



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:58 PM UTC

PDB ID : 8RG3 / pdb_00008rg3
Title : Crystal structure of PbFucA from Planctomycetes bacterium K23_9 in P 1 21
1
Authors : Perez-Curz, C.; Moraleda-Montoya, A.; Liebana, R.; Lorizate, M.; Arrizabalaga, U.; Garcia-Alija, M.; Terrones, O.; Contreras, F.X.; Guerin, M.E.; Trastoy, B.; Alonso-Saez, L.
Deposited on : 2023-12-13
Resolution : 2.50 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:

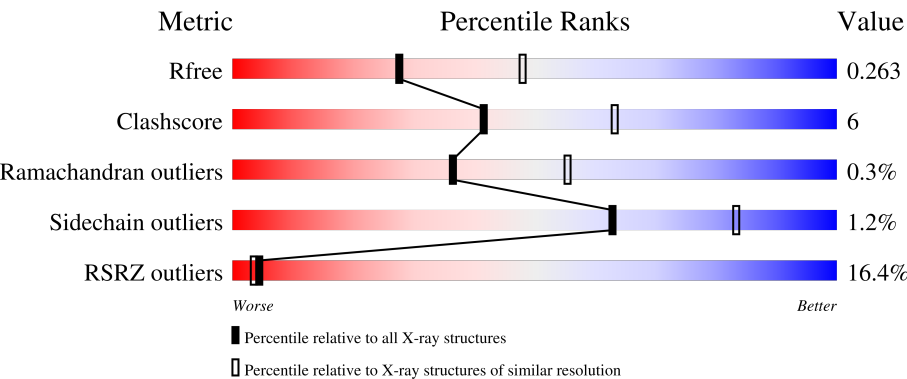
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	373	86%9%5%
1	B	373	83%12%5%
1	C	373	6% 84%11%5%
1	D	373	14% 85%10%5%

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Mol	Chain	Length	Quality of chain
1	E	373	
1	F	373	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16917 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 Glycoside-hydrolase family GH114 TIM-barrel domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	1	0
			2853	1831	501	506	15			
1	B	355	Total	C	N	O	S	0	1	0
			2813	1805	485	508	15			
1	C	356	Total	C	N	O	S	0	1	0
			2809	1806	484	504	15			
1	D	356	Total	C	N	O	S	0	0	0
			2733	1758	468	492	15			
1	E	355	Total	C	N	O	S	0	3	0
			2792	1793	479	504	16			
1	F	356	Total	C	N	O	S	0	1	0
			2739	1765	467	493	14			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP A0A517NMB4
A	21	HIS	-	expression tag	UNP A0A517NMB4
A	22	HIS	-	expression tag	UNP A0A517NMB4
A	23	HIS	-	expression tag	UNP A0A517NMB4
A	24	HIS	-	expression tag	UNP A0A517NMB4
A	25	HIS	-	expression tag	UNP A0A517NMB4
A	26	HIS	-	expression tag	UNP A0A517NMB4
A	27	GLU	-	expression tag	UNP A0A517NMB4
A	28	ASN	-	expression tag	UNP A0A517NMB4
A	29	LEU	-	expression tag	UNP A0A517NMB4
A	30	TYR	-	expression tag	UNP A0A517NMB4
A	31	PHE	-	expression tag	UNP A0A517NMB4
A	32	GLN	-	expression tag	UNP A0A517NMB4
A	33	GLY	-	expression tag	UNP A0A517NMB4
A	34	SER	-	expression tag	UNP A0A517NMB4
A	35	GLY	-	expression tag	UNP A0A517NMB4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	20	MET	-	initiating methionine	UNP A0A517NMB4
B	21	HIS	-	expression tag	UNP A0A517NMB4
B	22	HIS	-	expression tag	UNP A0A517NMB4
B	23	HIS	-	expression tag	UNP A0A517NMB4
B	24	HIS	-	expression tag	UNP A0A517NMB4
B	25	HIS	-	expression tag	UNP A0A517NMB4
B	26	HIS	-	expression tag	UNP A0A517NMB4
B	27	GLU	-	expression tag	UNP A0A517NMB4
B	28	ASN	-	expression tag	UNP A0A517NMB4
B	29	LEU	-	expression tag	UNP A0A517NMB4
B	30	TYR	-	expression tag	UNP A0A517NMB4
B	31	PHE	-	expression tag	UNP A0A517NMB4
B	32	GLN	-	expression tag	UNP A0A517NMB4
B	33	GLY	-	expression tag	UNP A0A517NMB4
B	34	SER	-	expression tag	UNP A0A517NMB4
B	35	GLY	-	expression tag	UNP A0A517NMB4
C	20	MET	-	initiating methionine	UNP A0A517NMB4
C	21	HIS	-	expression tag	UNP A0A517NMB4
C	22	HIS	-	expression tag	UNP A0A517NMB4
C	23	HIS	-	expression tag	UNP A0A517NMB4
C	24	HIS	-	expression tag	UNP A0A517NMB4
C	25	HIS	-	expression tag	UNP A0A517NMB4
C	26	HIS	-	expression tag	UNP A0A517NMB4
C	27	GLU	-	expression tag	UNP A0A517NMB4
C	28	ASN	-	expression tag	UNP A0A517NMB4
C	29	LEU	-	expression tag	UNP A0A517NMB4
C	30	TYR	-	expression tag	UNP A0A517NMB4
C	31	PHE	-	expression tag	UNP A0A517NMB4
C	32	GLN	-	expression tag	UNP A0A517NMB4
C	33	GLY	-	expression tag	UNP A0A517NMB4
C	34	SER	-	expression tag	UNP A0A517NMB4
C	35	GLY	-	expression tag	UNP A0A517NMB4
D	20	MET	-	initiating methionine	UNP A0A517NMB4
D	21	HIS	-	expression tag	UNP A0A517NMB4
D	22	HIS	-	expression tag	UNP A0A517NMB4
D	23	HIS	-	expression tag	UNP A0A517NMB4
D	24	HIS	-	expression tag	UNP A0A517NMB4
D	25	HIS	-	expression tag	UNP A0A517NMB4
D	26	HIS	-	expression tag	UNP A0A517NMB4
D	27	GLU	-	expression tag	UNP A0A517NMB4
D	28	ASN	-	expression tag	UNP A0A517NMB4
D	29	LEU	-	expression tag	UNP A0A517NMB4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	30	TYR	-	expression tag	UNP A0A517NMB4
D	31	PHE	-	expression tag	UNP A0A517NMB4
D	32	GLN	-	expression tag	UNP A0A517NMB4
D	33	GLY	-	expression tag	UNP A0A517NMB4
D	34	SER	-	expression tag	UNP A0A517NMB4
D	35	GLY	-	expression tag	UNP A0A517NMB4
E	20	MET	-	initiating methionine	UNP A0A517NMB4
E	21	HIS	-	expression tag	UNP A0A517NMB4
E	22	HIS	-	expression tag	UNP A0A517NMB4
E	23	HIS	-	expression tag	UNP A0A517NMB4
E	24	HIS	-	expression tag	UNP A0A517NMB4
E	25	HIS	-	expression tag	UNP A0A517NMB4
E	26	HIS	-	expression tag	UNP A0A517NMB4
E	27	GLU	-	expression tag	UNP A0A517NMB4
E	28	ASN	-	expression tag	UNP A0A517NMB4
E	29	LEU	-	expression tag	UNP A0A517NMB4
E	30	TYR	-	expression tag	UNP A0A517NMB4
E	31	PHE	-	expression tag	UNP A0A517NMB4
E	32	GLN	-	expression tag	UNP A0A517NMB4
E	33	GLY	-	expression tag	UNP A0A517NMB4
E	34	SER	-	expression tag	UNP A0A517NMB4
E	35	GLY	-	expression tag	UNP A0A517NMB4
F	20	MET	-	initiating methionine	UNP A0A517NMB4
F	21	HIS	-	expression tag	UNP A0A517NMB4
F	22	HIS	-	expression tag	UNP A0A517NMB4
F	23	HIS	-	expression tag	UNP A0A517NMB4
F	24	HIS	-	expression tag	UNP A0A517NMB4
F	25	HIS	-	expression tag	UNP A0A517NMB4
F	26	HIS	-	expression tag	UNP A0A517NMB4
F	27	GLU	-	expression tag	UNP A0A517NMB4
F	28	ASN	-	expression tag	UNP A0A517NMB4
F	29	LEU	-	expression tag	UNP A0A517NMB4
F	30	TYR	-	expression tag	UNP A0A517NMB4
F	31	PHE	-	expression tag	UNP A0A517NMB4
F	32	GLN	-	expression tag	UNP A0A517NMB4
F	33	GLY	-	expression tag	UNP A0A517NMB4
F	34	SER	-	expression tag	UNP A0A517NMB4
F	35	GLY	-	expression tag	UNP A0A517NMB4

