



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:52 PM UTC

PDB ID : 3C5M / pdb_00003c5m
Title : Crystal structure of oligogalacturonate lyase (VPA0088) from *Vibrio parahaemolyticus*. Northeast Structural Genomics Consortium Target VpR199
Authors : Forouhar, F.; Abashidze, M.; Seetharaman, J.; Janjua, H.; Mao, L.; Xiao, R.; Owens, L.A.; Wang, D.; Baran, M.C.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2008-01-31
Resolution : 2.60 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

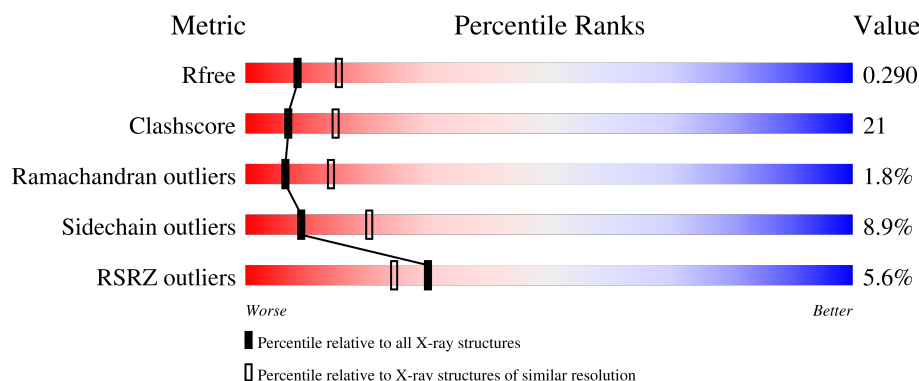
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	396	3% 54% 36% • 5%
1	B	396	9% 54% 36% 5% 5%
1	C	396	4% 55% 35% 5% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9292 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 Oligogalacturonate lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	Se	0	0	0
			3022	1919	494	593	9	7			
1	B	378	Total	C	N	O	S	Se	0	0	0
			3036	1929	496	595	9	7			
1	C	376	Total	C	N	O	S	Se	0	0	0
			3022	1919	494	593	9	7			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ILE	VAL	SEE REMARK 999	UNP Q87K10
A	389	LEU	-	expression tag	UNP Q87K10
A	390	GLU	-	expression tag	UNP Q87K10
A	391	HIS	-	expression tag	UNP Q87K10
A	392	HIS	-	expression tag	UNP Q87K10
A	393	HIS	-	expression tag	UNP Q87K10
A	394	HIS	-	expression tag	UNP Q87K10
A	395	HIS	-	expression tag	UNP Q87K10
A	396	HIS	-	expression tag	UNP Q87K10
B	31	ILE	VAL	SEE REMARK 999	UNP Q87K10
B	389	LEU	-	expression tag	UNP Q87K10
B	390	GLU	-	expression tag	UNP Q87K10
B	391	HIS	-	expression tag	UNP Q87K10
B	392	HIS	-	expression tag	UNP Q87K10
B	393	HIS	-	expression tag	UNP Q87K10
B	394	HIS	-	expression tag	UNP Q87K10
B	395	HIS	-	expression tag	UNP Q87K10
B	396	HIS	-	expression tag	UNP Q87K10
C	31	ILE	VAL	SEE REMARK 999	UNP Q87K10
C	389	LEU	-	expression tag	UNP Q87K10
C	390	GLU	-	expression tag	UNP Q87K10
C	391	HIS	-	expression tag	UNP Q87K10
C	392	HIS	-	expression tag	UNP Q87K10

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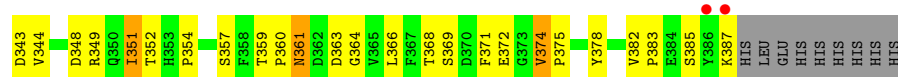
Chain	Residue	Modelled	Actual	Comment	Reference
C	393	HIS	-	expression tag	UNP Q87K10
C	394	HIS	-	expression tag	UNP Q87K10
C	395	HIS	-	expression tag	UNP Q87K10
C	396	HIS	-	expression tag	UNP Q87K10

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

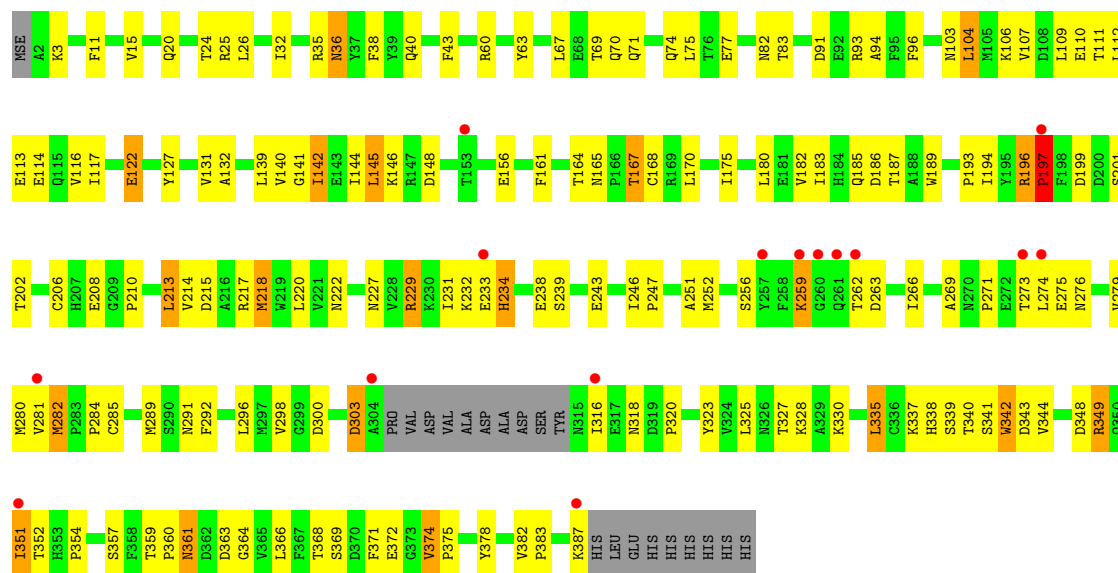
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	87	Total 87	O 87	0	0
3	B	69	Total 69	O 69	0	0
3	C	53	Total 53	O 53	0	0



