



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:36 AM UTC

PDB ID : 9FI3 / pdb_00009fi3
Title : Bacteroides ovatus polysaccharide lyase family 38 (BoPL38) mutant Q173N in complex with tetraguluronic acid at pH 3.5
Authors : Tandrup, T.; Wilkens, C.
Deposited on : 2024-05-28
Resolution : 1.99 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

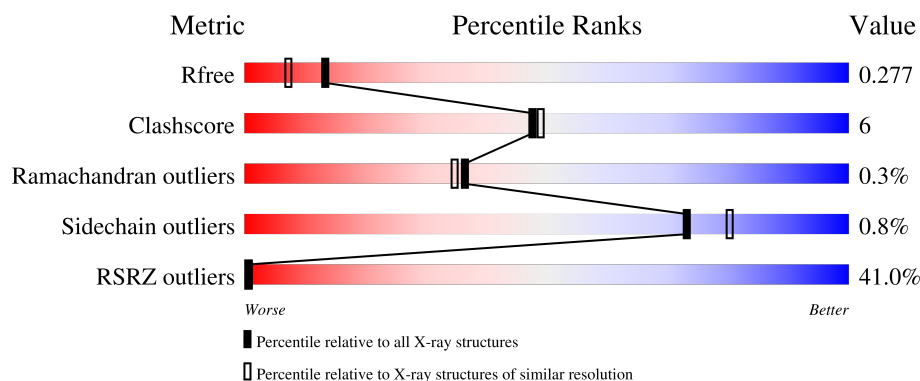
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	
1	B	404	
1	C	404	
1	D	404	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12549 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	379	Total	C	N	O	S	0	1	0
			3051	1952	515	571	13			
1	B	380	Total	C	N	O	S	0	0	0
			3051	1951	516	571	13			
1	C	380	Total	C	N	O	S	0	0	0
			3051	1951	516	571	13			
1	D	381	Total	C	N	O	S	0	0	0
			3056	1954	517	572	13			

There are 96 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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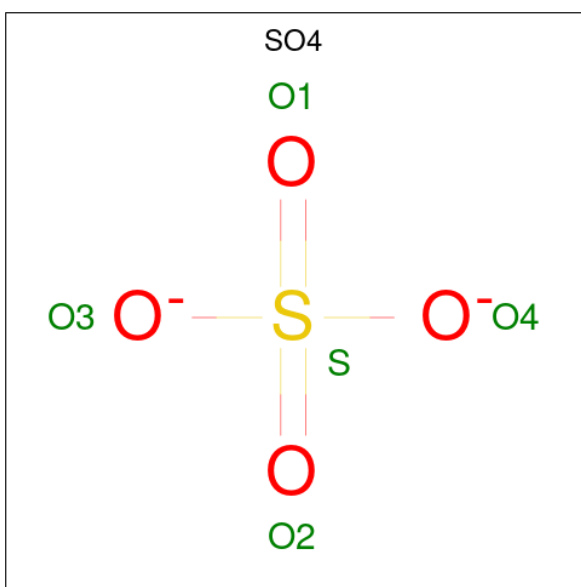
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	-	expression tag	UNP A0A5M5BWR5
A	23	SER	-	expression tag	UNP A0A5M5BWR5
A	173	ASN	GLN	engineered mutation	UNP A0A5M5BWR5
B	1	MET	-	initiating methionine	UNP A0A5M5BWR5
B	2	GLY	-	expression tag	UNP A0A5M5BWR5
B	3	SER	-	expression tag	UNP A0A5M5BWR5
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
B	173	ASN	GLN	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	16	PRO	-	expression tag	UNP A0A5M5BWR5
C	17	ARG	-	expression tag	UNP A0A5M5BWR5
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
C	173	ASN	GLN	engineered mutation	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
D	173	ASN	GLN	engineered mutation	UNP A0A5M5BWR5

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

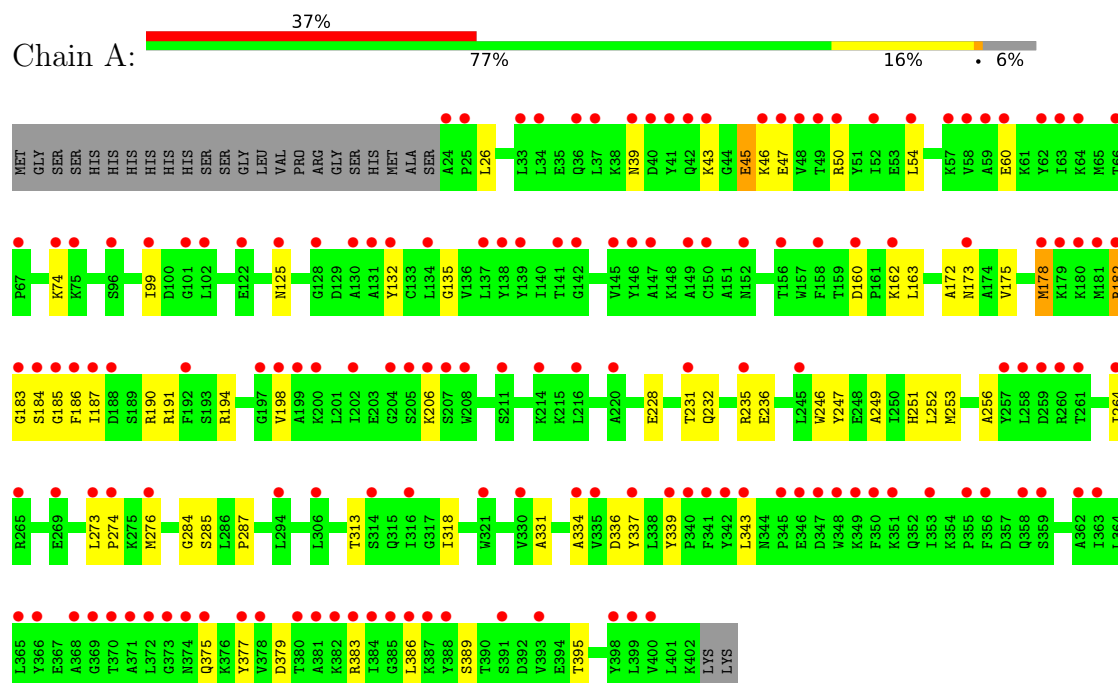
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total	O	0	0
			100	100		
3	B	95	Total	O	0	0
			95	95		
3	C	63	Total	O	0	0
			63	63		
3	D	72	Total	O	0	0
			72	72		