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is water.

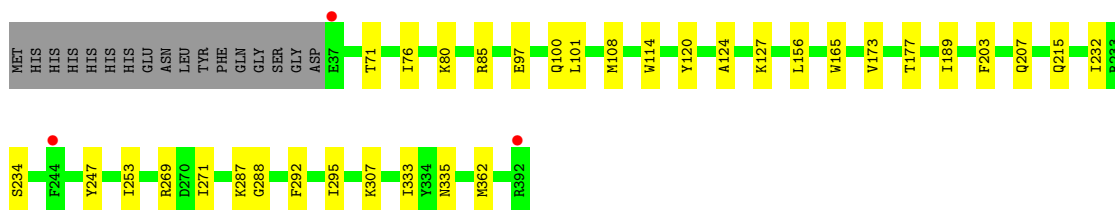
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	47	Total	O	0	0
			47	47		
3	C	32	Total	O	0	0
			32	32		
3	D	27	Total	O	0	0
			27	27		
3	E	22	Total	O	0	0
			22	22		
3	F	5	Total	O	0	0
			5	5		

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.

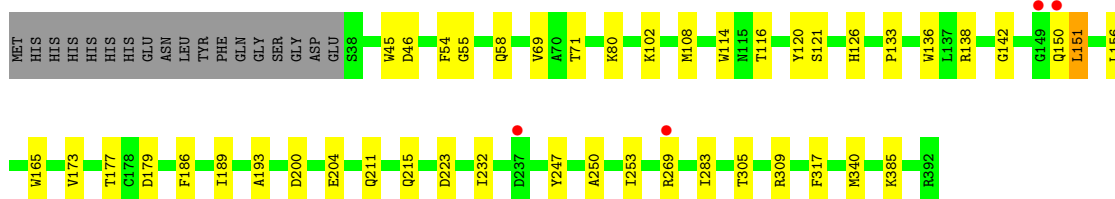
- Molecule 1: Glycoside-hydrolase family GH114 TIM-barrel domain-containing protein

Chain A: 



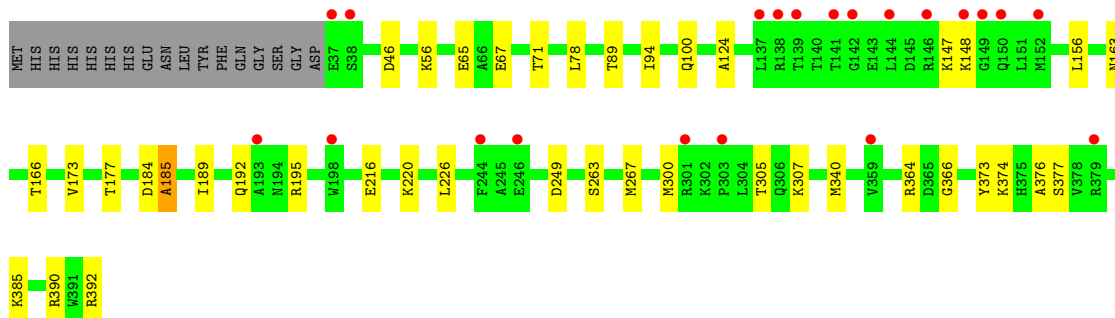
- Molecule 1: Glycoside-hydrolase family GH114 TIM-barrel domain-containing protein

Chain B: 

