



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 29, 2025 – 08:13 am BST

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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
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

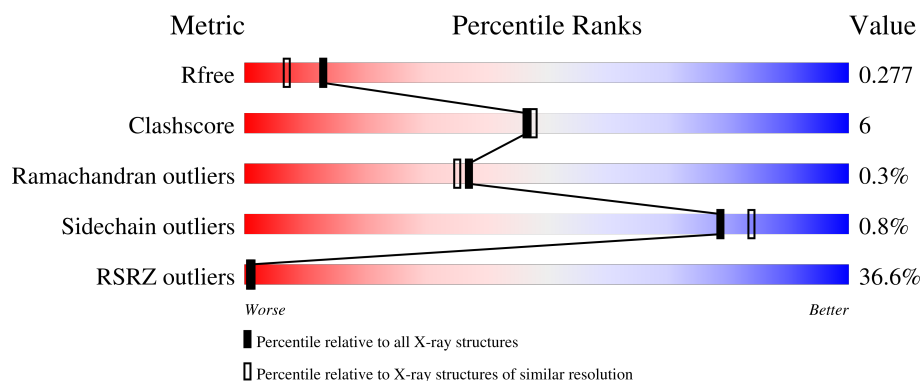
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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		

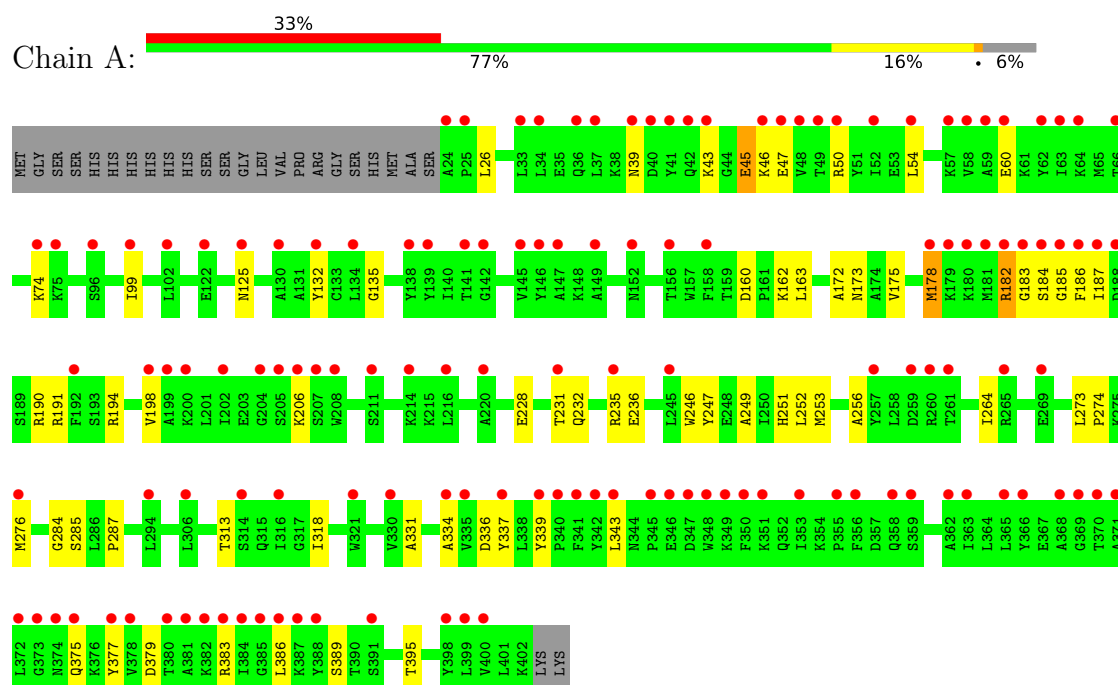
- Molecule 3 is water.

