB3	1:C:338:LEU:HD11	1.91	0.52
1:C:336:ASP:OD2	1:C:377:TYR:OH	2.27	0.52
1:D:375:GLN:NE2	1:D:379:ASP:OD2	2.44	0.51
1:A:70:VAL:CG2	1:A:120:GLU:HG2	2.41	0.51
1:A:319:ASN:HD22	1:A:321:TRP:H	1.60	0.50
1:A:228:GLU:OE2	1:A:251:HIS:NE2	2.41	0.50
1:D:275:LYS:O	1:D:279:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:TYR:CE1	1:D:343:LEU:HD11	2.48	0.49
1:C:340:PRO:HA	1:C:343:LEU:HD12	1.93	0.49
1:A:73:LYS:NZ	1:A:120:GLU:OE2	2.32	0.49
1:A:54:LEU:HD21	1:A:389:SER:HA	1.95	0.49
1:A:214:LYS:HE2	1:A:218:ASP:OD2	2.12	0.49
1:B:182:ARG:HH11	1:B:183:GLY:H	1.60	0.49
1:B:357:ASP:OD1	1:B:359:SER:OG	2.24	0.49
1:A:125:ASN:OD1	1:A:191:ARG:HD3	2.12	0.49
1:A:155:ARG:HE	1:A:212:ASP:CG	2.21	0.48
1:A:195:ALA:O	1:A:198:VAL:HG12	2.14	0.48
1:D:249:ALA:O	1:D:253:MET:HG3	2.13	0.48
1:B:276:MET:HA	1:B:276:MET:HE3	1.96	0.47
1:B:383:ARG:NH1	1:B:383:ARG:HB3	2.28	0.47
1:A:46:LYS:O	1:A:50:ARG:HG3	2.14	0.47
1:C:346:GLU:H	1:C:346:GLU:CD	2.21	0.46
1:D:34:LEU:HD11	1:D:136:VAL:HG13	1.97	0.46
1:A:394:GLU:OE1	1:A:394:GLU:N	2.37	0.46
1:A:125:ASN:CG	1:A:191:ARG:HD3	2.41	0.46
1:B:239:ALA:O	1:B:244:GLY:HA3	2.16	0.46
1:B:265:ARG:HG3	1:B:318:ILE:HD11	1.98	0.45
1:B:386:LEU:HD13	1:B:395:THR:HB	1.98	0.45
1:D:54:LEU:O	1:D:58:VAL:HG23	2.16	0.45
1:D:189:SER:HB2	1:D:250:ILE:HD13	1.98	0.45
1:B:70:VAL:HG23	1:B:120:GLU:HG2	1.98	0.45
1:D:387:LYS:O	1:D:390:THR:HG22	2.16	0.45
1:C:339:TYR:CE2	1:C:343:LEU:HD11	2.52	0.45
1:D:262:ASP:OD1	1:D:262:ASP:N	2.49	0.45
1:D:332:SER:OG	1:D:372:LEU:HD21	2.17	0.45
1:D:370:THR:HG23	1:D:378:VAL:HG21	1.99	0.45
1:C:339:TYR:CE2	1:C:376:LYS:HD3	2.52	0.45
1:B:230:SER:O	1:B:234:GLN:HG3	2.16	0.45
1:C:195:ALA:O	1:C:198:VAL:HG12	2.17	0.45
1:B:182:ARG:HH11	1:B:235:ARG:HD2	1.82	0.44
1:B:73:LYS:NZ	1:B:82:PRO:O	2.49	0.44
1:A:230:SER:O	1:A:234:GLN:HG3	2.17	0.44
1:D:29:PHE:O	1:D:311:GLN:HB3	2.17	0.44
1:D:51:TYR:O	1:D:55:GLN:HG2	2.17	0.44
1:B:227:MET:HE1	1:B:251:HIS:HA	1.99	0.44
1:C:27:GLY:HA3	1:C:29:PHE:CZ	2.53	0.44
1:D:341:PHE:CD2	1:D:348:TRP:HE3	2.35	0.44
1:B:33:LEU:HD11	1:B:366:TYR:HE1	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:GLN:HG3	1:C:354:LYS:O	2.18	0.44
1:D:354:LYS:HE2	1:D:354:LYS:HB3	1.80	0.44
1:D:202:ILE:HD12	1:D:208:TRP:HB2	1.99	0.43
1:D:403:LYS:HB3	1:D:403:LYS:HE3	1.73	0.43
1:B:95:ASP:O	1:B:101:GLY:HA2	2.17	0.43
1:D:388:TYR:HA	1:D:402:LYS:HB3	2.00	0.43
1:B:394:GLU:OE1	1:B:394:GLU:N	2.42	0.43
1:C:276:MET:SD	1:C:306:LEU:HD13	2.58	0.43
1:A:173:GLN:HB2	1:A:185:GLY:HA3	2.00	0.43
1:B:307:MET:SD	1:B:367:GLU:HG3	2.58	0.43
1:C:173:GLN:HB2	1:C:185:GLY:HA3	2.01	0.43
1:A:33:LEU:HD11	1:A:366:TYR:CE1	2.54	0.43
1:A:366:TYR:HB2	1:A:401:LEU:HD21	2.01	0.43
1:B:179:LYS:HE2	1:B:179:LYS:HB2	1.90	0.42
1:C:70:VAL:CG2	1:C:120:GLU:HG2	2.49	0.42
1:C:33:LEU:HD11	1:C:366:TYR:CE2	2.54	0.42
1:D:178:MET:SD	1:D:182:ARG:HD3	2.60	0.42
1:B:187:ILE:HD11	1:B:301:PHE:CE2	2.54	0.42
1:C:45:GLU:OE1	1:C:47:GLU:HB3	2.20	0.42
1:D:73:LYS:NZ	1:D:84:ASP:O	2.52	0.42
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.88	0.42
1:C:307:MET:O	1:C:311:GLN:HG3	2.20	0.42
1:D:251:HIS:O	1:D:255:LEU:HG	2.20	0.42
1:D:366:TYR:C	1:D:366:TYR:CD2	2.98	0.42
1:D:387:LYS:HD3	1:D:387:LYS:HA	1.78	0.42
1:B:252:LEU:HD22	1:B:264:ILE:HG23	2.02	0.42
1:C:252:LEU:HD12	1:C:309:ALA:HB1	2.02	0.42
1:D:85:TYR:OH	1:D:191:ARG:NH1	2.53	0.42
1:B:182:ARG:NH1	1:B:235:ARG:HD2	2.35	0.41
1:B:313:THR:HB	1:B:318:ILE:HB	2.02	0.41
1:C:65:MET:HE3	1:C:65:MET:HB2	1.91	0.41
1:C:303:LEU:HD23	1:C:303:LEU:HA	1.85	0.41
1:D:191:ARG:H	1:D:191:ARG:HG3	1.64	0.41
1:D:224:CYS:O	1:D:228:GLU:HG3	2.21	0.41
1:C:255:LEU:HD23	1:C:255:LEU:HA	1.90	0.41
1:A:276:MET:HE3	1:A:276:MET:HB3	1.96	0.41
1:A:74:LYS:HA	1:A:74:LYS:HD3	1.75	0.41
1:C:284:GLY:O	1:C:334:ALA:HA	2.20	0.41
1:C:296:LEU:HD13	1:C:348:TRP:CD2	2.55	0.41
1:A:165:MET:HE1	1:A:192:PHE:CZ	2.55	0.41
1:D:258:LEU:HD23	1:D:258:LEU:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LYS:HB2	1:A:180:LYS:HE3	1.98	0.40
1:A:353:ILE:O	1:A:354:LYS:HG3	2.21	0.40
1:C:403:LYS:HE2	1:C:403:LYS:HB3	1.83	0.40
1:D:70:VAL:HG23	1:D:120:GLU:HG2	2.03	0.40
1:D:339:TYR:HB3	1:D:340:PRO:HD3	2.02	0.40
1:A:319:ASN:ND2	1:A:321:TRP:H	2.20	0.40
1:B:248:GLU:HA	1:B:248:GLU:OE1	2.22	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	381/404 (94%)	368 (97%)	13 (3%)	0	100	100
1	B	379/404 (94%)	368 (97%)	11 (3%)	0	100	100
1	C	379/404 (94%)	367 (97%)	12 (3%)	0	100	100
1	D	379/404 (94%)	368 (97%)	10 (3%)	1 (0%)	37	57
All	All	1518/1616 (94%)	1471 (97%)	46 (3%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	353	ILE