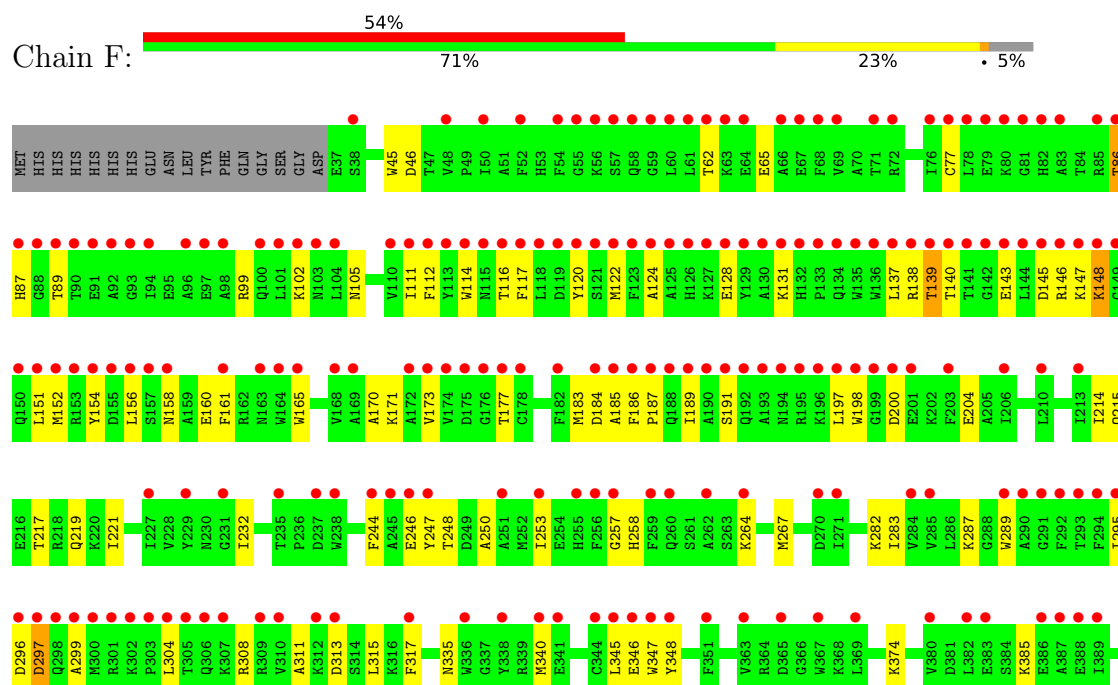


- Molecule 1: Glycoside-hydrolase family GH114 TIM-barrel domain-containing protein

Chain C: 



- Molecule 1: Glycoside-hydrolase family GH114 TIM-barrel domain-containing protein