• Molecule 1: Oligogalacturonate lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.23Å 115.23Å 209.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 2.60 19.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.8 (19.96-2.60) 96.7 (19.96-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.234 , 0.277 0.249 , 0.290	Depositor DCC
R_{free} test set	9235 reflections (9.73%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9292	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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 39.21 % 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 3.2840e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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](#)

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

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	0.49	0/3093	0.87	2/4191 (0.0%)
1	B	0.49	0/3108	0.86	2/4213 (0.0%)
1	C	0.49	0/3093	0.86	3/4191 (0.1%)
All	All	0.49	0/9294	0.86	7/12595 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	246	ILE	N-CA-C	-7.11	102.52	108.63
1	B	246	ILE	N-CA-C	-6.95	102.65	108.63
1	A	246	ILE	N-CA-C	-6.89	102.71	108.63
1	C	82	ASN	N-CA-C	-5.50	98.32	107.99
1	A	103	ASN	N-CA-C	5.25	117.08	108.52
1	B	82	ASN	N-CA-C	-5.16	98.92	107.99
1	C	103	ASN	N-CA-C	5.14	116.90	108.52

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	3022	0	2853	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3036	0	2869	127	0
1	C	3022	0	2853	120	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	87	0	0	5	0
3	B	69	0	0	4	0
3	C	53	0	0	2	0
All	All	9292	0	8575	371	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 21.