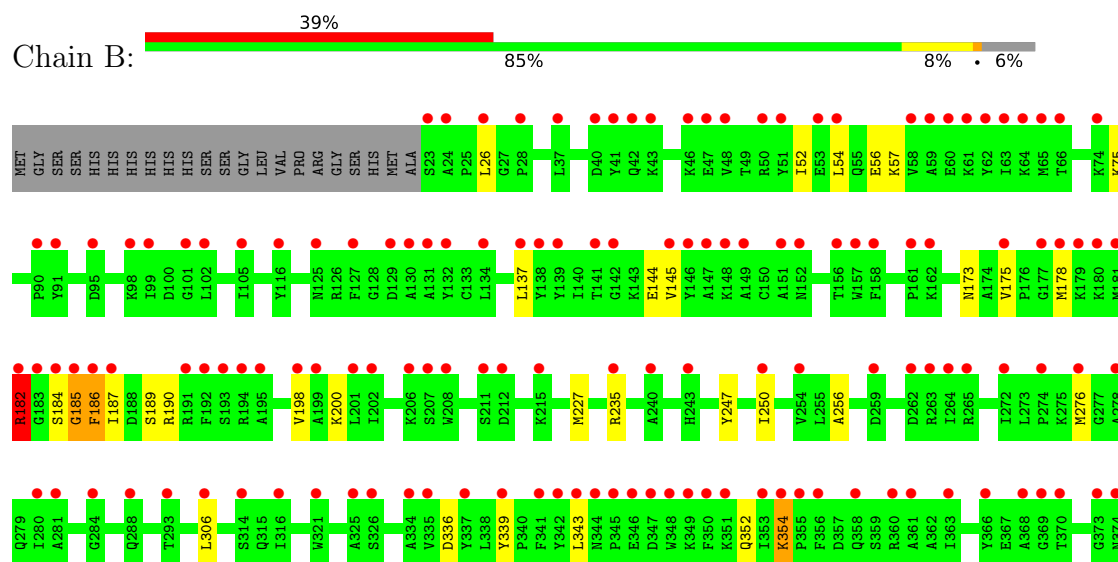
3 Residue-property plots

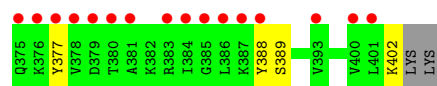
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Alginate lyase family protein

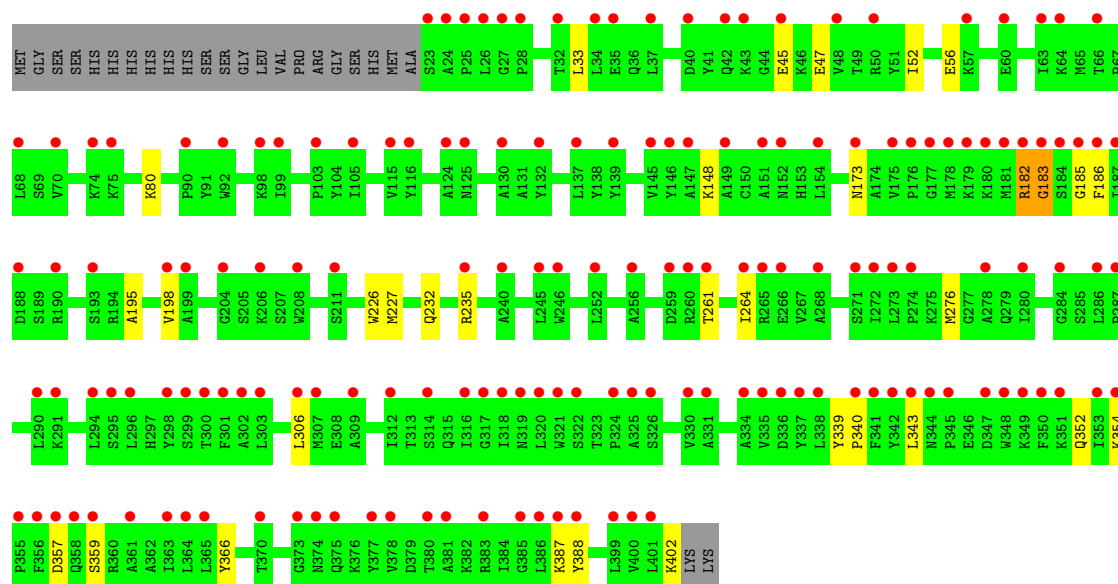
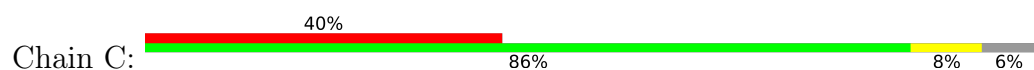


• Molecule 1: Alginate lyase family protein

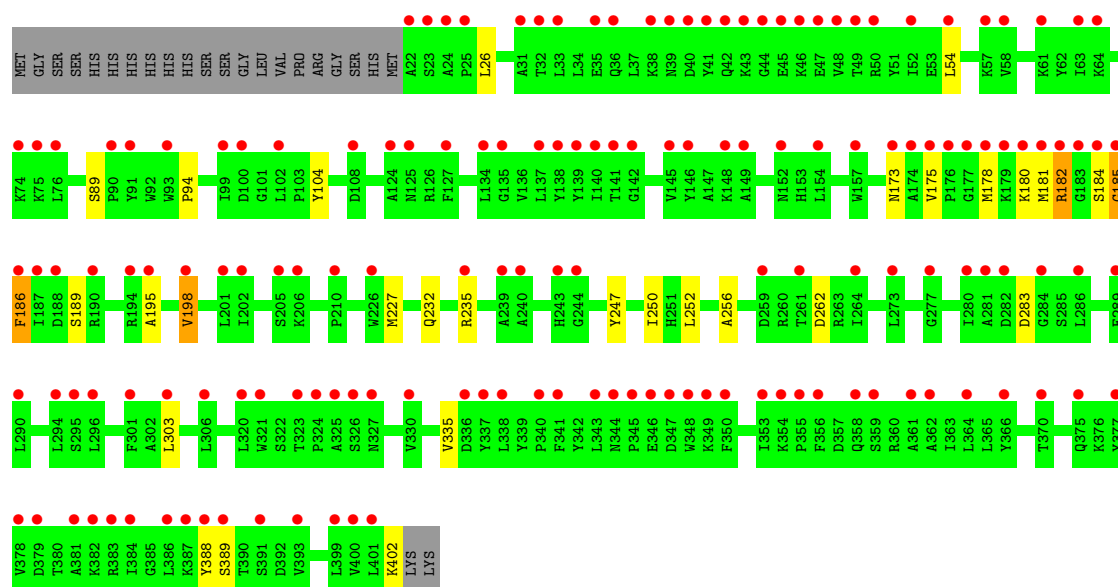
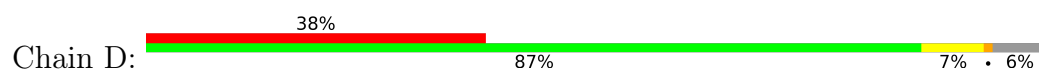