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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.84Å 81.90Å 160.31Å 90.00° 95.49° 90.00°	Depositor
Resolution (Å)	91.42 – 2.50 91.42 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (91.42-2.50) 89.5 (91.42-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.203 , 0.253 0.227 , 0.263	Depositor DCC
R_{free} test set	1983 reflections (2.41%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16917	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.66	0/2932	0.75	0/3965
1	B	0.63	1/2892 (0.0%)	0.76	0/3921
1	C	0.59	0/2888	0.72	0/3915
1	D	0.55	0/2810	0.68	1/3821 (0.0%)
1	E	0.54	0/2881	0.69	0/3909
1	F	0.45	0/2818	0.61	0/3834
All	All	0.58	1/17221 (0.0%)	0.70	1/23365 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	GLY	CA-C	-5.14	1.47	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	253	ILE	CA-C-O	-5.41	117.92	122.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	269	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	2853	0	2729	19	0
1	B	2813	0	2643	29	0
1	C	2809	0	2644	22	0
1	D	2733	0	2507	22	0
1	E	2792	0	2595	47	0
1	F	2739	0	2510	71	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
2	C	4	0	6	0	0
3	A	33	0	0	1	0
3	B	47	0	0	0	0
3	C	32	0	0	0	0
3	D	27	0	0	0	0
3	E	22	0	0	1	0
3	F	5	0	0	0	0
All	All	16917	0	15646	207	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 (207) 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:E:221:ILE:HD12	1:E:225:LYS:HB2	1.54	0.88
1:E:156:LEU:HD11	1:E:189:ILE:HD13	1.61	0.81
1:F:257:GLY:C	1:F:258:HIS:HD1	1.96	0.73
1:E:136:TRP:CG	1:E:152:MET:HE1	2.24	0.73
1:F:183:MET:HE1	1:F:214:ILE:HG12	1.69	0.72
1:F:102:LYS:HE3	1:F:177:THR:HG22	1.71	0.72
1:F:147:LYS:N	1:F:151:LEU:O	2.26	0.69
1:F:137:LEU:HD23	1:F:138:ARG:N	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:GLN:O	1:F:219:GLN:HG3	1.92	0.68
1:D:287:LYS:HE2	1:D:335:ASN:OD1	1.94	0.68
1:E:98:ALA:HB1	1:E:177:THR:HG22	1.76	0.67
1:E:215:GLN:HG3	1:E:247:TYR:CE2	2.29	0.67
1:F:215:GLN:HG2	1:F:219:GLN:NE2	2.10	0.66
1:F:65:GLU:CD	1:F:340:MET:HE1	2.21	0.66
1:F:120:TYR:HB3	1:F:122:MET:SD	2.38	0.63
1:F:137:LEU:HD22	1:F:145:ASP:CB	2.28	0.63
1:B:250:ALA:HB2	1:B:283:ILE:HB	1.82	0.62
1:E:132:HIS:CD2	1:E:135:TRP:CZ2	2.88	0.61
1:E:258[B]:HIS:NE2	1:E:259:PHE:CE1	2.69	0.61
1:D:67:GLU:O	1:D:71:THR:HG22	2.00	0.61
1:F:139:THR:HG22	1:F:143:GLU:O	2.01	0.60
1:E:274:MET:HG3	1:E:284:VAL:HG11	1.82	0.60
1:F:258:HIS:CD2	1:F:289:TRP:HB2	2.38	0.59
1:F:146:ARG:HA	1:F:152:MET:HA	1.83	0.59
1:F:287:LYS:HE3	1:F:335:ASN:OD1	2.02	0.59
1:A:287:LYS:NZ	1:A:335:ASN:OD1	2.27	0.58
1:F:244:PHE:O	1:F:248:THR:OG1	2.21	0.58
1:B:71:THR:O	1:B:71:THR:HG22	2.03	0.58
1:C:78:LEU:HD12	1:C:94:ILE:HG23	1.85	0.58
1:F:62:THR:HG23	1:F:65:GLU:OE1	2.03	0.58
1:F:304:LEU:HD21	1:F:308:ARG:NH2	2.20	0.57
1:E:377:SER:OG	1:E:392:ARG:NH1	2.37	0.57
1:F:296:ASP:O	1:F:297:ASP:C	2.48	0.57
1:C:166:THR:HG21	1:C:216:GLU:HB3	1.86	0.56
1:E:132:HIS:HB3	1:E:135:TRP:CE2	2.40	0.56
1:E:140:THR:HG23	1:E:197:LEU:O	2.05	0.56
1:D:68:PHE:O	1:D:72:ARG:HG3	2.05	0.56
1:F:308:ARG:NE	1:F:346:GLU:OE2	2.40	0.54
1:F:128:GLU:HA	1:F:131:LYS:HD3	1.90	0.54
1:B:69:VAL:HG12	1:B:108:MET:HE1	1.89	0.54
1:C:263:SER:O	1:C:267:MET:HG3	2.08	0.54
1:A:177:THR:O	1:A:177:THR:HG22	2.08	0.53
1:D:129:TYR:HE2	1:D:152:MET:HE3	1.73	0.53
1:E:252[B]:MET:SD	1:E:285:VAL:HB	2.47	0.53
1:E:132:HIS:HB3	1:E:135:TRP:NE1	2.23	0.53
1:E:257:GLY:O	1:E:258[A]:HIS:CD2	2.62	0.53
1:F:177:THR:HG22	1:F:177:THR:O	2.08	0.53
1:F:147:LYS:O	1:F:148:LYS:C	2.52	0.52