All (371) 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:38:PHE:HD1	1:A:289:MSE:HE3	1.38	0.89
1:A:374:VAL:HG22	1:A:375:PRO:HD2	1.56	0.87
1:C:38:PHE:HD1	1:C:289:MSE:HE3	1.38	0.86
1:C:213:LEU:H	1:C:213:LEU:HD23	1.42	0.85
1:B:107:VAL:HG22	1:B:114:GLU:HG2	1.59	0.84
1:C:374:VAL:HG22	1:C:375:PRO:HD2	1.57	0.84
1:B:374:VAL:HG22	1:B:375:PRO:HD2	1.58	0.84
1:A:38:PHE:CD1	1:A:289:MSE:HE3	2.13	0.83
1:B:213:LEU:HD23	1:B:213:LEU:H	1.42	0.83
1:A:213:LEU:H	1:A:213:LEU:HD23	1.43	0.82
1:A:107:VAL:HG22	1:A:114:GLU:HG2	1.62	0.82
1:A:218:MSE:HE1	1:A:243:GLU:HB3	1.60	0.82
1:A:180:LEU:HD22	3:A:467:HOH:O	1.80	0.81
1:C:218:MSE:HE1	1:C:243:GLU:HB3	1.61	0.81
1:C:38:PHE:CD1	1:C:289:MSE:HE3	2.15	0.81
1:B:32:ILE:HG23	1:B:375:PRO:HG2	1.63	0.79
1:C:107:VAL:HG22	1:C:114:GLU:HG2	1.64	0.79
1:B:218:MSE:HE1	1:B:243:GLU:HB3	1.63	0.78
1:B:38:PHE:HD1	1:B:289:MSE:HE3	1.50	0.77
1:C:32:ILE:HG23	1:C:375:PRO:HG2	1.67	0.76
1:A:161:PHE:O	1:A:164:THR:HG22	1.86	0.75
1:A:218:MSE:HB3	1:A:231:ILE:HB	1.67	0.75
1:C:161:PHE:O	1:C:164:THR:HG22	1.85	0.75
1:B:218:MSE:HB3	1:B:231:ILE:HB	1.70	0.74
1:B:343:ASP:O	1:B:352:THR:HG21	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:MSE:HB3	1:C:231:ILE:HB	1.70	0.73
1:C:343:ASP:O	1:C:352:THR:HG21	1.88	0.73
1:C:60:ARG:HG3	1:C:83:THR:HG21	1.69	0.73
1:A:359:THR:HG21	1:A:363:ASP:OD1	1.88	0.73
1:B:161:PHE:O	1:B:164:THR:HG22	1.88	0.72
1:B:359:THR:HG21	1:B:363:ASP:OD1	1.89	0.72
1:A:343:ASP:O	1:A:352:THR:HG21	1.89	0.72
1:A:199:ASP:OD1	1:A:201:SER:HB3	1.90	0.72
1:B:38:PHE:CD1	1:B:289:MSE:HE3	2.24	0.72
1:C:199:ASP:OD1	1:C:201:SER:HB3	1.90	0.71
1:A:60:ARG:HG3	1:A:83:THR:HG21	1.72	0.71
1:C:280:MSE:HE2	1:C:327:THR:HA	1.73	0.71
1:A:341:SER:O	1:A:343:ASP:N	2.22	0.70
1:B:199:ASP:OD1	1:B:201:SER:HB3	1.91	0.70
1:A:170:LEU:HD22	1:A:183:ILE:HD11	1.73	0.70
1:B:170:LEU:HD22	1:B:183:ILE:HD11	1.73	0.70
1:B:60:ARG:HG3	1:B:83:THR:HG21	1.73	0.70
1:C:359:THR:HG21	1:C:363:ASP:OD1	1.90	0.70
1:C:69:THR:HG22	1:C:71:GLN:HG3	1.74	0.70
1:C:170:LEU:HD22	1:C:183:ILE:HD11	1.73	0.69
1:A:32:ILE:HG23	1:A:375:PRO:HG2	1.75	0.69
1:B:69:THR:HG22	1:B:71:GLN:HG3	1.75	0.69
1:C:148:ASP:OD2	1:C:167:THR:HG22	1.93	0.68
1:A:15:VAL:HB	1:B:8:THR:HG21	1.74	0.68
1:C:341:SER:O	1:C:343:ASP:N	2.25	0.68
1:B:147:ARG:HG3	3:B:462:HOH:O	1.94	0.67
1:A:148:ASP:OD2	1:A:167:THR:HG22	1.94	0.67
1:B:275:GLU:O	1:B:275:GLU:HG3	1.93	0.67
1:C:275:GLU:HG3	1:C:275:GLU:O	1.95	0.67
1:A:139:LEU:HG	1:A:175:ILE:HD11	1.77	0.67
1:B:104:LEU:HD13	1:B:117:ILE:HD11	1.75	0.67
1:B:148:ASP:OD2	1:B:167:THR:HG22	1.94	0.67
1:C:182:VAL:HG21	3:C:424:HOH:O	1.94	0.66
1:A:232:LYS:HE2	1:A:238:GLU:OE1	1.94	0.66
1:B:132:ALA:HA	1:B:139:LEU:HD23	1.77	0.66
1:C:144:ILE:HG12	1:C:168:CYS:SG	2.35	0.66
1:A:132:ALA:HA	1:A:139:LEU:HD23	1.78	0.66
1:A:69:THR:HG22	1:A:71:GLN:HG3	1.77	0.66
1:C:232:LYS:HE2	1:C:238:GLU:OE1	1.97	0.66
1:B:232:LYS:HE2	1:B:238:GLU:OE1	1.95	0.65
1:C:359:THR:OG1	1:C:360:PRO:HD2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:MSE:HE2	1:B:327:THR:HA	1.78	0.65
1:A:359:THR:OG1	1:A:360:PRO:HD2	1.96	0.65
1:C:222:ASN:HB3	3:C:428:HOH:O	1.96	0.65
1:C:104:LEU:HD13	1:C:117:ILE:HD11	1.79	0.65
1:B:144:ILE:HG12	1:B:168:CYS:SG	2.36	0.64
1:C:139:LEU:HG	1:C:175:ILE:HD11	1.79	0.64
1:A:280:MSE:HE2	1:A:327:THR:HA	1.79	0.64
1:A:279:VAL:O	1:A:330:LYS:HE3	1.96	0.64
1:A:275:GLU:HG3	1:A:275:GLU:O	1.96	0.64
1:C:132:ALA:HA	1:C:139:LEU:HD23	1.79	0.63
1:B:266:ILE:CG1	1:B:282:MSE:HG2	2.28	0.63
1:B:359:THR:OG1	1:B:360:PRO:HD2	1.97	0.63
1:C:180:LEU:HD23	1:C:180:LEU:H	1.63	0.63
1:A:104:LEU:HD13	1:A:117:ILE:HD11	1.79	0.63
1:B:139:LEU:HG	1:B:175:ILE:HD11	1.80	0.62
1:B:104:LEU:HD11	1:B:139:LEU:HD13	1.80	0.62
1:C:338:HIS:CE1	1:C:340:THR:HG22	2.35	0.62
1:B:210:PRO:HG2	1:B:213:LEU:HG	1.81	0.62
1:C:303:ASP:HB3	1:C:318:ASN:ND2	2.15	0.62
1:A:180:LEU:HD23	1:A:180:LEU:H	1.65	0.62
1:B:180:LEU:H	1:B:180:LEU:HD23	1.64	0.62
1:A:210:PRO:HG2	1:A:213:LEU:HG	1.82	0.61
1:A:266:ILE:CG1	1:A:282:MSE:HG2	2.30	0.61
1:B:338:HIS:CE1	1:B:340:THR:HG22	2.35	0.61
1:B:341:SER:O	1:B:343:ASP:N	2.29	0.61
1:C:210:PRO:HG2	1:C:213:LEU:HG	1.83	0.61