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		

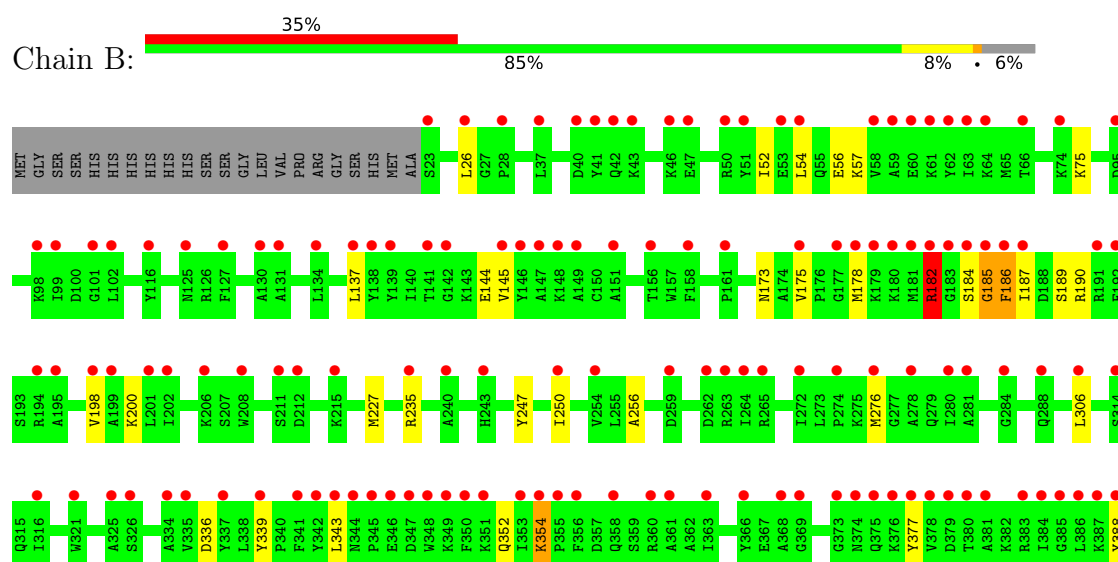
3 Residue-property plots [i](#)

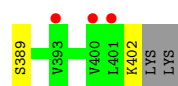
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

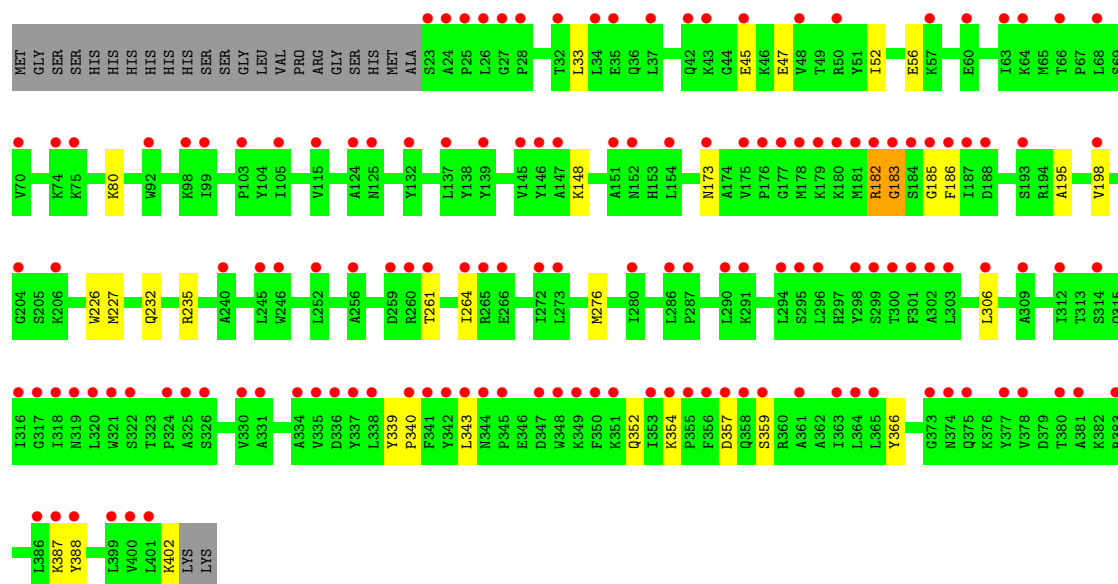
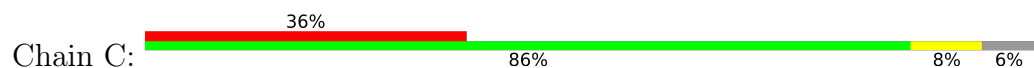