1:D:300:MET:O	1:D:307:LYS:HE3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:385:LYS:HD2	1:F:385:LYS:O	2.09	0.52
1:B:69:VAL:CG1	1:B:108:MET:HE1	2.40	0.52
1:B:121:SER:HA	1:B:126:HIS:CG	2.45	0.52
1:A:234:SER:OG	1:A:269[B]:ARG:NE	2.37	0.51
1:F:313:ASP:O	1:F:313:ASP:OD1	2.28	0.51
1:D:243:ASP:OD2	1:D:244:PHE:N	2.38	0.51
1:C:67:GLU:O	1:C:71:THR:HG23	2.09	0.51
1:D:147:LYS:N	1:D:151:LEU:O	2.43	0.51
1:B:150:GLN:O	1:B:151:LEU:HB2	2.10	0.51
1:F:200:ASP:O	1:F:204:GLU:HG2	2.11	0.51
1:F:317:PHE:CE1	1:F:385:LYS:HA	2.46	0.51
1:B:177:THR:HG22	1:B:177:THR:O	2.10	0.51
1:F:137:LEU:HD23	1:F:137:LEU:C	2.35	0.51
1:F:184:ASP:OD1	1:F:185:ALA:N	2.42	0.51
1:F:215:GLN:HG2	1:F:219:GLN:HE21	1.75	0.51
1:B:200:ASP:O	1:B:204:GLU:HG3	2.10	0.50
1:E:247:TYR:N	1:E:247:TYR:CD1	2.80	0.50
1:A:215:GLN:HG3	1:A:247:TYR:CZ	2.47	0.50
1:F:154:TYR:HB3	1:F:161:PHE:CE2	2.46	0.50
1:F:315:LEU:HD22	1:F:348:TYR:CD2	2.47	0.50
1:D:69:VAL:HG12	1:D:108:MET:HE1	1.93	0.50
1:E:373:TYR:O	1:E:392:ARG:NH2	2.44	0.50
1:F:258:HIS:CD2	1:F:289:TRP:CB	2.95	0.49
1:B:156:LEU:HD11	1:B:189:ILE:HD13	1.95	0.49
1:F:217:THR:O	1:F:221:ILE:HG13	2.12	0.49
1:A:203:PHE:O	1:A:207:GLN:HG2	2.13	0.49
1:D:129:TYR:CE2	1:D:152:MET:HE3	2.48	0.49
1:A:287:LYS:HE2	3:A:512:HOH:O	2.13	0.48
1:F:77:CYS:HA	1:F:111:ILE:HB	1.94	0.48
1:F:158:ASN:OD1	1:F:161:PHE:N	2.37	0.48
1:C:184:ASP:O	1:C:185:ALA:HB3	2.12	0.48
1:E:215:GLN:HA	1:E:247:TYR:CD2	2.48	0.48
1:F:158:ASN:OD1	1:F:158:ASN:C	2.57	0.48
1:E:200:ASP:O	1:E:204:GLU:HG2	2.13	0.48
1:E:147:LYS:N	1:E:151:LEU:O	2.45	0.48
1:C:192:GLN:NE2	1:C:195:ARG:HE	2.11	0.48
1:E:53:HIS:CD2	1:E:252[A]:MET:HE1	2.48	0.47
1:F:296:ASP:O	1:F:299:ALA:N	2.45	0.47
1:E:243:ASP:OD2	1:E:244:PHE:CZ	2.67	0.47
1:F:86:THR:HG23	1:F:87:HIS:ND1	2.29	0.47
1:F:158:ASN:OD1	1:F:160:GLU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLU:OE2	1:A:100:GLN:NE2	2.44	0.47
1:A:232:ILE:HB	1:A:253:ILE:HG12	1.96	0.47
1:D:78:LEU:HD12	1:D:94:ILE:HG23	1.95	0.47
1:F:214:ILE:CD1	1:F:244:PHE:CD2	2.98	0.47
1:E:40:TYR:CG	1:E:283:ILE:HD11	2.50	0.47
1:E:184:ASP:O	1:E:185:ALA:HB3	2.14	0.47
1:A:101:LEU:HD13	1:A:108:MET:HE3	1.96	0.46
1:B:102:LYS:HE3	1:B:179:ASP:OD2	2.15	0.46
1:F:62:THR:HG23	1:F:65:GLU:CD	2.40	0.46
1:F:311:ALA:HB1	1:F:348:TYR:OH	2.15	0.46
1:B:80:LYS:HE2	1:B:120:TYR:CZ	2.50	0.46
1:D:133:PRO:HA	1:D:136:TRP:CE2	2.51	0.46
1:E:45:TRP:O	1:E:46:ASP:C	2.58	0.46
1:F:89:THR:HG21	1:F:124:ALA:HB2	1.97	0.46
1:F:112:PHE:CE1	1:F:114:TRP:HB2	2.51	0.46
1:F:250:ALA:HB2	1:F:283:ILE:HB	1.96	0.46
1:B:133:PRO:HA	1:B:136:TRP:CE2	2.50	0.46
1:A:288:GLY:N	1:A:333:ILE:O	2.43	0.46
1:D:120:TYR:CE1	1:D:151:LEU:HD11	2.51	0.46
1:D:133:PRO:HA	1:D:136:TRP:CD2	2.51	0.46
1:C:177:THR:HG22	1:C:177:THR:O	2.16	0.45
1:B:309:ARG:O	1:B:309:ARG:HD3	2.17	0.45
1:E:258[B]:HIS:CE1	1:E:259:PHE:CZ	3.04	0.45
1:E:317:PHE:CE1	1:E:385:LYS:HA	2.51	0.45
1:F:186:PHE:N	1:F:187:PRO:CD	2.79	0.45
1:F:248:THR:O	1:F:282:LYS:NZ	2.45	0.45
1:F:246:GLU:HG2	1:F:247:TYR:CE2	2.51	0.45
1:F:257:GLY:C	1:F:258:HIS:ND1	2.71	0.45
1:A:76:ILE:O	1:A:76:ILE:HG23	2.17	0.45
1:C:46:ASP:OD1	1:F:374:LYS:HE2	2.17	0.45
1:C:147:LYS:O	1:C:148:LYS:C	2.60	0.45
1:E:57:SER:HA	1:E:81:GLY:O	2.16	0.45
1:E:69:VAL:HG12	1:E:108:MET:HE1	1.98	0.45
1:E:182:PHE:CE1	1:E:252[B]:MET:HG3	2.52	0.45
1:F:161:PHE:CE1	1:F:165:TRP:HB2	2.52	0.45
1:E:45:TRP:CE2	1:E:358:PRO:HD3	2.52	0.45
1:D:80:LYS:HE2	1:D:120:TYR:CZ	2.51	0.45
1:E:210:LEU:O	1:E:213:ILE:HG22	2.17	0.45
1:E:152:MET:HE3	3:E:411:HOH:O	2.17	0.44
1:E:314:SER:HB2	1:E:334:TYR:OH	2.16	0.44
1:C:300:MET:HA	1:C:307:LYS:NZ	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:HIS:HB3	1:E:135:TRP:CD1	2.52	0.44