1:A:338:HIS:CE1	1:A:340:THR:HG22	2.36	0.60
1:C:227:ASN:O	1:C:229:ARG:HG3	2.02	0.60
1:C:279:VAL:O	1:C:330:LYS:HE3	2.00	0.60
1:A:104:LEU:HD11	1:A:139:LEU:HD13	1.84	0.60
1:B:227:ASN:O	1:B:229:ARG:HG3	2.02	0.60
1:B:247:PRO:HB2	1:B:292:PHE:HA	1.84	0.60
1:A:266:ILE:HG13	1:A:282:MSE:HG2	1.84	0.59
1:C:383:PRO:HG2	1:C:387:LYS:H	1.67	0.59
1:A:144:ILE:HG12	1:A:168:CYS:SG	2.42	0.59
1:C:104:LEU:HD11	1:C:139:LEU:HD13	1.85	0.59
1:B:145:LEU:HB2	1:B:167:THR:HG23	1.84	0.58
1:C:266:ILE:CG1	1:C:282:MSE:HG2	2.33	0.58
1:A:247:PRO:HB2	1:A:292:PHE:HA	1.86	0.58
1:A:218:MSE:HB2	3:A:430:HOH:O	2.02	0.58
1:A:145:LEU:HB2	1:A:167:THR:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:PRO:HB2	1:C:292:PHE:HA	1.86	0.58
1:A:141:GLY:HA2	1:A:193:PRO:HG3	1.85	0.58
1:B:25:ARG:HG3	1:B:378:TYR:CE2	2.39	0.58
1:C:145:LEU:HB2	1:C:167:THR:HG23	1.86	0.58
1:A:213:LEU:HD23	1:A:213:LEU:N	2.17	0.58
1:B:266:ILE:HG13	1:B:282:MSE:HG2	1.86	0.58
1:A:104:LEU:HD22	1:A:117:ILE:HD11	1.85	0.58
1:C:289:MSE:HE2	1:C:289:MSE:HA	1.85	0.57
1:A:289:MSE:HE2	1:A:289:MSE:HA	1.86	0.57
1:A:227:ASN:O	1:A:229:ARG:HG3	2.04	0.57
1:C:25:ARG:HG3	1:C:378:TYR:CE2	2.39	0.57
1:B:141:GLY:HA2	1:B:193:PRO:HG3	1.87	0.56
1:B:251:ALA:HA	1:B:271:PRO:HD3	1.85	0.56
1:B:348:ASP:HB3	1:B:351:ILE:HD11	1.87	0.56
1:A:383:PRO:HG3	1:A:387:LYS:HB2	1.88	0.56
1:B:145:LEU:HD12	1:B:167:THR:HG21	1.88	0.56
1:A:266:ILE:O	1:A:279:VAL:HG12	2.06	0.55
1:C:251:ALA:HA	1:C:271:PRO:HD3	1.88	0.55
1:A:325:LEU:N	1:A:325:LEU:HD12	2.22	0.55
1:B:104:LEU:HD13	1:B:117:ILE:CD1	2.37	0.55
1:B:344:VAL:HG23	1:B:344:VAL:O	2.06	0.55
1:C:344:VAL:HG23	1:C:344:VAL:O	2.06	0.55
1:C:325:LEU:N	1:C:325:LEU:HD12	2.21	0.55
1:C:348:ASP:HB3	1:C:351:ILE:HD11	1.89	0.55
1:C:361:ASN:HD22	1:C:361:ASN:H	1.54	0.55
1:A:104:LEU:HD13	1:A:117:ILE:CD1	2.37	0.55
1:A:361:ASN:HD22	1:A:361:ASN:H	1.55	0.55
1:B:213:LEU:HD23	1:B:213:LEU:N	2.18	0.55
1:A:251:ALA:HA	1:A:271:PRO:HD3	1.88	0.54
1:B:325:LEU:HD12	1:B:325:LEU:N	2.22	0.54
1:C:383:PRO:HG3	1:C:387:LYS:HB2	1.88	0.54
1:C:339:SER:O	1:C:371:PHE:HB3	2.07	0.54
1:A:145:LEU:HD12	1:A:167:THR:HG21	1.90	0.54
1:A:348:ASP:HB3	1:A:351:ILE:HD11	1.89	0.54
1:B:291:ASN:HB2	1:B:296:LEU:HB2	1.90	0.54
1:C:291:ASN:HB2	1:C:296:LEU:HB2	1.90	0.53
1:A:131:VAL:O	1:A:140:VAL:HG12	2.08	0.53
1:A:359:THR:CG2	1:A:364:GLY:H	2.21	0.53
1:C:145:LEU:HD12	1:C:167:THR:HG21	1.91	0.53
1:C:231:ILE:HD13	1:C:252:MSE:HG2	1.90	0.53
1:A:291:ASN:HB2	1:A:296:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ILE:O	1:B:279:VAL:HG12	2.07	0.53
1:A:344:VAL:O	1:A:344:VAL:HG23	2.08	0.53
1:C:213:LEU:HD23	1:C:213:LEU:N	2.17	0.53
1:C:141:GLY:HA2	1:C:193:PRO:HG3	1.90	0.53
1:A:359:THR:HG22	1:A:364:GLY:H	1.73	0.53
1:B:341:SER:O	1:B:341:SER:OG	2.27	0.53
1:A:231:ILE:HD13	1:A:252:MSE:HG2	1.91	0.53
1:C:36:ASN:N	1:C:36:ASN:HD22	2.07	0.53
1:A:25:ARG:HG3	1:A:378:TYR:CE2	2.44	0.52
1:C:266:ILE:O	1:C:279:VAL:HG12	2.09	0.52
1:C:341:SER:C	1:C:343:ASP:H	2.15	0.52
1:B:359:THR:CG2	1:B:364:GLY:H	2.22	0.52
1:B:231:ILE:HD13	1:B:252:MSE:HG2	1.91	0.52
1:C:32:ILE:HG23	1:C:375:PRO:CG	2.37	0.52
1:A:341:SER:C	1:A:343:ASP:H	2.15	0.52
1:C:111:THR:O	1:C:112:LEU:HB2	2.10	0.52
1:C:266:ILE:HG13	1:C:282:MSE:HG2	1.90	0.52
1:C:269:ALA:HB2	1:C:276:ASN:ND2	2.24	0.52
1:C:280:MSE:CE	1:C:327:THR:HA	2.40	0.52
1:A:341:SER:O	1:A:341:SER:OG	2.27	0.51
1:C:131:VAL:O	1:C:140:VAL:HG12	2.10	0.51
1:A:339:SER:O	1:A:371:PHE:HB3	2.10	0.51
1:B:35:ARG:HE	1:B:366:LEU:HD23	1.74	0.51
1:B:335:LEU:HD11	1:B:382:VAL:HG22	1.92	0.51
1:C:335:LEU:HA	1:C:387:LYS:O	2.10	0.51
1:A:15:VAL:HB	1:B:8:THR:CG2	2.38	0.51
1:C:335:LEU:HD11	1:C:382:VAL:HG22	1.93	0.51
1:B:341:SER:C	1:B:343:ASP:H	2.17	0.51
1:C:359:THR:CG2	1:C:364:GLY:H	2.23	0.51
1:B:131:VAL:O	1:B:140:VAL:HG12	2.11	0.51
1:B:300:ASP:OD1	1:B:354:PRO:HB2	2.11	0.51
1:A:269:ALA:HB2	1:A:276:ASN:ND2	2.26	0.51
1:B:91:ASP:OD2	1:B:93:ARG:HB2	2.11	0.50
1:B:339:SER:O	1:B:371:PHE:HB3	2.11	0.50
1:B:361:ASN:H	1:B:361:ASN:HD22	1.59	0.50
1:A:342:TRP:H	1:A:342:TRP:CD1	2.28	0.50
1:B:359:THR:HG22	1:B:364:GLY:H	1.75	0.50
1:C:35:ARG:HH12	1:C:38:PHE:HA	1.77	0.50