• Molecule 1: Alginate lyase family protein

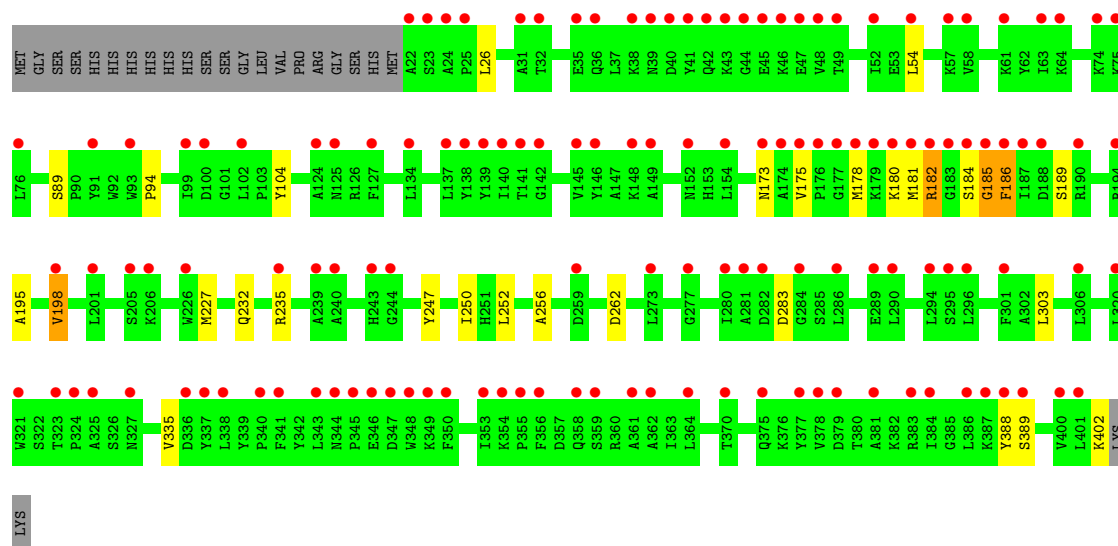
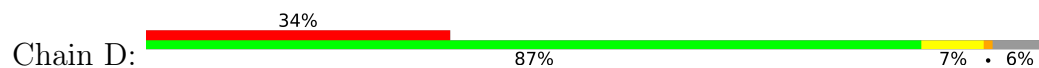




• Molecule 1: Alginate lyase family protein



• 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	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	7298 reflections (4.91%)	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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%)	25	21
1	C	378/404 (94%)	369 (98%)	8 (2%)	1 (0%)	37	35
1	D	379/404 (94%)	368 (97%)	10 (3%)	1 (0%)	37	35
All	All	1513/1616 (94%)	1469 (97%)	40 (3%)	4 (0%)	37	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%)	75	81
1	B	324/344 (94%)	319 (98%)	5 (2%)	60	66
1	C	324/344 (94%)	323 (100%)	1 (0%)	91	94
1	D	324/344 (94%)	322 (99%)	2 (1%)	84	88
All	All	1296/1376 (94%)	1285 (99%)	11 (1%)	79	84