1:E:117:PHE:C	1:E:118:LEU:HD23	2.43	0.44
1:A:156:LEU:HD11	1:A:189:ILE:HD13	2.00	0.44
1:C:300:MET:O	1:C:307:LYS:NZ	2.51	0.44
1:F:139:THR:OG1	1:F:140:THR:N	2.50	0.44
1:C:56:LYS:HD2	1:C:340:MET:HE2	2.00	0.44
1:B:45:TRP:O	1:B:46:ASP:C	2.61	0.43
1:D:129:TYR:HB2	1:D:164:TRP:CH2	2.53	0.43
1:E:255:HIS:O	1:E:256:PHE:C	2.59	0.43
1:F:264:LYS:HA	1:F:267:MET:HE3	2.00	0.43
1:F:295:ILE:C	1:F:295:ILE:HD12	2.43	0.43
1:C:184:ASP:OD1	1:C:185:ALA:N	2.51	0.43
1:C:373:TYR:O	1:C:374:LYS:C	2.60	0.43
1:E:177:THR:O	1:E:177:THR:CG2	2.67	0.43
1:E:184:ASP:O	1:E:185:ALA:CB	2.66	0.43
1:B:138:ARG:HD3	1:B:142:GLY:O	2.18	0.43
1:E:174:VAL:HG12	1:E:175:ASP:N	2.34	0.43
1:F:137:LEU:HD23	1:F:138:ARG:O	2.18	0.43
1:A:292:PHE:CZ	1:A:307:LYS:HG2	2.53	0.43
1:C:364:ARG:HD2	1:C:366:GLY:O	2.19	0.43
1:D:364:ARG:HG3	1:D:365:ASP:N	2.34	0.43
1:E:117:PHE:O	1:E:118:LEU:HD23	2.19	0.43
1:C:163:ASN:OD1	1:C:220:LYS:NZ	2.42	0.43
1:B:232:ILE:HB	1:B:253:ILE:HG12	2.01	0.43
1:B:71:THR:O	1:B:71:THR:CG2	2.67	0.42
1:C:65:GLU:OE2	1:C:340:MET:HE1	2.19	0.42
1:E:252[B]:MET:HE1	1:E:285:VAL:HG11	2.02	0.42
1:F:137:LEU:HD11	1:F:198:TRP:CE2	2.54	0.42
1:C:377:SER:OG	1:C:392:ARG:NH1	2.53	0.42
1:D:380:VAL:HG22	1:D:381:ASP:N	2.34	0.42
1:F:116:THR:HA	1:F:165:TRP:CZ2	2.55	0.42
1:A:80:LYS:HE2	1:A:120:TYR:CZ	2.54	0.42
1:D:235:THR:HB	1:D:236:PRO:CD	2.49	0.42
1:A:124:ALA:O	1:A:127:LYS:HG3	2.19	0.42
1:E:200:ASP:O	1:E:201:GLU:C	2.62	0.42
1:F:347:TRP:C	1:F:348:TYR:CD1	2.97	0.42
1:D:194:ASN:HB3	1:D:198:TRP:CZ3	2.55	0.42
1:D:156:LEU:O	1:D:162:ARG:HD3	2.19	0.42
1:B:54:PHE:CE1	1:B:340:MET:HG3	2.55	0.42
1:B:114:TRP:CD1	1:B:165:TRP:CZ2	3.08	0.42
1:B:211:GLN:HE21	1:B:211:GLN:HB2	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:PHE:CE1	1:B:385:LYS:HA	2.55	0.42
1:F:246:GLU:O	1:F:246:GLU:HG3	2.18	0.42
1:F:183:MET:HE2	1:F:186:PHE:HZ	1.84	0.41
1:D:114:TRP:HA	1:D:114:TRP:CE3	2.55	0.41
1:F:122:MET:SD	1:F:122:MET:N	2.93	0.41
1:F:156:LEU:HD11	1:F:189:ILE:HD13	2.02	0.41
1:B:215:GLN:HG3	1:B:247:TYR:CZ	2.56	0.41
1:A:271:ILE:HG22	1:A:362:MET:HE1	2.01	0.41
1:A:114:TRP:CD1	1:A:165:TRP:CZ2	3.08	0.41
1:B:193:ALA:HB1	1:E:106:PRO:HD3	2.03	0.41
1:F:170:ALA:O	1:F:171:LYS:C	2.64	0.41
1:F:287:LYS:CE	1:F:335:ASN:OD1	2.67	0.41
1:E:135:TRP:CD1	1:E:135:TRP:N	2.88	0.41
1:A:71:THR:O	1:A:71:THR:CG2	2.68	0.41
1:B:186:PHE:N	1:B:186:PHE:CD1	2.89	0.41
1:F:340:MET:HE3	1:F:345:LEU:HD12	2.01	0.41
1:B:133:PRO:HA	1:B:136:TRP:CD2	2.55	0.41
1:B:186:PHE:N	1:B:186:PHE:HD1	2.19	0.41
1:E:53:HIS:CE1	1:E:79:GLU:HG2	2.56	0.41
1:E:192:GLN:OE1	1:E:195:ARG:HD2	2.20	0.41
1:F:45:TRP:O	1:F:46:ASP:C	2.63	0.41
1:F:99:ARG:HH11	1:F:99:ARG:HG3	1.86	0.41
1:F:102:LYS:HA	1:F:105:ASN:O	2.21	0.41
1:F:140:THR:HG23	1:F:197:LEU:O	2.21	0.41
1:A:85:ARG:NE	1:B:223:ASP:OD2	2.54	0.40
1:C:89:THR:HG21	1:C:124:ALA:HB2	2.03	0.40
1:D:144:LEU:HD23	1:D:144:LEU:HA	1.94	0.40
1:E:286:LEU:HD23	1:E:286:LEU:C	2.46	0.40
1:C:156:LEU:HD11	1:C:189:ILE:HD13	2.02	0.40
1:C:226:LEU:HA	1:C:249:ASP:OD2	2.21	0.40
1:C:376:ALA:HA	1:C:390:ARG:O	2.21	0.40
1:F:117:PHE:CD2	1:F:189:ILE:HG13	2.57	0.40
1:F:137:LEU:HD23	1:F:138:ARG:C	2.47	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	355/373 (95%)	347 (98%)	8 (2%)	0	100	100
1	B	354/373 (95%)	341 (96%)	12 (3%)	1 (0%)	36	55
1	C	355/373 (95%)	345 (97%)	9 (2%)	1 (0%)	36	55
1	D	354/373 (95%)	344 (97%)	10 (3%)	0	100	100
1	E	356/373 (95%)	345 (97%)	9 (2%)	2 (1%)	21	38
1	F	355/373 (95%)	335 (94%)	18 (5%)	2 (1%)	21	38
All	All	2129/2238 (95%)	2057 (97%)	66 (3%)	6 (0%)	36	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	LEU
1	E	185	ALA
1	C	185	ALA
1	F	148	LYS
1	F	297	ASP
1	E	335	ASN