1:C:361:ASN:HD22	1:C:361:ASN:N	2.10	0.50
1:A:91:ASP:OD2	1:A:93:ARG:HB2	2.11	0.50
1:B:289:MSE:HA	1:B:289:MSE:HE2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASN:HD22	1:A:36:ASN:N	2.10	0.50
1:A:208:GLU:OE2	1:A:208:GLU:HA	2.11	0.50
1:B:269:ALA:HB2	1:B:276:ASN:ND2	2.26	0.50
1:B:296:LEU:HD11	3:B:465:HOH:O	2.10	0.50
1:B:266:ILE:HB	1:B:279:VAL:CG1	2.42	0.50
1:C:342:TRP:H	1:C:342:TRP:CD1	2.29	0.50
1:B:208:GLU:OE2	1:B:208:GLU:HA	2.10	0.49
1:C:285:CYS:HA	1:C:300:ASP:O	2.12	0.49
1:C:298:VAL:HA	1:C:323:TYR:O	2.13	0.49
1:C:359:THR:HG22	1:C:364:GLY:H	1.75	0.49
1:A:206:CYS:HB2	1:A:217:ARG:HB2	1.94	0.49
1:B:35:ARG:HH12	1:B:38:PHE:HA	1.78	0.49
1:B:104:LEU:HD22	1:B:117:ILE:HD11	1.95	0.49
1:B:36:ASN:N	1:B:36:ASN:HD22	2.10	0.49
1:B:69:THR:HG22	1:B:71:GLN:CG	2.42	0.49
1:C:69:THR:HG22	1:C:71:GLN:CG	2.42	0.49
1:C:104:LEU:HD13	1:C:117:ILE:CD1	2.42	0.49
1:B:40:GLN:HE21	1:B:40:GLN:HA	1.77	0.49
1:B:226:SER:OG	3:B:439:HOH:O	2.20	0.49
1:B:142:ILE:HG23	1:B:193:PRO:HD3	1.94	0.48
1:C:142:ILE:HG23	1:C:193:PRO:HD3	1.95	0.48
1:A:298:VAL:HA	1:A:323:TYR:O	2.14	0.48
1:A:361:ASN:HD22	1:A:361:ASN:N	2.11	0.48
1:A:383:PRO:HG2	1:A:387:LYS:H	1.76	0.48
1:A:386:TYR:HB2	3:A:440:HOH:O	2.14	0.48
1:A:35:ARG:HH12	1:A:38:PHE:HA	1.79	0.48
1:B:11:PHE:CE1	1:B:70:GLN:HG2	2.49	0.48
1:A:335:LEU:HD11	1:A:382:VAL:HG22	1.96	0.48
1:C:206:CYS:HB2	1:C:217:ARG:HB2	1.95	0.48
1:B:280:MSE:CE	1:B:327:THR:HA	2.41	0.48
1:B:342:TRP:H	1:B:342:TRP:CD1	2.31	0.48
1:C:266:ILE:HB	1:C:279:VAL:CG1	2.43	0.48
1:B:280:MSE:HG3	1:B:281:VAL:O	2.13	0.47
1:B:285:CYS:HA	1:B:300:ASP:O	2.14	0.47
1:C:11:PHE:CE1	1:C:70:GLN:HG2	2.49	0.47
1:A:11:PHE:CE1	1:A:70:GLN:HG2	2.50	0.47
1:A:285:CYS:HA	1:A:300:ASP:O	2.14	0.47
1:A:266:ILE:HB	1:A:279:VAL:CG1	2.44	0.47
1:A:94:ALA:HA	1:A:109:LEU:HG	1.96	0.47
1:A:142:ILE:HG23	1:A:193:PRO:HD3	1.97	0.47
1:A:300:ASP:OD1	1:A:354:PRO:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:CYS:HB2	1:B:217:ARG:HB2	1.95	0.47
1:C:208:GLU:OE2	1:C:208:GLU:HA	2.13	0.47
1:B:291:ASN:ND2	1:B:292:PHE:H	2.12	0.47
1:C:196:ARG:HB2	1:C:202:THR:HB	1.96	0.47
1:B:196:ARG:O	1:B:197:PRO:C	2.56	0.47
1:A:63:TYR:CZ	1:A:74:GLN:HG3	2.50	0.46
1:A:185:GLN:O	1:A:186:ASP:HB2	2.15	0.46
1:A:111:THR:O	1:A:112:LEU:HB2	2.14	0.46
1:C:91:ASP:OD2	1:C:93:ARG:HB2	2.15	0.46
1:C:279:VAL:HG13	1:C:280:MSE:N	2.30	0.46
1:A:280:MSE:HG3	1:A:281:VAL:O	2.16	0.46
1:B:239:SER:O	1:B:256:SER:HA	2.16	0.46
1:C:196:ARG:HH11	1:C:271:PRO:HG2	1.80	0.46
1:A:35:ARG:NH2	1:A:357:SER:HB3	2.30	0.46
1:B:164:THR:O	1:B:165:ASN:C	2.59	0.46
1:B:279:VAL:HG13	1:B:280:MSE:N	2.31	0.46
1:B:111:THR:O	1:B:112:LEU:HB2	2.15	0.46
1:B:241:THR:O	1:B:242:HIS:HB2	2.16	0.46
1:B:132:ALA:CA	1:B:139:LEU:HD23	2.45	0.46
1:B:196:ARG:HB2	1:B:202:THR:HB	1.97	0.46
1:B:196:ARG:HH11	1:B:271:PRO:HG2	1.81	0.46
1:C:280:MSE:HG3	1:C:281:VAL:O	2.16	0.45
1:A:196:ARG:O	1:A:197:PRO:C	2.59	0.45
1:B:383:PRO:HG2	1:B:387:LYS:H	1.81	0.45
1:C:35:ARG:NH2	1:C:357:SER:HB3	2.32	0.45
1:B:15:VAL:HG13	1:B:20:GLN:O	2.17	0.45
1:C:196:ARG:O	1:C:197:PRO:C	2.59	0.45
1:A:14:PHE:HB3	1:B:10:ASN:ND2	2.31	0.45
1:A:280:MSE:CE	1:A:327:THR:HA	2.45	0.45
1:C:11:PHE:CZ	1:C:26:LEU:HD12	2.52	0.45
1:A:11:PHE:CZ	1:A:26:LEU:HD12	2.52	0.45
1:A:196:ARG:HB2	1:A:202:THR:HB	1.97	0.45
1:B:94:ALA:HA	1:B:109:LEU:HG	1.99	0.45
1:C:164:THR:O	1:C:165:ASN:C	2.60	0.45
1:C:214:VAL:O	1:C:214:VAL:HG13	2.17	0.45
1:A:279:VAL:HG13	1:A:280:MSE:N	2.31	0.45
1:B:215:ASP:OD2	1:B:215:ASP:N	2.49	0.45
1:C:35:ARG:HE	1:C:366:LEU:HD23	1.82	0.45
1:C:63:TYR:CZ	1:C:74:GLN:HG3	2.51	0.45
1:C:104:LEU:HD22	1:C:117:ILE:HD11	1.99	0.45
1:A:368:THR:HG22	1:A:369:SER:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ARG:HD3	1:B:372:GLU:OE2	2.17	0.45
1:B:335:LEU:HA	1:B:387:LYS:O	2.16	0.45
1:C:239:SER:O	1:C:256:SER:HA	2.17	0.45
1:C:291:ASN:ND2	1:C:292:PHE:H	2.15	0.45
1:C:318:ASN:O	1:C:320:PRO:HD3	2.17	0.45
1:A:239:SER:O	1:A:256:SER:HA	2.17	0.45
1:B:63:TYR:CZ	1:B:74:GLN:HG3	2.51	0.45
1:A:69:THR:HG22	1:A:71:GLN:CG	2.45	0.44
1:B:40:GLN:HA	1:B:40:GLN:NE2	2.33	0.44
1:C:40:GLN:HE21	1:C:40:GLN:HA	1.83	0.44
