Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 09:20 AM EST

PDB ID	:	3RO8
Title	:	Crystal structure of the catalytic domain of XynA1 from Paenibacillus sp. JDR-2
Authors	:	Pozharski, E.; St John, F.J.
Deposited on	:	2011-04-25
Resolution	:	1.34 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:

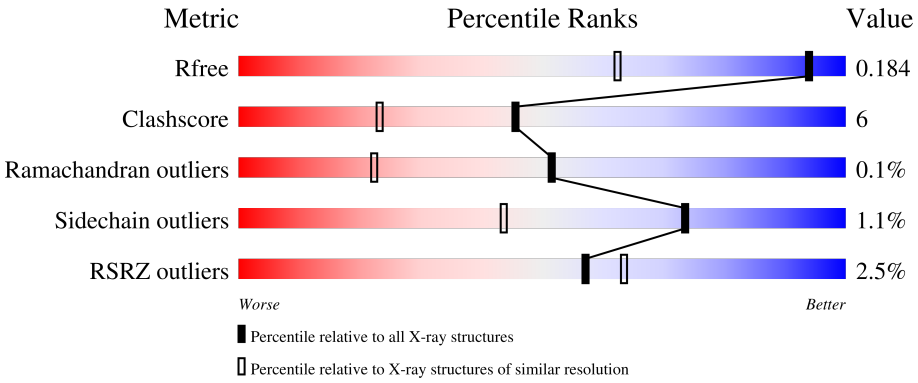
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.34 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}	130704	1385 (1.36-1.32)
Clashscore	141614	1417 (1.36-1.32)
Ramachandran outliers	138981	1397 (1.36-1.32)
Sidechain outliers	138945	1397 (1.36-1.32)
RSRZ outliers	127900	1369 (1.36-1.32)

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 <=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	341	2% 76% 12% • 11%
1	B	341	2% 76% 12% • 11%
1	C	341	% 77% 10% • 11%
1	D	341	% 77% 12% 12%
1	E	341	2% 76% 11% • 12%

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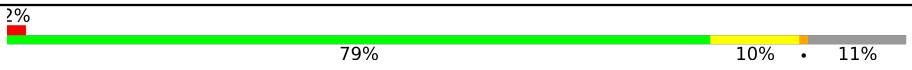
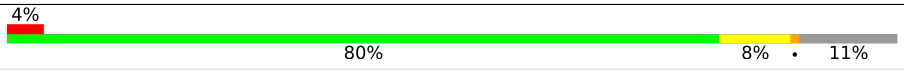
Mol	Chain	Length	Quality of chain
1	F	341	
1	G	341	
1	H	341	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23733 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 Endo-1,4-beta-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	19	0
			2575	1626	442	496	11			
1	B	304	Total	C	N	O	S	0	17	0
			2571	1625	444	489	13			
1	C	302	Total	C	N	O	S	0	14	0
			2507	1582	432	481	12			
1	D	301	Total	C	N	O	S	0	17	0
			2530	1594	438	486	12			
1	E	301	Total	C	N	O	S	0	16	0
			2530	1594	439	486	11			
1	F	304	Total	C	N	O	S	0	18	0
			2575	1622	447	494	12			
1	G	304	Total	C	N	O	S	0	13	0
			2527	1592	438	486	11			
1	H	304	Total	C	N	O	S	0	20	0
			2585	1629	446	498	12			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP C6CRV0
A	2	SER	-	expression tag	UNP C6CRV0
A	3	HIS	-	expression tag	UNP C6CRV0
A	4	MET	-	expression tag	UNP C6CRV0
A	339	ALA	-	expression tag	UNP C6CRV0
A	340	GLU	-	expression tag	UNP C6CRV0
A	341	GLN	-	expression tag	UNP C6CRV0
B	1	GLY	-	expression tag	UNP C6CRV0
B	2	SER	-	expression tag	UNP C6CRV0
B	3	HIS	-	expression tag	UNP C6CRV0
B	4	MET	-	expression tag	UNP C6CRV0
B	339	ALA	-	expression tag	UNP C6CRV0
B	340	GLU	-	expression tag	UNP C6CRV0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	341	GLN	-	expression tag	UNP C6CRV0
C	1	GLY	-	expression tag	UNP C6CRV0
C	2	SER	-	expression tag	UNP C6CRV0
C	3	HIS	-	expression tag	UNP C6CRV0
C	4	MET	-	expression tag	UNP C6CRV0
C	339	ALA	-	expression tag	UNP C6CRV0
C	340	GLU	-	expression tag	UNP C6CRV0
C	341	GLN	-	expression tag	UNP C6CRV0
D	1	GLY	-	expression tag	UNP C6CRV0
D	2	SER	-	expression tag	UNP C6CRV0
D	3	HIS	-	expression tag	UNP C6CRV0
D	4	MET	-	expression tag	UNP C6CRV0
D	339	ALA	-	expression tag	UNP C6CRV0
D	340	GLU	-	expression tag	UNP C6CRV0
D	341	GLN	-	expression tag	UNP C6CRV0
E	1	GLY	-	expression tag	UNP C6CRV0
E	2	SER	-	expression tag	UNP C6CRV0
E	3	HIS	-	expression tag	UNP C6CRV0
E	4	MET	-	expression tag	UNP C6CRV0
E	339	ALA	-	expression tag	UNP C6CRV0
E	340	GLU	-	expression tag	UNP C6CRV0
E	341	GLN	-	expression tag	UNP C6CRV0
F	1	GLY	-	expression tag	UNP C6CRV0
F	2	SER	-	expression tag	UNP C6CRV0
F	3	HIS	-	expression tag	UNP C6CRV0
F	4	MET	-	expression tag	UNP C6CRV0
F	339	ALA	-	expression tag	UNP C6CRV0
F	340	GLU	-	expression tag	UNP C6CRV0
F	341	GLN	-	expression tag	UNP C6CRV0
G	1	GLY	-	expression tag	UNP C6CRV0
G	2	SER	-	expression tag	UNP C6CRV0
G	3	HIS	-	expression tag	UNP C6CRV0
G	4	MET	-	expression tag	UNP C6CRV0
G	339	ALA	-	expression tag	UNP C6CRV0
G	340	GLU	-	expression tag	UNP C6CRV0
G	341	GLN	-	expression tag	UNP C6CRV0
H	1	GLY	-	expression tag	UNP C6CRV0
H	2	SER	-	expression tag	UNP C6CRV0
H	3	HIS	-	expression tag	UNP C6CRV0
H	4	MET	-	expression tag	UNP C6CRV0
H	339	ALA	-	expression tag	UNP C6CRV0
H	340	GLU	-	expression tag	UNP C6CRV0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	341	GLN	-	expression tag	UNP C6CRV0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	C	1	Total Mg 2 2	0	1
2	D	1	Total Mg 1 1	0	0
2	E	2	Total Mg 2 2	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	1
3	B	1	Total Cl 1 1	0	1
3	C	1	Total Cl 1 1	0	1
3	D	1	Total Cl 1 1	0	1
3	E	2	Total Cl 2 2	0	1
3	F	1	Total Cl 1 1	0	1
3	G	1	Total Cl 1 1	0	1
3	H	1	Total Cl 1 1	0	1