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

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	0.64	0	6,6,6	0.14	0
2	SO4	D	501	-	4,4,4	0.61	0	6,6,6	0.10	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	379/404 (93%)	1.71	135 (35%) 1 1	26, 36, 55, 96	1 (0%)
1	B	380/404 (94%)	1.79	141 (37%) 1 1	26, 38, 53, 100	0
1	C	380/404 (94%)	1.83	144 (37%) 1 1	28, 40, 57, 97	0
1	D	381/404 (94%)	1.84	136 (35%) 1 1	27, 42, 63, 120	0
All	All	1520/1616 (94%)	1.79	556 (36%) 1 1	26, 39, 58, 120	1 (0%)

All (556) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	22	ALA	12.6
1	B	186	PHE	9.8
1	B	185	GLY	9.1
1	D	186	PHE	8.9
1	C	186	PHE	8.6
1	A	182	ARG	8.6
1	C	185	GLY	8.3
1	B	145	VAL	7.8
1	A	183	GLY	7.6
1	C	381	ALA	6.9
1	A	180	LYS	6.8
1	B	182	ARG	6.6
1	B	180	LYS	6.5
1	C	182	ARG	6.5
1	B	183	GLY	6.4
1	D	43	LYS	6.3
1	B	187	ILE	6.2
1	D	39	ASN	6.2
1	D	44	GLY	6.1
1	C	180	LYS	6.1
1	D	187	ILE	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	178	MET	5.9
1	A	349	LYS	5.9
1	D	179	LYS	5.9
1	D	102	LEU	5.8
1	C	378	VAL	5.8
1	C	353	ILE	5.8
1	B	385	GLY	5.6
1	D	42	GLN	5.5
1	D	182	ARG	5.5
1	C	184	SER	5.5
1	C	179	LYS	5.5
1	C	99	ILE	5.5
1	D	183	GLY	5.4
1	D	184	SER	5.3
1	D	180	LYS	5.1
1	C	183	GLY	5.1
1	B	184	SER	5.1
1	C	306	LEU	5.1
1	B	202	ILE	5.1
1	C	356	PHE	5.0
1	D	185	GLY	4.9
1	A	179	LYS	4.9
1	A	187	ILE	4.8
1	D	378	VAL	4.8
1	D	178	MET	4.8
1	B	339	TYR	4.8
1	C	303	LEU	4.7
1	A	186	PHE	4.7
1	A	378	VAL	4.6
1	B	349	LYS	4.6
1	D	243	HIS	4.6
1	C	400	VAL	4.6
1	C	345	PRO	4.5
1	B	384	ILE	4.5
1	C	175	VAL	4.5
1	D	99	ILE	4.5
1	A	345	PRO	4.4
1	D	149	ALA	4.4
1	C	401	LEU	4.4
1	A	145	VAL	4.3
1	B	179	LYS	4.3
1	D	46	LYS	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	369	GLY	4.2
1	A	294	LEU	4.2
1	A	102	LEU	4.2
1	A	64	LYS	4.2
1	B	326	SER	4.2
1	C	321	TRP	4.1
1	C	364	LEU	4.1
1	D	138	TYR	4.1
1	D	140	ILE	4.1
1	C	348	TRP	4.1
1	C	342	TYR	4.1
1	C	25	PRO	4.1
1	A	381	ALA	4.1
1	C	300	THR	4.0
1	B	147	ALA	4.0
1	D	341	PHE	4.0
1	C	50	ARG	4.0
1	B	321	TRP	4.0
1	D	23	SER	3.9
1	D	175	VAL	3.9
1	D	348	TRP	3.9
1	A	43	LYS	3.9
1	D	24	ALA	3.9