1:C:215:ASP:N	1:C:215:ASP:OD2	2.50	0.44
1:A:196:ARG:HH11	1:A:271:PRO:HG2	1.82	0.44
1:B:35:ARG:NH2	1:B:357:SER:HB3	2.33	0.44
1:B:185:GLN:O	1:B:186:ASP:HB2	2.16	0.44
1:C:94:ALA:HA	1:C:109:LEU:HG	1.99	0.44
1:A:40:GLN:HE21	1:A:40:GLN:HA	1.83	0.44
1:B:180:LEU:H	1:B:180:LEU:CD2	2.30	0.44
1:C:300:ASP:OD1	1:C:354:PRO:HB2	2.17	0.44
1:A:164:THR:O	1:A:165:ASN:C	2.61	0.44
1:B:11:PHE:CZ	1:B:26:LEU:HD12	2.53	0.44
1:B:259:LYS:HB2	1:B:259:LYS:NZ	2.33	0.44
1:B:385:SER:OG	1:B:387:LYS:HG3	2.17	0.44
1:B:229:ARG:HD3	1:B:274:LEU:HD21	2.00	0.44
1:C:185:GLN:O	1:C:186:ASP:HB2	2.17	0.44
1:C:180:LEU:H	1:C:180:LEU:CD2	2.30	0.44
1:A:132:ALA:CA	1:A:139:LEU:HD23	2.45	0.43
1:A:229:ARG:HD3	1:A:274:LEU:HD21	2.00	0.43
1:B:318:ASN:O	1:B:320:PRO:HD3	2.17	0.43
1:B:368:THR:HG22	1:B:369:SER:N	2.33	0.43
1:C:361:ASN:H	1:C:361:ASN:ND2	2.16	0.43
1:A:35:ARG:HE	1:A:366:LEU:HD23	1.83	0.43
1:B:59:ASN:HD22	1:B:59:ASN:HA	1.66	0.43
1:C:368:THR:HG22	1:C:369:SER:N	2.32	0.43
1:A:15:VAL:HG13	1:A:20:GLN:O	2.19	0.43
1:A:335:LEU:HA	1:A:387:LYS:O	2.18	0.43
1:B:113:GLU:HG3	1:C:113:GLU:HG3	2.00	0.43
1:A:215:ASP:OD2	1:A:215:ASP:N	2.50	0.43
1:B:214:VAL:HG13	1:B:214:VAL:O	2.18	0.43
1:C:132:ALA:CA	1:C:139:LEU:HD23	2.47	0.43
1:A:241:THR:O	1:A:242:HIS:HB2	2.19	0.43
1:B:21:VAL:HG11	1:B:335:LEU:CD2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:VAL:HG11	1:B:335:LEU:HD22	2.01	0.43
1:C:15:VAL:HG13	1:C:20:GLN:O	2.18	0.43
1:C:43:PHE:CE2	1:C:366:LEU:HD22	2.54	0.43
1:A:3:LYS:HB3	1:A:77:GLU:OE2	2.18	0.43
1:A:32:ILE:HG23	1:A:375:PRO:CG	2.48	0.42
1:B:3:LYS:HB3	1:B:77:GLU:OE2	2.19	0.42
1:B:32:ILE:HG23	1:B:375:PRO:CG	2.42	0.42
1:B:298:VAL:HA	1:B:323:TYR:O	2.19	0.42
1:B:279:VAL:O	1:B:330:LYS:HE3	2.18	0.42
1:A:59:ASN:HD22	1:A:59:ASN:HA	1.71	0.42
1:A:214:VAL:O	1:A:214:VAL:HG13	2.20	0.42
1:A:259:LYS:NZ	1:A:259:LYS:HB2	2.34	0.42
1:C:3:LYS:HB3	1:C:77:GLU:OE2	2.19	0.42
1:A:40:GLN:HA	1:A:40:GLN:NE2	2.34	0.42
1:B:361:ASN:HD22	1:B:361:ASN:N	2.16	0.42
1:C:229:ARG:HD3	1:C:274:LEU:HD21	2.02	0.42
1:A:351:ILE:H	1:A:351:ILE:HG12	1.60	0.42
1:A:52:PHE:HE2	1:A:65:LEU:HB2	1.85	0.42
1:A:180:LEU:H	1:A:180:LEU:CD2	2.31	0.42
1:C:259:LYS:HB2	1:C:259:LYS:NZ	2.34	0.42
1:A:43:PHE:CE2	1:A:366:LEU:HD22	2.54	0.42
1:B:163:HIS:C	1:B:165:ASN:H	2.28	0.42
1:B:170:LEU:O	1:B:183:ILE:HG12	2.20	0.42
1:A:101:GLU:HG2	3:A:432:HOH:O	2.19	0.41
1:B:233:GLU:O	1:B:234:HIS:HB3	2.20	0.41
1:A:318:ASN:O	1:A:320:PRO:HD3	2.19	0.41
1:B:35:ARG:HE	1:B:366:LEU:CD2	2.33	0.41
1:B:273:THR:CG2	1:B:275:GLU:HG2	2.50	0.41
1:C:122:GLU:O	1:C:146:LYS:HD2	2.20	0.41
1:A:383:PRO:CG	1:A:387:LYS:HB2	2.49	0.41
1:C:25:ARG:HD3	1:C:372:GLU:OE2	2.20	0.41
1:B:189:TRP:CD2	1:B:208:GLU:HB2	2.55	0.41
1:C:189:TRP:CD2	1:C:208:GLU:HB2	2.55	0.41
1:C:233:GLU:O	1:C:234:HIS:HB3	2.20	0.41
1:A:229:ARG:HE	1:A:274:LEU:HD11	1.85	0.41
1:A:353:HIS:HA	1:A:354:PRO:HD3	1.95	0.41
1:A:170:LEU:O	1:A:183:ILE:HG12	2.21	0.41
1:A:189:TRP:CD2	1:A:208:GLU:HB2	2.56	0.41
1:A:196:ARG:HG2	1:A:245:TRP:CZ2	2.56	0.41
1:A:291:ASN:ND2	1:A:292:PHE:H	2.19	0.41
1:B:124:TRP:CH2	1:B:169:ARG:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ASN:N	3:B:414:HOH:O	2.54	0.41
1:B:279:VAL:O	1:B:280:MSE:HB3	2.21	0.41
1:A:303:ASP:HB3	1:A:318:ASN:ND2	2.36	0.41
1:C:127:TYR:CD1	1:C:142:ILE:HD11	2.55	0.41
1:C:273:THR:CG2	1:C:275:GLU:HG2	2.51	0.41
1:A:4:GLY:HA2	1:A:112:LEU:CD1	2.51	0.40
1:B:4:GLY:HA2	1:B:112:LEU:CD1	2.52	0.40
1:B:163:HIS:CE1	1:B:213:LEU:HD12	2.57	0.40
1:C:344:VAL:HG11	1:C:349:ARG:NH1	2.36	0.40
1:A:19:THR:O	1:A:20:GLN:HB2	2.20	0.40
1:A:252:MSE:HE3	3:A:424:HOH:O	2.21	0.40
1:A:361:ASN:H	1:A:361:ASN:ND2	2.18	0.40
1:C:341:SER:C	1:C:343:ASP:N	2.78	0.40
1:C:40:GLN:HA	1:C:40:GLN:NE2	2.36	0.40
1:C:325:LEU:HD12	1:C:325:LEU:H	1.85	0.40
1:A:36:ASN:C	1:A:36:ASN:ND2	2.80	0.40
1:C:96:PHE:CZ	1:C:106:LYS:HG3	2.56	0.40
1:C:167:THR:HA	1:C:187:THR:HA	2.04	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	372/396 (94%)	336 (90%)	30 (8%)	6 (2%)	7	16
1	B	374/396 (94%)	334 (89%)	33 (9%)	7 (2%)	6	13
1	C	372/396 (94%)	332 (89%)	33 (9%)	7 (2%)	6	13
All	All	1118/1188 (94%)	1002 (90%)	96 (9%)	20 (2%)	6	14