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	282/313 (90%)	280 (99%)	2 (1%)	76	89
1	B	276/313 (88%)	273 (99%)	3 (1%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	274/313 (88%)	270 (98%)	4 (2%)	57	80
1	D	255/313 (82%)	253 (99%)	2 (1%)	73	88
1	E	270/313 (86%)	268 (99%)	2 (1%)	76	89
1	F	257/313 (82%)	251 (98%)	6 (2%)	44	72
All	All	1614/1878 (86%)	1595 (99%)	19 (1%)	63	83

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	VAL
1	A	295	ILE
1	B	116	THR
1	B	173	VAL
1	B	305	THR
1	C	100	GLN
1	C	173	VAL
1	C	305	THR
1	C	385	LYS
1	D	38	SER
1	D	258	HIS
1	E	38	SER
1	E	173	VAL
1	F	86	THR
1	F	139	THR
1	F	173	VAL
1	F	191	SER
1	F	232	ILE
1	F	253	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	GLN
1	A	215	GLN
1	A	375	HIS
1	B	39	HIS
1	E	53	HIS
1	E	211	GLN
1	F	219	GLN
1	F	255	HIS

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Mol	Chain	Res	Type
1	F	329	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](#)

3 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	EDO	C	401	-	3,3,3	0.66	0	2,2,2	0.70	0
2	EDO	A	401	-	3,3,3	0.61	0	2,2,2	0.98	0
2	EDO	B	401	-	3,3,3	0.54	0	2,2,2	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	C	401	-	-	0/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	401	-	-	0/1/1/1	-

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	356/373 (95%)	0.23	3 (0%) 82 80	18, 34, 46, 54	1 (0%)
1	B	355/373 (95%)	0.37	4 (1%) 78 75	19, 38, 48, 56	1 (0%)
1	C	356/373 (95%)	0.85	21 (5%) 28 24	23, 45, 68, 86	1 (0%)
1	D	356/373 (95%)	1.07	54 (15%) 5 4	34, 51, 69, 81	0
1	E	355/373 (95%)	1.15	67 (18%) 3 2	25, 49, 83, 97	3 (0%)
1	F	356/373 (95%)	2.33	201 (56%) 0 0	48, 75, 103, 122	1 (0%)
All	All	2134/2238 (95%)	1.00	350 (16%) 4 3	18, 45, 86, 122	7 (0%)