1	B	341	PHE	3.9
1	A	343	LEU	3.9
1	D	40	ASP	3.8
1	B	64	LYS	3.8
1	C	318	ILE	3.8
1	C	181	MET	3.8
1	C	280	ILE	3.8
1	A	374	ASN	3.8
1	D	181	MET	3.8
1	A	371	ALA	3.8
1	A	377	TYR	3.7
1	D	377	TYR	3.7
1	C	45	GLU	3.7
1	A	181	MET	3.7
1	A	138	TYR	3.7
1	B	53	GLU	3.7
1	D	301	PHE	3.7
1	B	130	ALA	3.7
1	D	239	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	374	ASN	3.7
1	A	142	GLY	3.7
1	A	385	GLY	3.7
1	C	359	SER	3.7
1	B	348	TRP	3.7
1	C	246	TRP	3.7
1	D	383	ARG	3.7
1	D	296	LEU	3.6
1	B	99	ILE	3.6
1	C	34	LEU	3.6
1	A	99	ILE	3.6
1	D	31	ALA	3.6
1	D	240	ALA	3.6
1	D	194	ARG	3.6
1	C	28	PRO	3.6
1	B	134	LEU	3.6
1	B	142	GLY	3.6
1	D	290	LEU	3.5
1	D	280	ILE	3.5
1	B	191	ARG	3.5
1	A	58	VAL	3.5
1	A	391	SER	3.5
1	C	290	LEU	3.5
1	C	325	ALA	3.5
1	B	250	ILE	3.5
1	B	400	VAL	3.5
1	C	23	SER	3.5
1	A	365	LEU	3.5
1	C	57	LYS	3.5
1	A	184	SER	3.5
1	D	370	THR	3.5
1	B	388	TYR	3.5
1	A	178	MET	3.5
1	D	353	ILE	3.4
1	A	46	LYS	3.4
1	C	299	SER	3.4
1	C	336	ASP	3.4
1	A	149	ALA	3.4
1	D	388	TYR	3.4
1	D	32	THR	3.4
1	C	240	ALA	3.4
1	B	335	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	130	ALA	3.4
1	D	306	LEU	3.4
1	D	325	ALA	3.4
1	D	384	ILE	3.4
1	B	346	GLU	3.3
1	A	380	THR	3.3
1	D	321	TRP	3.3
1	B	151	ALA	3.3
1	B	181	MET	3.3
1	D	346	GLU	3.3
1	D	74	LYS	3.3
1	B	350	PHE	3.3
1	B	42	GLN	3.3
1	C	344	ASN	3.3
1	A	400	VAL	3.3
1	D	336	ASP	3.3
1	C	178	MET	3.3
1	C	286	LEU	3.3
1	C	320	LEU	3.3
1	D	349	LYS	3.3
1	B	51	TYR	3.3
1	C	42	GLN	3.3
1	A	334	ALA	3.2
1	D	340	PRO	3.2
1	D	359	SER	3.2
1	A	60[A]	GLU	3.2
1	A	220	ALA	3.2
1	D	273	LEU	3.2
1	D	36	GLN	3.2
1	A	146	TYR	3.2
1	D	139	TYR	3.2
1	D	350	PHE	3.2
1	B	199	ALA	3.2
1	D	343	LEU	3.2
1	B	353	ILE	3.2
1	A	62	TYR	3.2
1	B	383	ARG	3.2
1	A	348	TRP	3.1
1	A	339	TYR	3.1
1	C	176	PRO	3.1
1	D	355	PRO	3.1
1	A	34	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	347	ASP	3.1
1	A	205	SER	3.1
1	C	380	THR	3.1
1	C	388	TYR	3.1
1	A	59	ALA	3.1
1	A	134	LEU	3.1
1	A	386	LEU	3.1
1	B	387	LYS	3.1
1	A	47	GLU	3.1
1	C	187	ILE	3.1
1	C	361	ALA	3.1
1	B	74	LYS	3.1
1	C	343	LEU	3.1
1	D	137	LEU	3.1
1	C	132	TYR	3.0
1	D	142	GLY	3.0