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	PRO
1	A	316	ILE
1	A	342	TRP
1	B	197	PRO
1	B	316	ILE
1	B	342	TRP
1	C	197	PRO
1	C	316	ILE
1	C	342	TRP
1	A	262	THR
1	B	262	THR
1	C	262	THR
1	A	284	PRO
1	A	234	HIS
1	B	218	MSE
1	B	284	PRO
1	C	284	PRO
1	B	234	HIS
1	C	218	MSE
1	C	234	HIS

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	334/344 (97%)	303 (91%)	31 (9%)	8	18
1	B	336/344 (98%)	307 (91%)	29 (9%)	10	22
1	C	334/344 (97%)	305 (91%)	29 (9%)	9	21
All	All	1004/1032 (97%)	915 (91%)	89 (9%)	9	20

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	36	ASN
1	A	67	LEU

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Mol	Chain	Res	Type
1	A	75	LEU
1	A	104	LEU
1	A	110	GLU
1	A	116	VAL
1	A	122	GLU
1	A	136	CYS
1	A	142	ILE
1	A	145	LEU
1	A	167	THR
1	A	194	ILE
1	A	196	ARG
1	A	197	PRO
1	A	213	LEU
1	A	220	LEU
1	A	229	ARG
1	A	259	LYS
1	A	263	ASP
1	A	282	MSE
1	A	303	ASP
1	A	315	ASN
1	A	320	PRO
1	A	328	LYS
1	A	335	LEU
1	A	337	LYS
1	A	349	ARG
1	A	351	ILE
1	A	361	ASN
1	A	374	VAL
1	B	24	THR
1	B	36	ASN
1	B	67	LEU
1	B	75	LEU
1	B	104	LEU
1	B	110	GLU
1	B	116	VAL
1	B	122	GLU
1	B	136	CYS
1	B	142	ILE
1	B	145	LEU
1	B	167	THR
1	B	194	ILE
1	B	196	ARG