• Molecule 1: Alginate lyase family protein



• 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	196.78Å 89.13Å 145.83Å 90.00° 120.38° 90.00°	Depositor
Resolution (Å)	70.34 – 1.99 70.34 – 1.99	Depositor EDS
% Data completeness (in resolution range)	96.6 (70.34-1.99) 96.7 (70.34-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.250 , 0.277 0.250 , 0.277	Depositor DCC
R_{free} test set	7067 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.4	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	0.90	EDS
Total number of atoms	12549	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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 25.69 % 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 3.0229e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.38	0/3132	0.59	0/4245
1	B	0.39	0/3129	0.59	0/4241
1	C	0.38	0/3129	0.58	0/4241
1	D	0.34	0/3134	0.55	0/4248
All	All	0.37	0/12524	0.58	0/16975

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	182	ARG	Sidechain
1	D	182	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3051	0	3021	48	0
1	B	3051	0	3020	30	0
1	C	3051	0	3020	29	0
1	D	3056	0	3025	31	0
2	B	5	0	0	0	0
2	D	5	0	0	0	0
3	A	100	0	0	9	0
3	B	95	0	0	2	0
3	C	63	0	0	2	0
3	D	72	0	0	1	0
All	All	12549	0	12086	137	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 (137) 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:C:173:ASN:HD22	1:C:185:GLY:HA2	1.29	0.95
1:B:186:PHE:CZ	1:B:247:TYR:HA	2.04	0.93
1:C:173:ASN:ND2	1:C:185:GLY:HA2	1.95	0.81
1:A:175:VAL:N	3:A:503:HOH:O	2.13	0.79
1:B:186:PHE:HE1	1:B:227:MET:HE3	1.48	0.77
1:A:178:MET:SD	3:A:503:HOH:O	2.43	0.76
1:C:186:PHE:CZ	1:C:227:MET:HG2	2.22	0.74
1:B:186:PHE:CE2	1:B:247:TYR:HA	2.23	0.74
1:A:383:ARG:NH1	3:A:504:HOH:O	2.21	0.73
1:D:173:ASN:HB2	1:D:185:GLY:HA2	1.70	0.73
1:D:175:VAL:HG23	1:D:178:MET:HB2	1.72	0.72
1:A:60[A]:GLU:OE1	3:A:501:HOH:O	2.07	0.71
1:A:182:ARG:HG2	1:A:232:GLN:HG2	1.74	0.69
1:B:339:TYR:CZ	1:B:343:LEU:HD21	2.29	0.69
1:A:160:ASP:OD1	3:A:502:HOH:O	2.12	0.67
1:D:186:PHE:HE1	1:D:247:TYR:HA	1.59	0.66
1:B:336:ASP:OD1	1:B:377:TYR:OH	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASN:OD1	1:A:191:ARG:HD3	1.99	0.64
1:B:186:PHE:CE2	1:B:250:ILE:HD12	2.33	0.63
1:A:386:LEU:HD13	1:A:395:THR:HB	1.80	0.63
1:B:186:PHE:HZ	1:B:250:ILE:HB	1.64	0.62
1:C:148:LYS:NZ	3:C:503:HOH:O	2.32	0.62
1:A:191:ARG:NE	3:A:506:HOH:O	2.31	0.62
1:B:189:SER:HB2	1:B:250:ILE:HD13	1.82	0.62
1:B:182:ARG:HA	1:B:235:ARG:HH12	1.65	0.61
1:D:182:ARG:HH21	1:D:235:ARG:HD2	1.65	0.60
1:C:340:PRO:HA	1:C:343:LEU:HD12	1.83	0.60
1:A:39:ASN:OD1	1:A:43:LYS:NZ	2.29	0.60
1:A:375:GLN:HE22	1:A:379:ASP:CG	2.08	0.59
1:D:186:PHE:CE1	1:D:247:TYR:HA	2.37	0.59
1:A:54:LEU:HD21	1:A:389:SER:HA	1.86	0.58
1:C:339:TYR:CE2	1:C:343:LEU:HD11	2.41	0.55
1:B:200:LYS:NZ	3:B:606:HOH:O	2.39	0.55
1:B:276:MET:SD	1:B:306:LEU:HD13	2.47	0.55
1:B:182:ARG:HA	1:B:235:ARG:NH1	2.21	0.55
1:C:276:MET:SD	1:C:306:LEU:HD13	2.47	0.55
1:D:182:ARG:HD3	1:D:182:ARG:H	1.72	0.54
1:A:228:GLU:OE2	1:A:251:HIS:NE2	2.34	0.54
1:A:183:GLY:HA3	3:A:503:HOH:O	2.08	0.54
1:A:182:ARG:HG2	1:A:232:GLN:CG	2.39	0.53
1:B:186:PHE:CZ	1:B:250:ILE:HB	2.44	0.53
1:A:182:ARG:CG	1:A:232:GLN:HG2	2.39	0.53
1:A:26:LEU:HG	1:A:256:ALA:HB1	1.91	0.53
1:C:388:TYR:HA	1:C:402:LYS:HB3	1.90	0.53
1:D:178:MET:HG2	1:D:180:LYS:H	1.73	0.52
1:D:182:ARG:HD2	1:D:232:GLN:HG2	1.92	0.52
1:A:60[B]:GLU:HG3	3:A:501:HOH:O	2.10	0.52
1:A:173:ASN:HB3	1:A:184:SER:HB3	1.92	0.52
1:C:195:ALA:O	1:C:198:VAL:HG12	2.09	0.52
1:B:185:GLY:O	1:B:187:ILE:N	2.43	0.51
1:A:379:ASP:O	1:A:383:ARG:HD2	2.10	0.51
1:C:354:LYS:NZ	3:C:505:HOH:O	2.44	0.51
1:A:336:ASP:OD1	1:A:377:TYR:OH	2.28	0.51
1:A:276:MET:SD	1:A:331:ALA:HB2	2.51	0.51
1:D:89:SER:HB3	1:D:175:VAL:HG12	1.91	0.51
1:D:182:ARG:HG2	1:D:184:SER:H	1.76	0.51
1:D:178:MET:HG2	1:D:180:LYS:HB2	1.92	0.50