1	D	356	PHE	3.0
1	A	276	MET	3.0
1	D	38	LYS	3.0
1	D	176	PRO	3.0
1	C	272	ILE	3.0
1	C	295	SER	3.0
1	A	372	LEU	3.0
1	B	354	LYS	3.0
1	A	40	ASP	3.0
1	C	27	GLY	3.0
1	C	316	ILE	3.0
1	D	54	LEU	3.0
1	B	351	LYS	3.0
1	C	198	VAL	3.0
1	D	57	LYS	3.0
1	C	259	ASP	3.0
1	B	63	ILE	2.9
1	B	240	ALA	2.9
1	C	147	ALA	2.9
1	B	342	TYR	2.9
1	B	215	LYS	2.9
1	C	60	GLU	2.9
1	A	185	GLY	2.9
1	A	211	SER	2.9
1	A	152	ASN	2.9
1	A	351	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	23	SER	2.9
1	A	147	ALA	2.9
1	B	43	LYS	2.9
1	C	291	LYS	2.9
1	A	122	GLU	2.9
1	B	40	ASP	2.9
1	B	379	ASP	2.9
1	B	138	TYR	2.9
1	B	337	TYR	2.9
1	B	343	LEU	2.9
1	C	350	PHE	2.9
1	A	235	ARG	2.9
1	C	383	ARG	2.9
1	D	145	VAL	2.9
1	A	362	ALA	2.9
1	A	52	ILE	2.8
1	A	260	ARG	2.8
1	B	201	LEU	2.8
1	C	296	LEU	2.8
1	D	41	TYR	2.8
1	B	175	VAL	2.8
1	D	324	PRO	2.8
1	D	93	TRP	2.8
1	A	259	ASP	2.8
1	C	260	ARG	2.8
1	B	386	LEU	2.8
1	A	257	TYR	2.8
1	B	46	LYS	2.8
1	B	98	LYS	2.8
1	C	354	LYS	2.8
1	B	344	ASN	2.8
1	A	48	VAL	2.8
1	C	151	ALA	2.8
1	C	302	ALA	2.8
1	B	272	ILE	2.8
1	B	211	SER	2.8
1	C	386	LEU	2.8
1	D	154	LEU	2.8
1	D	177	GLY	2.8
1	C	152	ASN	2.8
1	A	340	PRO	2.8
1	C	103	PRO	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	341	PHE	2.8
1	A	350	PHE	2.8
1	D	127	PHE	2.8
1	D	48	VAL	2.8
1	D	58	VAL	2.8
1	B	361	ALA	2.8
1	B	380	THR	2.8
1	A	382	LYS	2.8
1	B	148	LYS	2.8
1	C	74	LYS	2.8
1	B	102	LEU	2.7
1	A	139	TYR	2.7
1	D	337	TYR	2.7
1	C	335	VAL	2.7
1	D	400	VAL	2.7
1	B	195	ALA	2.7
1	C	334	ALA	2.7
1	D	281	ALA	2.7
1	D	206	LYS	2.7
1	D	45	GLU	2.7
1	B	363	ILE	2.7
1	A	208	TRP	2.7
1	A	321	TRP	2.7
1	B	208	TRP	2.7
1	C	26	LEU	2.7
1	A	41	TYR	2.7
1	B	139	TYR	2.7
1	C	337	TYR	2.7
1	D	358	GLN	2.7
1	D	64	LYS	2.7
1	C	322	SER	2.7
1	B	369	GLY	2.7
1	B	373	GLY	2.7
1	C	177	GLY	2.7
1	A	54	LEU	2.7
1	D	286	LEU	2.7
1	A	74	LYS	2.7
1	C	298	TYR	2.7
1	D	198	VAL	2.7
1	D	284	GLY	2.7
1	A	63	ILE	2.7
1	A	375	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	280	ILE	2.7
1	B	37	LEU	2.7
1	C	273	LEU	2.7
1	D	338	LEU	2.7
1	C	387	LYS	2.7
1	B	41	TYR	2.6
1	A	57	LYS	2.6
1	A	206	LYS	2.6
1	B	401	LEU	2.6