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Mol	Chain	Res	Type
1	B	197	PRO
1	B	213	LEU
1	B	220	LEU
1	B	229	ARG
1	B	247	PRO
1	B	259	LYS
1	B	263	ASP
1	B	282	MSE
1	B	328	LYS
1	B	335	LEU
1	B	337	LYS
1	B	349	ARG
1	B	351	ILE
1	B	361	ASN
1	B	374	VAL
1	C	24	THR
1	C	36	ASN
1	C	67	LEU
1	C	75	LEU
1	C	104	LEU
1	C	110	GLU
1	C	116	VAL
1	C	122	GLU
1	C	142	ILE
1	C	145	LEU
1	C	156	GLU
1	C	167	THR
1	C	194	ILE
1	C	196	ARG
1	C	197	PRO
1	C	213	LEU
1	C	220	LEU
1	C	229	ARG
1	C	259	LYS
1	C	263	ASP
1	C	282	MSE
1	C	303	ASP
1	C	328	LYS
1	C	335	LEU
1	C	337	LYS
1	C	349	ARG
1	C	351	ILE

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Mol	Chain	Res	Type
1	C	361	ASN
1	C	374	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	40	GLN
1	A	59	ASN
1	A	74	GLN
1	A	100	ASN
1	A	115	GLN
1	A	184	HIS
1	A	227	ASN
1	A	242	HIS
1	A	261	GLN
1	A	276	ASN
1	A	291	ASN
1	A	318	ASN
1	A	333	GLN
1	A	361	ASN
1	B	10	ASN
1	B	34	HIS
1	B	36	ASN
1	B	40	GLN
1	B	59	ASN
1	B	100	ASN
1	B	115	GLN
1	B	165	ASN
1	B	184	HIS
1	B	211	HIS
1	B	227	ASN
1	B	242	HIS
1	B	261	GLN
1	B	276	ASN
1	B	291	ASN
1	B	318	ASN
1	B	333	GLN
1	B	361	ASN
1	C	36	ASN
1	C	40	GLN
1	C	59	ASN

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Mol	Chain	Res	Type
1	C	70	GLN
1	C	100	ASN
1	C	115	GLN
1	C	163	HIS
1	C	165	ASN
1	C	184	HIS
1	C	227	ASN
1	C	242	HIS
1	C	276	ASN
1	C	291	ASN
1	C	315	ASN
1	C	318	ASN
1	C	333	GLN
1	C	361	ASN

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	369/396 (93%)	0.09	13 (3%) 47 41	20, 44, 81, 98	0
1	B	371/396 (93%)	0.51	34 (9%) 14 11	17, 53, 86, 105	0
1	C	369/396 (93%)	0.15	15 (4%) 41 36	19, 46, 85, 100	0
All	All	1109/1188 (93%)	0.25	62 (5%) 30 24	17, 47, 85, 105	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	387	LYS	5.8
1	B	259	LYS	4.3
1	B	387	LYS	4.3
1	B	260	GLY	4.3
1	B	274	LEU	4.2
1	A	387	LYS	4.2
1	B	306	VAL	4.2
1	B	251	ALA	4.1
1	B	272	GLU	4.1
1	C	261	GLN	3.6
1	A	236	GLU	3.5
1	B	273	THR	3.5
1	B	235	ALA	3.4
1	B	257	TYR	3.3
1	B	216	ALA	3.3
1	A	260	GLY	3.2
1	B	316	ILE	3.2
1	B	276	ASN	3.1
1	B	271	PRO	3.1
1	B	202	THR	3.0
1	B	188	ALA	3.0
1	C	304	ALA	3.0
1	C	197	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	351	ILE	2.9
1	B	269	ALA	2.8
1	B	204	GLY	2.8
1	C	259	LYS	2.7
1	C	233	GLU	2.7
1	B	262	THR	2.7
1	A	259	LYS	2.7
1	C	257	TYR	2.6
1	C	274	LEU	2.6
1	C	260	GLY	2.5
1	A	281	VAL	2.5
1	B	267	TYR	2.5
1	B	221	VAL	2.5
1	B	227	ASN	2.4
1	B	281	VAL	2.4
1	B	386	TYR	2.4
1	B	304	ALA	2.4
1	A	274	LEU	2.4
1	B	222	ASN	2.3
1	B	155	TRP	2.3
1	C	262	THR	2.3
1	A	160	GLU	2.3
1	A	262	THR	2.2
1	B	258	PHE	2.2
1	A	233	GLU	2.2
1	C	281	VAL	2.2
1	B	305	PRO	2.2
1	B	284	PRO	2.2
1	C	316	ILE	2.2
1	A	263	ASP	2.1
1	A	316	ILE	2.1
1	B	239	SER	2.1
1	C	273	THR	2.1
1	B	189	TRP	2.1
1	B	270	ASN	2.1
1	A	315	ASN	2.0
1	A	197	PRO	2.0
1	C	153	THR	2.0
1	B	183	ILE	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](#)

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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	A	401	1/1	0.99	0.05	30,30,30,30	0
2	MN	B	401	1/1	0.99	0.03	20,20,20,20	0
2	MN	C	401	1/1	0.99	0.06	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.