1:A:186:PHE:HE2	1:A:236:GLU:HG2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:PHE:CE2	1:D:227:MET:HE3	2.47	0.50
1:B:352:GLN:HG3	1:B:354:LYS:O	2.11	0.49
1:C:186:PHE:CE1	1:C:226:TRP:HZ3	2.30	0.49
1:C:186:PHE:CD1	1:C:226:TRP:HZ3	2.31	0.49
1:A:206:LYS:N	1:A:206:LYS:HD2	2.27	0.49
1:D:186:PHE:CZ	1:D:227:MET:HE3	2.47	0.49
1:A:339:TYR:CE2	1:A:343:LEU:HD11	2.47	0.49
1:B:26:LEU:HG	1:B:256:ALA:HB1	1.95	0.49
1:C:182:ARG:O	1:C:232:GLN:NE2	2.24	0.48
1:D:388:TYR:HA	1:D:402:LYS:HB3	1.95	0.48
1:B:175:VAL:HB	1:B:178:MET:SD	2.53	0.48
1:D:283:ASP:OD2	3:D:601:HOH:O	2.19	0.48
1:B:388:TYR:HA	1:B:402:LYS:HB3	1.96	0.47
1:A:46:LYS:HE2	1:A:50:ARG:NH1	2.29	0.47
1:A:187:ILE:HD11	1:A:246:TRP:CD1	2.49	0.47
1:B:52:ILE:O	1:B:56:GLU:HG3	2.14	0.47
1:B:173:ASN:HD22	1:B:185:GLY:HA2	1.80	0.47
1:D:26:LEU:HG	1:D:256:ALA:HB1	1.97	0.47
1:D:173:ASN:HD22	1:D:185:GLY:HA2	1.80	0.47
1:D:180:LYS:HB3	1:D:181:MET:H	1.51	0.47
1:B:144:GLU:OE1	3:B:601:HOH:O	2.20	0.47
1:A:190:ARG:O	1:A:194:ARG:HG3	2.15	0.47
1:C:182:ARG:HA	1:C:235:ARG:HH12	1.80	0.47
1:C:183:GLY:N	1:C:235:ARG:HH12	2.14	0.46
1:D:303:LEU:HD13	1:D:335:VAL:HG22	1.97	0.46
1:A:182:ARG:HD3	1:A:185:GLY:H	1.81	0.46
1:B:185:GLY:O	1:B:186:PHE:C	2.58	0.45
1:D:195:ALA:O	1:D:198:VAL:HG12	2.17	0.45
1:A:45:GLU:OE1	1:A:47:GLU:HB3	2.16	0.45
1:C:173:ASN:HB2	1:C:185:GLY:CA	2.46	0.45
1:C:186:PHE:CE2	1:C:227:MET:HE3	2.52	0.45
1:C:387:LYS:HA	1:C:387:LYS:HD2	1.66	0.45
1:A:186:PHE:CE2	1:A:236:GLU:HG2	2.52	0.45
1:A:284:GLY:O	1:A:334:ALA:HA	2.18	0.44
1:C:186:PHE:HZ	1:C:227:MET:HG2	1.80	0.44
1:A:74:LYS:HE2	1:A:74:LYS:HB3	1.79	0.44
1:D:186:PHE:CD1	1:D:186:PHE:C	2.96	0.44
1:C:45:GLU:OE2	1:C:47:GLU:HB3	2.18	0.44
1:A:162:LYS:HG2	1:A:163:LEU:HG	1.99	0.43
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.78	0.43
1:D:189:SER:HB2	1:D:250:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LEU:HD21	1:B:389:SER:HA	2.01	0.43
1:D:182:ARG:HB3	1:D:232:GLN:OE1	2.18	0.43
1:A:178:MET:HE1	3:A:593:HOH:O	2.19	0.43
1:A:285:SER:O	1:A:287:PRO:HD3	2.18	0.43
1:B:339:TYR:CE2	1:B:343:LEU:HD21	2.54	0.43
1:D:182:ARG:HH21	1:D:235:ARG:HB3	1.82	0.43
1:C:182:ARG:HA	1:C:182:ARG:HD3	1.82	0.43
1:A:273:LEU:HB2	1:A:274:PRO:HD3	2.01	0.43
1:A:273:LEU:HD23	1:A:276:MET:HE2	2.01	0.43
1:D:54:LEU:HD21	1:D:389:SER:HA	2.00	0.43
1:A:231:THR:HG22	1:A:235:ARG:HD3	2.00	0.42
1:A:249:ALA:O	1:A:253:MET:HG3	2.19	0.42
1:B:173:ASN:ND2	1:B:185:GLY:HA2	2.33	0.42
1:A:252:LEU:HD22	1:A:264:ILE:HG12	2.00	0.42
1:B:186:PHE:C	1:B:186:PHE:CD2	2.96	0.42
1:B:190:ARG:HB3	1:B:250:ILE:HD11	2.00	0.42
1:C:182:ARG:HA	1:C:235:ARG:NH1	2.35	0.42
1:C:357:ASP:OD1	1:C:359:SER:HB3	2.19	0.42
1:C:182:ARG:HD3	1:C:235:ARG:NH1	2.35	0.41
1:C:352:GLN:HG3	1:C:354:LYS:O	2.20	0.41
1:C:80:LYS:HA	1:C:80:LYS:HD3	1.93	0.41
1:A:285:SER:HB3	1:A:337:TYR:CE1	2.56	0.41
1:A:172:ALA:O	1:A:182:ARG:NH2	2.54	0.41
1:D:94:PRO:HG3	1:D:104:TYR:CZ	2.55	0.41
1:A:135:GLY:HA3	1:A:198:VAL:CG1	2.50	0.41
1:D:262:ASP:N	1:D:262:ASP:OD1	2.53	0.41
1:B:184:SER:O	1:B:185:GLY:C	2.64	0.41
1:A:99:ILE:HD11	1:B:57:LYS:C	2.46	0.41
1:D:173:ASN:ND2	1:D:185:GLY:HA2	2.36	0.41
1:D:227:MET:HE2	1:D:227:MET:HB3	1.89	0.41
1:D:252:LEU:HD23	1:D:252:LEU:HA	1.85	0.40
1:A:186:PHE:CE2	1:A:247:TYR:HD2	2.39	0.40
1:C:261:THR:HA	1:C:264:ILE:HD12	2.02	0.40
1:A:313:THR:HB	1:A:318:ILE:HB	2.03	0.40
1:C:52:ILE:O	1:C:56:GLU:HG3	2.21	0.40
1:D:182:ARG:NH2	1:D:235:ARG:HD2	2.36	0.40
1:A:132:TYR:CD1	1:A:198:VAL:HG21	2.57	0.40
1:C:33:LEU:HD11	1:C:366:TYR:CE2	2.57	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	378/404 (94%)	366 (97%)	12 (3%)	0	100	100
1	B	378/404 (94%)	366 (97%)	10 (3%)	2 (0%)	24	21
1	C	378/404 (94%)	369 (98%)	8 (2%)	1 (0%)	36	35
1	D	379/404 (94%)	368 (97%)	10 (3%)	1 (0%)	36	35
All	All	1513/1616 (94%)	1469 (97%)	40 (3%)	4 (0%)	36	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	PHE
1	B	185	GLY
1	D	185	GLY
1	C	183	GLY