1	D	141	THR	2.6
1	D	323	THR	2.6
1	C	24	ALA	2.6
1	D	375	GLN	2.6
1	C	347	ASP	2.6
1	A	214	LYS	2.6
1	D	345	PRO	2.6
1	C	252	LEU	2.6
1	C	193	SER	2.6
1	A	36	GLN	2.6
1	D	362	ALA	2.6
1	C	341	PHE	2.6
1	A	337	TYR	2.6
1	D	61	LYS	2.6
1	B	355	PRO	2.6
1	C	105	ILE	2.6
1	C	173	ASN	2.6
1	D	76	LEU	2.6
1	D	294	LEU	2.6
1	B	101	GLY	2.6
1	B	141	THR	2.6
1	B	60	GLU	2.6
1	B	278	ALA	2.6
1	A	335	VAL	2.5
1	B	127	PHE	2.5
1	B	192	PHE	2.5
1	C	75	LYS	2.5
1	B	146	TYR	2.5
1	D	235	ARG	2.5
1	C	363	ILE	2.5
1	C	365	LEU	2.5
1	A	49	THR	2.5
1	B	259	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	259	ASP	2.5
1	D	387	LYS	2.5
1	D	124	ALA	2.5
1	D	174	ALA	2.5
1	A	50	ARG	2.5
1	A	388	TYR	2.5
1	A	37	LEU	2.5
1	C	37	LEU	2.5
1	D	201	LEU	2.5
1	B	206	LYS	2.5
1	C	351	LYS	2.5
1	A	199	ALA	2.5
1	B	325	ALA	2.5
1	B	381	ALA	2.5
1	C	309	ALA	2.5
1	A	342	TYR	2.5
1	A	366	TYR	2.5
1	C	314	SER	2.5
1	D	205	SER	2.5
1	D	389	SER	2.5
1	C	206	LYS	2.5
1	A	245	LEU	2.5
1	A	353	ILE	2.5
1	C	204	GLY	2.5
1	C	373	GLY	2.5
1	A	231	THR	2.5
1	B	131	ALA	2.5
1	C	146	TYR	2.4
1	A	373	GLY	2.4
1	D	244	GLY	2.4
1	A	306	LEU	2.4
1	B	47	GLU	2.4
1	B	235	ARG	2.4
1	B	393	VAL	2.4
1	A	132	TYR	2.4
1	A	398	TYR	2.4
1	A	358	GLN	2.4
1	C	245	LEU	2.4
1	B	281	ALA	2.4
1	B	262	ASP	2.4
1	C	357	ASP	2.4
1	B	378	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	158	PHE	2.4
1	B	356	PHE	2.4
1	C	301	PHE	2.4
1	C	317	GLY	2.4
1	C	139	TYR	2.4
1	B	156	THR	2.4
1	D	47	GLU	2.4
1	D	364	LEU	2.4
1	A	368	ALA	2.4
1	C	331	ALA	2.4
1	C	64	LYS	2.4
1	C	287	PRO	2.4
1	A	198	VAL	2.4
1	B	58	VAL	2.4
1	B	177	GLY	2.4
1	C	145	VAL	2.4
1	D	277	GLY	2.4
1	A	356	PHE	2.4
1	B	366	TYR	2.4
1	C	66	THR	2.4
1	C	312	ILE	2.3
1	B	59	ALA	2.3
1	B	334	ALA	2.3
1	B	95	ASP	2.3
1	B	347	ASP	2.3
1	C	330	VAL	2.3
1	A	158	PHE	2.3
1	D	173	ASN	2.3
1	C	154	LEU	2.3
1	B	316	ILE	2.3
1	C	63	ILE	2.3
1	D	100	ASP	2.3
1	A	204	GLY	2.3
1	A	355	PRO	2.3
1	B	161	PRO	2.3
1	C	92	TRP	2.3
1	D	226	TRP	2.3
1	C	48	VAL	2.3
1	A	156	THR	2.3
1	B	62	TYR	2.3
1	C	377	TYR	2.3
1	A	33	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	134	LEU	2.3
1	D	401	LEU	2.3
1	A	316	ILE	2.3