All (350) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	144	LEU	5.8
1	F	152	MET	5.8
1	F	298	GLN	5.6
1	E	219	GLN	5.5
1	F	145	ASP	5.3
1	F	55	GLY	5.1
1	F	297	ASP	5.0
1	F	66	ALA	5.0
1	F	54	PHE	5.0
1	F	129	TYR	5.0
1	F	303	PRO	5.0
1	F	104	LEU	4.9
1	F	123	PHE	4.9
1	F	296	ASP	4.9
1	F	64	GLU	4.7
1	F	86	THR	4.7
1	F	150	GLN	4.7
1	F	57[A]	SER	4.6
1	F	134	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	153	ARG	4.5
1	F	237	ASP	4.5
1	F	112	PHE	4.4
1	F	114	TRP	4.4
1	F	118	LEU	4.4
1	F	60	LEU	4.3
1	F	130	ALA	4.3
1	F	188	GLN	4.3
1	F	78	LEU	4.2
1	F	122	MET	4.2
1	F	136	TRP	4.2
1	F	125	ALA	4.2
1	F	82	HIS	4.1
1	F	121	SER	4.1
1	F	61	LEU	4.1
1	F	156	LEU	4.0
1	F	120	TYR	4.0
1	F	119	ASP	4.0
1	F	347	TRP	4.0
1	F	143	GLU	3.9
1	F	142	GLY	3.9
1	F	198	TRP	3.9
1	F	300	MET	3.9
1	F	149	GLY	3.9
1	F	92	ALA	3.8
1	F	151	LEU	3.8
1	E	150	GLN	3.8
1	F	135	TRP	3.8
1	C	149	GLY	3.8
1	D	222	GLY	3.8
1	D	295	ILE	3.7
1	F	246	GLU	3.7
1	F	294	PHE	3.7
1	F	141	THR	3.7
1	C	148	LYS	3.7
1	D	64	GLU	3.6
1	E	134	GLN	3.6
1	F	113	TYR	3.6
1	E	159	ALA	3.5
1	F	154	TYR	3.5
1	F	90	THR	3.5
1	F	238	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	60	LEU	3.5
1	E	133	PRO	3.5
1	F	203	PHE	3.5
1	F	292	PHE	3.5
1	F	302	LYS	3.5
1	F	164	TRP	3.5
1	C	246	GLU	3.4
1	D	224	ASP	3.4
1	F	345	LEU	3.4
1	E	245	ALA	3.4
1	F	124	ALA	3.4
1	F	89	THR	3.4
1	F	197	LEU	3.4
1	E	220	LYS	3.4
1	F	189	ILE	3.4
1	E	135	TRP	3.4
1	F	137	LEU	3.4
1	F	190	ALA	3.4
1	E	142	GLY	3.4
1	F	140	THR	3.3
1	D	223	ASP	3.3
1	F	100	GLN	3.3
1	F	127	LYS	3.3
1	F	244	PHE	3.3
1	F	301	ARG	3.3
1	F	139	THR	3.3
1	F	76	ILE	3.3
1	E	137	LEU	3.2
1	D	71	THR	3.2
1	F	340	MET	3.2
1	F	264	LYS	3.2
1	F	94	ILE	3.2
1	C	150	GLN	3.2
1	F	191	SER	3.2
1	E	118	LEU	3.2
1	F	201	GLU	3.2
1	D	129	TYR	3.2
1	F	77	CYS	3.2
1	F	103	ASN	3.1
1	E	124	ALA	3.1
1	F	133	PRO	3.1
1	F	367	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	168	VAL	3.1
1	F	310	VAL	3.1
1	F	206	ILE	3.1
1	F	193	ALA	3.1
1	F	63	LYS	3.1
1	C	244	PHE	3.1
1	D	132	HIS	3.1
1	F	87	HIS	3.1
1	D	142	GLY	3.1
1	C	139	THR	3.1
1	F	293	THR	3.1
1	F	295	ILE	3.1
1	D	98	ALA	3.1
1	E	131	LYS	3.1
1	F	380	VAL	3.1
1	F	392	ARG	3.0
1	E	136	TRP	3.0
1	F	192	GLN	3.0
1	D	86	THR	3.0
1	F	96	ALA	3.0
1	D	131	LYS	3.0
1	F	115	ASN	3.0
1	F	117	PHE	3.0
1	E	148	LYS	3.0
1	E	158	ASN	3.0
1	D	134	GLN	3.0
1	F	172	ALA	3.0
1	F	148	LYS	3.0
1	E	174	VAL	2.9
1	F	165	TRP	2.9
1	C	146	ARG	2.9
1	F	50	ILE	2.9
1	E	138	ARG	2.9
1	F	185	ALA	2.9
1	E	164	TRP	2.9
1	F	101	LEU	2.9
1	F	382	LEU	2.9
1	F	58	GLN	2.9
1	E	167	ASN	2.9
1	F	85	ARG	2.9
1	D	220	LYS	2.9
1	F	306	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	93	GLY	2.9
1	F	195	ARG	2.9
1	E	130	ALA	2.9
1	D	215	GLN	2.9
1	C	37	GLU	2.9
1	C	38	SER	2.8
1	D	61	LEU	2.8
1	D	104	LEU	2.8
1	E	160	GLU	2.8
1	F	131	LYS	2.8
1	F	307	LYS	2.8
1	F	251	ALA	2.8
1	E	127	LYS	2.8
1	F	256	PHE	2.8
1	E	144	LEU	2.8
1	F	299	ALA	2.8
1	F	387	ALA	2.8
1	E	120	TYR	2.8
1	F	98	ALA	2.8
1	F	138	ARG	2.8
1	F	111	ILE	2.7
1	D	78	LEU	2.7
1	B	237	ASP	2.7
1	E	93	GLY	2.7
1	F	271	ILE	2.7
1	E	140	THR	2.7
1	F	71	THR	2.7
1	F	147	LYS	2.7
1	E	163	ASN	2.7
1	E	202	LYS	2.7
1	F	102	LYS	2.7
1	C	141	THR	2.7
1	F	388	GLU	2.7
1	F	126	HIS	2.7
1	F	270	ASP	2.7
1	E	216	GLU	2.7
1	F	229	TYR	2.7
1	F	182	PHE	2.6
1	C	144	LEU	2.6
1	D	57	SER	2.6
1	F	38	SER	2.6
1	F	116	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	148	LYS	2.6
1	E	162	ARG	2.6
1	F	194	ASN	2.6
1	D	199	GLY	2.6
1	F	227	ILE	2.6
1	C	137	LEU	2.6
1	F	79	GLU	2.6
1	F	178	CYS	2.6
1	E	173	VAL	2.6
1	F	157	SER	2.6
1	F	83	ALA	2.6
1	F	305	THR	2.6
1	D	85	ARG	2.6
1	F	313	ASP	2.6
1	D	221	ILE	2.6
1	D	260	GLN	2.6
1	F	173	VAL	2.6
1	F	177	THR	2.6
1	F	348	TYR	2.6
1	D	136	TRP	2.5
1	E	143	GLU	2.5
1	F	52	PHE	2.5
1	C	359	VAL	2.5
1	F	72	ARG	2.5
1	F	88	GLY	2.5
1	E	213	ILE	2.5
1	F	289	TRP	2.5
1	F	67	GLU	2.5
1	F	91	GLU	2.5
1	F	97	GLU	2.5
1	F	259	PHE	2.5
1	B	150	GLN	2.5
1	F	163	ASN	2.5
1	E	92	ALA	2.5
1	F	59	GLY	2.5
1	F	161	PHE	2.5
1	F	132	HIS	2.5
1	F	285	VAL	2.5
1	E	38	SER	2.5
1	E	89	THR	2.5
1	E	247	TYR	2.5
1	E	244	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	68	PHE	2.5
1	D	103	ASN	2.5
1	C	193	ALA	2.5
1	F	169	ALA	2.5
1	F	231	GLY	2.4
1	F	146	ARG	2.4
1	E	205	ALA	2.4
1	F	262	ALA	2.4
1	F	383	GLU	2.4
1	E	149	GLY	2.4
1	D	150	GLN	2.4
1	D	219	GLN	2.4
1	F	304	LEU	2.4
1	A	244	PHE	2.4
1	E	128	GLU	2.4
1	E	201	GLU	2.4
1	F	196	LYS	2.4
1	F	257	GLY	2.4
1	F	184	ASP	2.4
1	C	301	ARG	2.4
1	D	83	ALA	2.4
1	D	135	TRP	2.4
1	D	141	THR	2.4
1	F	56	LYS	2.4
1	D	149	GLY	2.4
1	E	129	TYR	2.4
1	E	161	PHE	2.4
1	F	338	TYR	2.4
1	D	127	LYS	2.4
1	E	206	ILE	2.3
1	F	200	ASP	2.3
1	F	255	HIS	2.3
1	F	80	LYS	2.3
1	F	389	ILE	2.3
1	F	175	ASP	2.3
1	F	309	ARG	2.3
1	E	199	GLY	2.3
1	F	253	ILE	2.3
1	F	344	CYS	2.3
1	F	245	ALA	2.3
1	F	290	ALA	2.3
1	F	235	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	37	GLU	2.3
1	F	128	GLU	2.3
1	F	317	PHE	2.3
1	F	69	VAL	2.3
1	D	99	ARG	2.3
1	E	151	LEU	2.2
1	E	156	LEU	2.2
1	E	212	ASP	2.2
1	B	269	ARG	2.2
1	F	110	VAL	2.2
1	F	247	TYR	2.2
1	D	97	GLU	2.2
1	E	259	PHE	2.2
1	D	66	ALA	2.2
1	D	63	LYS	2.2
1	F	176	GLY	2.2
1	E	119	ASP	2.2
1	E	243	ASP	2.2
1	F	346	GLU	2.2
1	E	85	ARG	2.2
1	E	238	TRP	2.2
1	F	336	TRP	2.2
1	E	117	PHE	2.2
1	F	174	VAL	2.2
1	E	58	GLN	2.2
1	D	101	LEU	2.2
1	F	213	ILE	2.2
1	F	155	ASP	2.2
1	D	133	PRO	2.2
1	D	292	PHE	2.2
1	D	174	VAL	2.1
1	F	284	VAL	2.1
1	D	177	THR	2.1
1	D	197	LEU	2.1
1	F	187	PRO	2.1
1	D	294	PHE	2.1
1	F	48	VAL	2.1
1	C	152	MET	2.1
1	D	152	MET	2.1
1	E	153	ARG	2.1
1	F	341	GLU	2.1
1	F	386	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	200	ASP	2.1
1	F	365	ASP	2.1
1	C	198	TRP	2.1
1	F	158	ASN	2.1
1	D	291	GLY	2.1
1	F	199	GLY	2.1
1	F	210	LEU	2.1
1	C	379	ARG	2.1
1	E	221	ILE	2.1
1	E	184	ASP	2.1
1	C	303	PRO	2.1
1	D	252	MET	2.1
1	F	186	PHE	2.1
1	F	351	PHE	2.1
1	F	363	VAL	2.1
1	D	392	ARG	2.1
1	D	37	GLU	2.1
1	E	166	THR	2.1
1	F	62	THR	2.1
1	E	147	LYS	2.1
1	D	243	ASP	2.1
1	E	154	TYR	2.1
1	D	377	SER	2.1
1	F	260	GLN	2.0
1	A	392	ARG	2.0
1	E	185	ALA	2.0
1	F	369	LEU	2.0
1	B	149	GLY	2.0
1	E	198	TRP	2.0
1	F	81	GLY	2.0
1	F	312	LYS	2.0
1	C	138	ARG	2.0
1	D	156	LEU	2.0
1	C	142	GLY	2.0
1	D	176	GLY	2.0
1	F	291	GLY	2.0
1	E	224	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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	EDO	C	401	4/4	0.84	0.14	43,45,45,46	0
2	EDO	B	401	4/4	0.94	0.10	37,38,39,40	0
2	EDO	A	401	4/4	0.94	0.10	34,36,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.