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	324/344 (94%)	321 (99%)	3 (1%)	70	78
1	B	324/344 (94%)	319 (98%)	5 (2%)	57	64
1	C	324/344 (94%)	323 (100%)	1 (0%)	86	91
1	D	324/344 (94%)	322 (99%)	2 (1%)	78	85
All	All	1296/1376 (94%)	1285 (99%)	11 (1%)	73	80

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

Mol	Chain	Res	Type
1	A	45	GLU
1	A	178	MET
1	A	182	ARG
1	B	75	LYS
1	B	145	VAL
1	B	182	ARG
1	B	198	VAL
1	B	354	LYS
1	C	182	ARG
1	D	186	PHE
1	D	198	VAL

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	42	GLN
1	A	242	ASN
1	A	358	GLN
1	A	375	GLN
1	B	375	GLN
1	C	125	ASN
1	D	42	GLN
1	D	152	ASN
1	D	243	HIS
1	D	375	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	501	-	4,4,4	0.71	0	6,6,6	0.11	0
2	SO4	D	501	-	4,4,4	0.68	0	6,6,6	0.13	0

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	379/404 (93%)	1.84	150 (39%) 1 1	26, 36, 55, 96	1 (0%)
1	B	380/404 (94%)	1.92	156 (41%) 0 1	26, 38, 53, 100	0
1	C	380/404 (94%)	1.97	162 (42%) 0 1	28, 40, 57, 97	0
1	D	381/404 (94%)	1.98	155 (40%) 0 1	27, 42, 63, 120	0
All	All	1520/1616 (94%)	1.93	623 (40%) 0 1	26, 39, 58, 120	1 (0%)