1	A	363	ILE	2.3
1	C	264	ILE	2.3
1	D	35	GLU	2.3
1	B	194	ARG	2.3
1	C	324	PRO	2.3
1	C	43	LYS	2.3
1	D	354	LYS	2.3
1	A	261	THR	2.3
1	B	66	THR	2.3
1	B	358	GLN	2.3
1	B	54	LEU	2.3
1	B	306	LEU	2.3
1	D	344	ASN	2.2
1	B	288	GLN	2.2
1	A	346	GLU	2.2
1	A	330	VAL	2.2
1	B	198	VAL	2.2
1	B	50	ARG	2.2
1	B	368	ALA	2.2
1	C	256	ALA	2.2
1	A	314	SER	2.2
1	B	26	LEU	2.2
1	C	68	LEU	2.2
1	A	200	LYS	2.2
1	B	149	ALA	2.2
1	C	349	LYS	2.2
1	A	202	ILE	2.2
1	C	35	GLU	2.2
1	B	212	ASP	2.2
1	D	379	ASP	2.2
1	A	66	THR	2.2
1	A	265	ARG	2.2
1	C	32	THR	2.2
1	C	261	THR	2.2
1	C	115	VAL	2.2
1	A	24	ALA	2.2
1	B	137	LEU	2.2
1	C	137	LEU	2.2
1	C	375	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	25	PRO	2.2
1	D	146	TYR	2.2
1	D	52	ILE	2.2
1	C	188	ASP	2.1
1	A	96	SER	2.1
1	C	326	SER	2.1
1	C	70	VAL	2.1
1	D	125	ASN	2.1
1	B	28	PRO	2.1
1	C	265	ARG	2.1
1	C	340	PRO	2.1
1	A	141	THR	2.1
1	B	314	SER	2.1
1	A	387	LYS	2.1
1	B	276	MET	2.1
1	A	39	ASN	2.1
1	A	42	GLN	2.1
1	B	375	GLN	2.1
1	C	374	ASN	2.1
1	A	399	LEU	2.1
1	C	124	ALA	2.1
1	C	294	LEU	2.1
1	C	399	LEU	2.1
1	D	347	ASP	2.1
1	D	91	TYR	2.1
1	A	370	THR	2.1
1	D	289	GLU	2.1
1	C	319	ASN	2.1
1	A	383	ARG	2.1
1	B	263	ARG	2.1
1	A	188	ASP	2.1
1	D	188	ASP	2.1
1	D	361	ALA	2.1
1	A	25	PRO	2.1
1	A	192	PHE	2.1
1	C	338	LEU	2.1
1	A	207	SER	2.1
1	C	98	LYS	2.1
1	D	148	LYS	2.1
1	A	384	ILE	2.1
1	C	266	GLU	2.1
1	D	63	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	116	TYR	2.1
1	D	49	THR	2.1
1	D	190	ARG	2.1
1	B	284	GLY	2.1
1	B	274	PRO	2.0
1	B	345	PRO	2.0
1	C	355	PRO	2.0
1	D	381	ALA	2.0
1	A	216	LEU	2.0
1	D	320	LEU	2.0
1	A	75	LYS	2.0
1	B	61	LYS	2.0
1	C	358	GLN	2.0
1	A	359	SER	2.0
1	B	125	ASN	2.0
1	B	264	ILE	2.0
1	D	327	ASN	2.0
1	B	377	TYR	2.0
1	B	243	HIS	2.0
1	D	282	ASP	2.0
1	A	269	GLU	2.0
1	B	254	VAL	2.0
1	B	376	LYS	2.0
1	D	75	LYS	2.0
1	D	295	SER	2.0
1	D	386	LEU	2.0
1	A	125	ASN	2.0
1	B	265	ARG	2.0
1	B	360	ARG	2.0
1	C	125	ASN	2.0
1	D	152	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](#)

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(Å 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.