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	325/344 (94%)	322 (99%)	3 (1%)	75	89
1	B	324/344 (94%)	317 (98%)	7 (2%)	47	70
1	C	324/344 (94%)	315 (97%)	9 (3%)	38	63
1	D	324/344 (94%)	320 (99%)	4 (1%)	67	84
All	All	1297/1376 (94%)	1274 (98%)	23 (2%)	54	75

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LYS
1	A	69	SER
1	A	291	LYS
1	B	99	ILE
1	B	137	LEU
1	B	179	LYS
1	B	200	LYS
1	B	306	LEU
1	B	330	VAL
1	B	389	SER
1	C	23	SER
1	C	47	GLU
1	C	70	VAL
1	C	180	LYS
1	C	200	LYS
1	C	211	SER
1	C	306	LEU
1	C	346	GLU
1	C	347	ASP
1	D	73	LYS
1	D	175	VAL
1	D	198	VAL
1	D	200	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	319	ASN

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Mol	Chain	Res	Type
1	A	358	GLN
1	B	288	GLN
1	C	125	ASN
1	C	153	HIS
1	C	243	HIS
1	D	232	GLN
1	D	241	ASN
1	D	288	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

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	382/404 (94%)	-0.04	3 (0%) 82 80	37, 56, 80, 115	1 (0%)
1	B	381/404 (94%)	-0.04	1 (0%) 90 89	38, 56, 81, 110	0
1	C	381/404 (94%)	0.09	6 (1%) 70 66	42, 59, 88, 110	0
1	D	381/404 (94%)	0.46	18 (4%) 37 33	39, 71, 107, 146	0
All	All	1525/1616 (94%)	0.12	28 (1%) 67 64	37, 59, 93, 146	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	353	ILE	4.0
1	D	403	LYS	3.4
1	C	353	ILE	3.3
1	D	343	LEU	3.2
1	D	371	ALA	3.2
1	A	22	ALA	3.1
1	D	342	TYR	3.1
1	D	281	ALA	3.0
1	D	260	ARG	2.9
1	D	369	GLY	2.7
1	D	355	PRO	2.6
1	C	45	GLU	2.6
1	D	356	PHE	2.6
1	C	351	LYS	2.5
1	D	345	PRO	2.5
1	D	379	ASP	2.4
1	D	373	GLY	2.2
1	D	206	LYS	2.2
1	C	291	LYS	2.2
1	D	388	TYR	2.1
1	D	191	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	284	GLY	2.1
1	A	355	PRO	2.1
1	C	403	LYS	2.1
1	D	362	ALA	2.1
1	C	179	LYS	2.1
1	A	187	ILE	2.1
1	D	374	ASN	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.