All (623) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	22	ALA	13.1
1	B	186	PHE	10.1
1	B	185	GLY	9.4
1	D	186	PHE	9.2
1	C	186	PHE	8.9
1	A	182	ARG	8.7
1	C	185	GLY	8.7
1	B	145	VAL	8.1
1	A	183	GLY	8.0
1	C	381	ALA	7.2
1	A	180	LYS	6.8
1	B	182	ARG	6.7
1	B	183	GLY	6.7
1	C	182	ARG	6.6
1	B	180	LYS	6.6
1	B	187	ILE	6.5
1	D	44	GLY	6.4
1	D	43	LYS	6.4
1	D	39	ASN	6.3
1	D	187	ILE	6.2
1	C	180	LYS	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	178	MET	6.1
1	D	102	LEU	6.1
1	C	378	VAL	6.0
1	C	353	ILE	6.0
1	A	349	LYS	6.0
1	D	179	LYS	5.9
1	B	385	GLY	5.9
1	C	99	ILE	5.7
1	C	184	SER	5.7
1	D	42	GLN	5.6
1	D	183	GLY	5.6
1	D	182	ARG	5.6
1	C	179	LYS	5.5
1	D	184	SER	5.4
1	C	183	GLY	5.4
1	C	306	LEU	5.3
1	B	202	ILE	5.3
1	B	184	SER	5.3
1	D	180	LYS	5.2
1	C	356	PHE	5.2
1	D	185	GLY	5.2
1	D	378	VAL	5.1
1	A	187	ILE	5.0
1	D	178	MET	5.0
1	B	339	TYR	5.0
1	C	303	LEU	4.9
1	A	179	LYS	4.9
1	A	186	PHE	4.9
1	A	378	VAL	4.9
1	C	400	VAL	4.8
1	D	243	HIS	4.7
1	C	345	PRO	4.7
1	C	175	VAL	4.7
1	B	384	ILE	4.7
1	B	349	LYS	4.7
1	D	99	ILE	4.7
1	A	345	PRO	4.6
1	D	149	ALA	4.6
1	C	401	LEU	4.6
1	A	145	VAL	4.5
1	A	369	GLY	4.4
1	C	321	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	294	LEU	4.4
1	B	179	LYS	4.4
1	A	102	LEU	4.4
1	C	364	LEU	4.3
1	D	138	TYR	4.3
1	C	348	TRP	4.3
1	B	326	SER	4.3
1	D	140	ILE	4.3
1	A	381	ALA	4.3
1	D	46	LYS	4.3
1	C	342	TYR	4.3
1	B	147	ALA	4.3
1	C	25	PRO	4.3
1	A	64	LYS	4.2
1	B	321	TRP	4.2
1	C	300	THR	4.2
1	D	341	PHE	4.2
1	D	348	TRP	4.2
1	D	175	VAL	4.1
1	D	24	ALA	4.1
1	C	50	ARG	4.1
1	D	23	SER	4.1
1	A	343	LEU	4.1
1	B	341	PHE	4.0
1	C	318	ILE	4.0
1	A	371	ALA	4.0
1	C	280	ILE	4.0
1	A	43	LYS	4.0
1	D	40	ASP	4.0
1	C	181	MET	4.0
1	A	377	TYR	3.9
1	D	377	TYR	3.9
1	D	181	MET	3.9
1	A	374	ASN	3.9
1	B	130	ALA	3.9
1	D	239	ALA	3.9
1	B	64	LYS	3.9
1	A	138	TYR	3.9
1	B	348	TRP	3.9
1	C	246	TRP	3.9
1	A	142	GLY	3.9
1	A	385	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	301	PHE	3.9
1	A	181	MET	3.9
1	D	296	LEU	3.8
1	D	31	ALA	3.8
1	D	240	ALA	3.8
1	B	99	ILE	3.8
1	B	374	ASN	3.8
1	C	45	GLU	3.8
1	C	359	SER	3.8
1	C	34	LEU	3.8
1	A	99	ILE	3.8
1	B	53	GLU	3.8
1	B	134	LEU	3.8
1	B	142	GLY	3.8
1	C	28	PRO	3.8
1	D	383	ARG	3.8
1	D	290	LEU	3.7
1	C	325	ALA	3.7
1	D	280	ILE	3.7
1	A	58	VAL	3.7
1	C	290	LEU	3.7
1	D	194	ARG	3.7
1	B	250	ILE	3.7
1	B	400	VAL	3.7
1	A	365	LEU	3.7
1	A	391	SER	3.7
1	C	23	SER	3.6
1	A	149	ALA	3.6
1	B	388	TYR	3.6
1	B	191	ARG	3.6
1	D	353	ILE	3.6
1	D	370	THR	3.6
1	A	184	SER	3.6
1	C	240	ALA	3.6
1	D	388	TYR	3.6
1	A	178	MET	3.6
1	C	299	SER	3.6
1	A	130	ALA	3.6
1	D	325	ALA	3.6
1	B	335	VAL	3.6
1	D	32	THR	3.6
1	C	336	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	57	LYS	3.6
1	D	306	LEU	3.6
1	D	321	TRP	3.5
1	D	384	ILE	3.5
1	A	46	LYS	3.5
1	B	151	ALA	3.5
1	A	380	THR	3.5
1	A	400	VAL	3.5
1	B	350	PHE	3.5
1	A	334	ALA	3.5
1	C	286	LEU	3.5
1	C	320	LEU	3.5
1	B	51	TYR	3.4
1	B	181	MET	3.4
1	A	220	ALA	3.4
1	C	344	ASN	3.4
1	D	340	PRO	3.4
1	C	178	MET	3.4
1	B	346	GLU	3.4
1	D	336	ASP	3.4
1	B	42	GLN	3.4
1	B	199	ALA	3.4
1	D	273	LEU	3.4
1	A	146	TYR	3.4
1	D	74	LYS	3.4
1	D	139	TYR	3.4
1	D	346	GLU	3.4
1	C	42	GLN	3.4
1	A	348	TRP	3.4
1	D	359	SER	3.4
1	D	343	LEU	3.4
1	D	350	PHE	3.4
1	D	349	LYS	3.3
1	A	62	TYR	3.3
1	B	353	ILE	3.3
1	D	36	GLN	3.3
1	A	339	TYR	3.3
1	A	59	ALA	3.3
1	A	60[A]	GLU	3.3
1	A	34	LEU	3.3
1	C	176	PRO	3.3
1	D	355	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	388	TYR	3.3
1	C	361	ALA	3.3
1	A	134	LEU	3.3
1	A	386	LEU	3.3
1	C	380	THR	3.3
1	B	383	ARG	3.3
1	A	205	SER	3.3
1	C	187	ILE	3.2
1	A	347	ASP	3.2
1	C	343	LEU	3.2
1	D	137	LEU	3.2
1	D	142	GLY	3.2
1	C	132	TYR	3.2
1	D	356	PHE	3.2
1	C	272	ILE	3.2
1	D	176	PRO	3.2
1	A	372	LEU	3.2
1	B	387	LYS	3.2
1	C	27	GLY	3.2
1	A	47	GLU	3.2
1	B	74	LYS	3.1
1	B	240	ALA	3.1
1	C	147	ALA	3.1
1	C	316	ILE	3.1
1	A	276	MET	3.1
1	C	198	VAL	3.1
1	C	295	SER	3.1
1	D	54	LEU	3.1
1	B	63	ILE	3.1
1	A	185	GLY	3.1
1	B	342	TYR	3.1
1	A	40	ASP	3.1
1	D	38	LYS	3.1
1	A	147	ALA	3.1
1	C	259	ASP	3.1
1	B	354	LYS	3.1
1	A	211	SER	3.1
1	A	362	ALA	3.1
1	B	343	LEU	3.0
1	B	138	TYR	3.0
1	B	337	TYR	3.0
1	B	351	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	57	LYS	3.0
1	D	145	VAL	3.0
1	D	93	TRP	3.0
1	A	152	ASN	3.0
1	C	350	PHE	3.0
1	B	23	SER	3.0
1	B	215	LYS	3.0
1	A	52	ILE	3.0
1	B	201	LEU	3.0
1	C	296	LEU	3.0
1	B	175	VAL	3.0
1	D	41	TYR	3.0
1	C	60	GLU	3.0
1	B	40	ASP	3.0
1	B	379	ASP	3.0
1	D	324	PRO	3.0
1	A	351	LYS	3.0
1	C	151	ALA	3.0
1	C	302	ALA	3.0
1	B	386	LEU	3.0
1	A	48	VAL	3.0
1	A	257	TYR	3.0
1	B	43	LYS	3.0
1	C	291	LYS	3.0
1	D	177	GLY	3.0
1	A	235	ARG	3.0
1	C	383	ARG	3.0
1	B	361	ALA	3.0
1	A	122	GLU	3.0
1	B	272	ILE	3.0
1	C	386	LEU	2.9
1	D	154	LEU	2.9
1	D	48	VAL	2.9
1	D	58	VAL	2.9
1	A	259	ASP	2.9
1	A	260	ARG	2.9
1	A	340	PRO	2.9
1	A	341	PHE	2.9
1	A	350	PHE	2.9
1	C	103	PRO	2.9
1	D	127	PHE	2.9
1	A	208	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	321	TRP	2.9
1	B	208	TRP	2.9
1	B	344	ASN	2.9
1	B	195	ALA	2.9
1	C	334	ALA	2.9
1	D	281	ALA	2.9
1	B	102	LEU	2.9
1	B	211	SER	2.9
1	C	260	ARG	2.9
1	C	335	VAL	2.9
1	D	400	VAL	2.9
1	A	139	TYR	2.9
1	D	337	TYR	2.9
1	B	380	THR	2.9
1	C	152	ASN	2.9
1	B	46	LYS	2.9
1	B	98	LYS	2.9
1	C	354	LYS	2.9
1	B	363	ILE	2.9
1	C	26	LEU	2.9
1	B	369	GLY	2.9
1	B	373	GLY	2.9
1	C	177	GLY	2.9
1	A	41	TYR	2.9
1	B	139	TYR	2.9
1	C	337	TYR	2.9
1	A	54	LEU	2.9
1	D	286	LEU	2.9
1	D	284	GLY	2.9
1	D	198	VAL	2.8
1	C	298	TYR	2.8
1	A	382	LYS	2.8
1	B	148	LYS	2.8
1	C	74	LYS	2.8
1	C	322	SER	2.8
1	A	63	ILE	2.8
1	B	37	LEU	2.8
1	B	280	ILE	2.8
1	C	273	LEU	2.8
1	D	338	LEU	2.8
1	D	358	GLN	2.8
1	D	206	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	41	TYR	2.8
1	D	45	GLU	2.8
1	C	24	ALA	2.8
1	B	401	LEU	2.8
1	D	64	LYS	2.8
1	D	362	ALA	2.8
1	A	375	GLN	2.8
1	A	74	LYS	2.8
1	C	252	LEU	2.8
1	D	141	THR	2.8
1	D	323	THR	2.8
1	D	345	PRO	2.8
1	A	337	TYR	2.7
1	B	278	ALA	2.7
1	C	341	PHE	2.7
1	C	387	LYS	2.7
1	B	101	GLY	2.7
1	D	76	LEU	2.7
1	D	294	LEU	2.7
1	C	105	ILE	2.7
1	C	347	ASP	2.7
1	B	355	PRO	2.7
1	C	193	SER	2.7
1	A	335	VAL	2.7
1	D	375	GLN	2.7
1	A	57	LYS	2.7
1	A	206	LYS	2.7
1	B	146	TYR	2.7
1	D	124	ALA	2.7
1	D	174	ALA	2.7
1	B	127	PHE	2.7
1	B	192	PHE	2.7
1	B	141	THR	2.7
1	C	365	LEU	2.7
1	C	363	ILE	2.7
1	A	36	GLN	2.7
1	C	173	ASN	2.7
1	A	214	LYS	2.7
1	A	199	ALA	2.7
1	B	325	ALA	2.7
1	B	381	ALA	2.7
1	C	309	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	388	TYR	2.7
1	A	49	THR	2.7
1	A	37	LEU	2.7
1	C	37	LEU	2.7
1	D	201	LEU	2.7
1	D	61	LYS	2.7
1	B	131	ALA	2.6
1	C	204	GLY	2.6
1	C	373	GLY	2.6
1	A	342	TYR	2.6
1	A	366	TYR	2.6
1	B	259	ASP	2.6
1	D	259	ASP	2.6
1	D	235	ARG	2.6
1	B	60	GLU	2.6
1	C	75	LYS	2.6
1	A	245	LEU	2.6
1	A	353	ILE	2.6
1	A	373	GLY	2.6
1	D	244	GLY	2.6
1	A	50	ARG	2.6
1	C	146	TYR	2.6
1	A	231	THR	2.6
1	D	387	LYS	2.6
1	C	314	SER	2.6
1	D	205	SER	2.6
1	D	389	SER	2.6
1	A	306	LEU	2.6
1	B	281	ALA	2.6
1	B	393	VAL	2.6
1	B	206	LYS	2.6
1	C	351	LYS	2.6
1	A	132	TYR	2.6
1	A	398	TYR	2.6
1	C	245	LEU	2.6
1	C	317	GLY	2.6
1	C	206	LYS	2.6
1	A	368	ALA	2.6
1	B	378	VAL	2.6
1	C	331	ALA	2.6
1	C	139	TYR	2.5
1	B	158	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	356	PHE	2.5
1	C	301	PHE	2.5
1	D	364	LEU	2.5
1	B	177	GLY	2.5
1	D	277	GLY	2.5
1	B	59	ALA	2.5
1	B	334	ALA	2.5
1	A	198	VAL	2.5
1	B	58	VAL	2.5
1	C	145	VAL	2.5
1	B	156	THR	2.5
1	B	235	ARG	2.5
1	A	358	GLN	2.5
1	B	47	GLU	2.5
1	C	287	PRO	2.5
1	B	262	ASP	2.5
1	B	366	TYR	2.5
1	C	357	ASP	2.5
1	A	356	PHE	2.5
1	C	92	TRP	2.5
1	C	312	ILE	2.5
1	D	226	TRP	2.5
1	C	66	THR	2.5
1	C	330	VAL	2.5
1	A	158	PHE	2.5
1	A	204	GLY	2.5
1	C	154	LEU	2.5
1	B	316	ILE	2.5
1	C	63	ILE	2.5
1	D	47	GLU	2.5
1	B	95	ASP	2.5
1	B	347	ASP	2.5
1	C	48	VAL	2.5
1	C	64	LYS	2.5
1	A	355	PRO	2.5
1	B	161	PRO	2.5
1	B	62	TYR	2.4
1	C	377	TYR	2.4
1	D	173	ASN	2.4
1	A	33	LEU	2.4
1	D	134	LEU	2.4
1	D	401	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	316	ILE	2.4
1	A	363	ILE	2.4
1	C	264	ILE	2.4
1	A	156	THR	2.4
1	D	100	ASP	2.4
1	C	324	PRO	2.4
1	B	54	LEU	2.4
1	B	306	LEU	2.4
1	A	261	THR	2.4
1	B	66	THR	2.4
1	B	368	ALA	2.4
1	C	256	ALA	2.4
1	A	330	VAL	2.4
1	B	198	VAL	2.4
1	B	194	ARG	2.4
1	B	149	ALA	2.4
1	D	35	GLU	2.4
1	B	358	GLN	2.4
1	D	344	ASN	2.4
1	C	43	LYS	2.4
1	D	354	LYS	2.4
1	B	26	LEU	2.3
1	C	68	LEU	2.3
1	B	288	GLN	2.3
1	A	24	ALA	2.3
1	A	202	ILE	2.3
1	A	314	SER	2.3
1	C	115	VAL	2.3
1	B	50	ARG	2.3
1	A	346	GLU	2.3
1	B	137	LEU	2.3
1	C	137	LEU	2.3
1	A	66	THR	2.3
1	C	32	THR	2.3
1	C	261	THR	2.3
1	D	146	TYR	2.3
1	D	52	ILE	2.3
1	D	25	PRO	2.3
1	B	212	ASP	2.3
1	C	70	VAL	2.3
1	D	379	ASP	2.3
1	A	200	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	349	LYS	2.3
1	B	28	PRO	2.3
1	C	124	ALA	2.3
1	C	340	PRO	2.3
1	A	265	ARG	2.3
1	A	96	SER	2.3
1	C	326	SER	2.3
1	C	35	GLU	2.3
1	C	188	ASP	2.3
1	C	375	GLN	2.3
1	D	125	ASN	2.3
1	A	141	THR	2.3
1	A	399	LEU	2.3
1	C	294	LEU	2.3
1	C	399	LEU	2.3
1	D	91	TYR	2.2
1	D	361	ALA	2.2
1	B	314	SER	2.2
1	A	39	ASN	2.2
1	C	374	ASN	2.2
1	B	276	MET	2.2
1	A	370	THR	2.2
1	C	265	ARG	2.2
1	C	338	LEU	2.2
1	A	25	PRO	2.2
1	A	42	GLN	2.2
1	B	284	GLY	2.2
1	B	375	GLN	2.2
1	D	347	ASP	2.2
1	D	381	ALA	2.2
1	A	192	PHE	2.2
1	B	116	TYR	2.2
1	A	384	ILE	2.2
1	D	63	ILE	2.2
1	A	387	LYS	2.2
1	C	319	ASN	2.2
1	D	49	THR	2.2
1	A	216	LEU	2.2
1	D	320	LEU	2.2
1	A	188	ASP	2.2
1	A	207	SER	2.2
1	D	188	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	274	PRO	2.2
1	B	345	PRO	2.2
1	C	355	PRO	2.2
1	B	377	TYR	2.2
1	B	264	ILE	2.2
1	D	157	TRP	2.2
1	A	383	ARG	2.2
1	B	263	ARG	2.2
1	D	289	GLU	2.2
1	B	254	VAL	2.2
1	A	359	SER	2.2
1	D	135	GLY	2.2
1	D	386	LEU	2.2
1	C	98	LYS	2.2
1	D	148	LYS	2.2
1	B	243	HIS	2.1
1	D	190	ARG	2.2
1	B	125	ASN	2.1
1	D	327	ASN	2.1
1	C	266	GLU	2.1
1	A	264	ILE	2.1
1	B	157	TRP	2.1
1	C	358	GLN	2.1
1	D	282	ASP	2.1
1	A	393	VAL	2.1
1	D	295	SER	2.1
1	C	385	GLY	2.1
1	A	137	LEU	2.1
1	A	75	LYS	2.1
1	B	61	LYS	2.1
1	A	125	ASN	2.1
1	C	125	ASN	2.1
1	C	130	ALA	2.1
1	C	268	ALA	2.1
1	D	152	ASN	2.1
1	B	132	TYR	2.1
1	D	202	ILE	2.1
1	D	366	TYR	2.1
1	D	108	ASP	2.1
1	B	193	SER	2.1
1	B	370	THR	2.1
1	A	101	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	265	ARG	2.1
1	B	360	ARG	2.1
1	B	376	LYS	2.1
1	D	75	LYS	2.1
1	A	269	GLU	2.1
1	A	258	LEU	2.1
1	A	273	LEU	2.1
1	C	90	PRO	2.1
1	C	274	PRO	2.1
1	D	33	LEU	2.1
1	D	303	LEU	2.1
1	A	131	ALA	2.1
1	D	195	ALA	2.1
1	B	129	ASP	2.1
1	C	40	ASP	2.1
1	C	116	TYR	2.1
1	B	207	SER	2.1
1	A	128	GLY	2.1
1	D	393	VAL	2.1
1	B	90	PRO	2.1
1	B	24	ALA	2.1
1	C	149	ALA	2.1
1	C	278	ALA	2.1
1	C	235	ARG	2.1
1	B	105	ILE	2.0
1	B	162	LYS	2.0
1	C	271	SER	2.0
1	D	264	ILE	2.0
1	B	91	TYR	2.0
1	B	65	MET	2.0
1	B	293	THR	2.0
1	C	307	MET	2.0
1	C	370	THR	2.0
1	C	284	GLY	2.0
1	B	152	ASN	2.0
1	A	67	PRO	2.0
1	A	274	PRO	2.0
1	B	48	VAL	2.0
1	D	330	VAL	2.0
1	A	150	CYS	2.0
1	C	208	TRP	2.0
1	D	399	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	199	ALA	2.0
1	A	160	ASP	2.0
1	A	162	LYS	2.0
1	D	382	LYS	2.0
1	C	211	SER	2.0
1	D	326	SER	2.0
1	D	391	SER	2.0
1	A	173	ASN	2.0
1	A	197	GLY	2.0
1	D	261	THR	2.0
1	D	90	PRO	2.0
1	D	210	PRO	2.0
1	C	190	ARG	2.0
1	D	50	ARG	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	SO4	D	501	5/5	0.35	0.24	108,113,122,124	0
2	SO4	B	501	5/5	0.62	0.17	64,66,80,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.