- Molecule 4 is water.

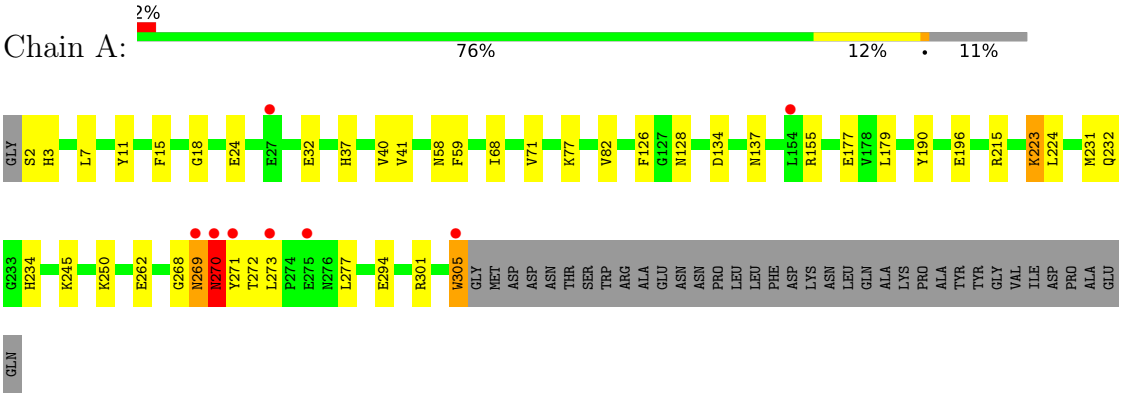
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	431	Total O 431 431	0	0
4	B	447	Total O 447 447	0	0
4	C	453	Total O 453 453	0	0
4	D	400	Total O 400 400	0	0
4	E	407	Total O 407 407	0	0
4	F	429	Total O 429 429	0	0
4	G	392	Total O 392 392	0	0
4	H	353	Total O 353 353	0	0

3 Residue-property plots (i)

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

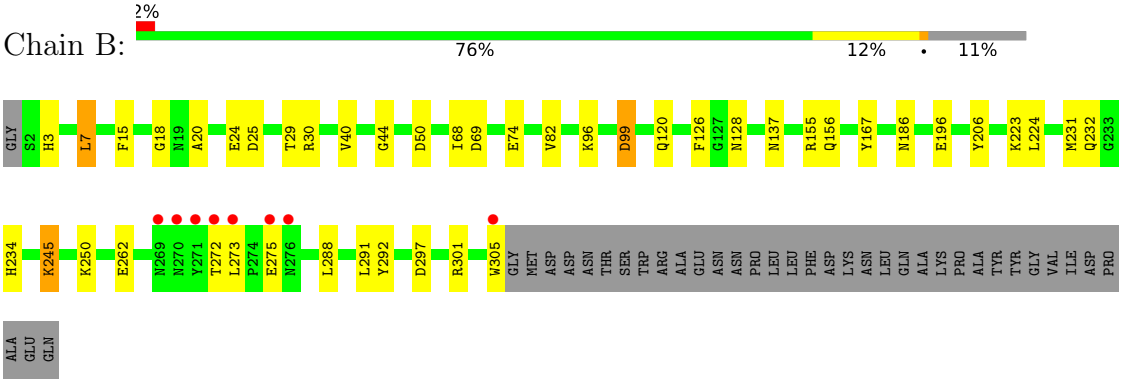
• Molecule 1: Endo-1,4-beta-xylanase

Chain A:



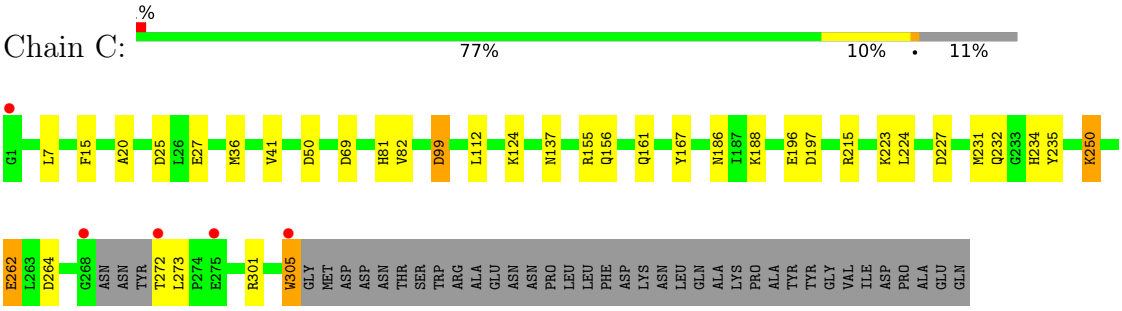
• Molecule 1: Endo-1,4-beta-xylanase

Chain B:

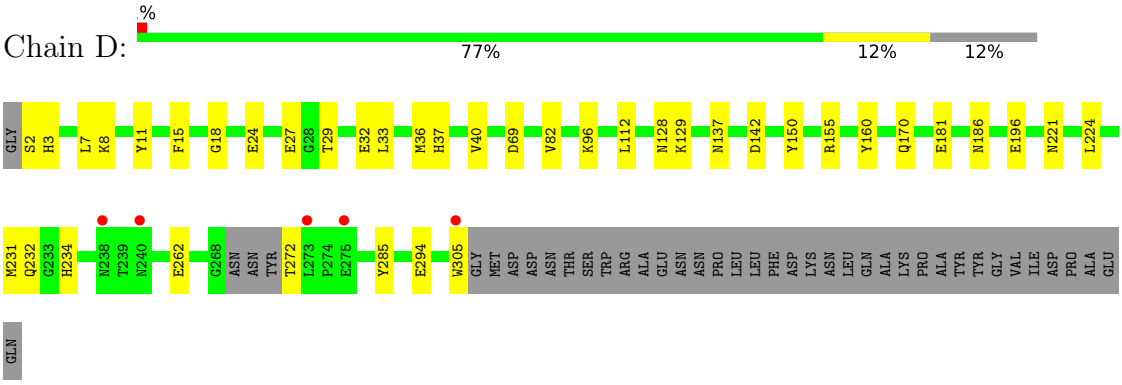


• Molecule 1: Endo-1,4-beta-xylanase

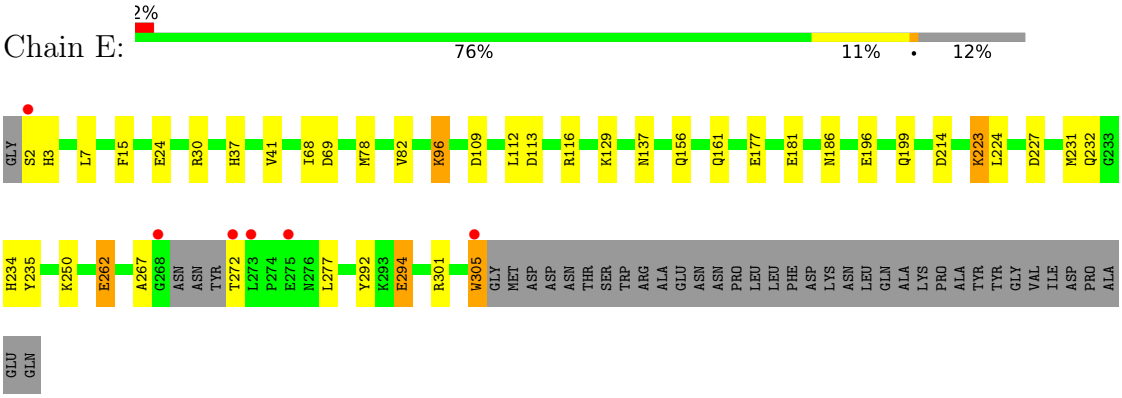
Chain C:



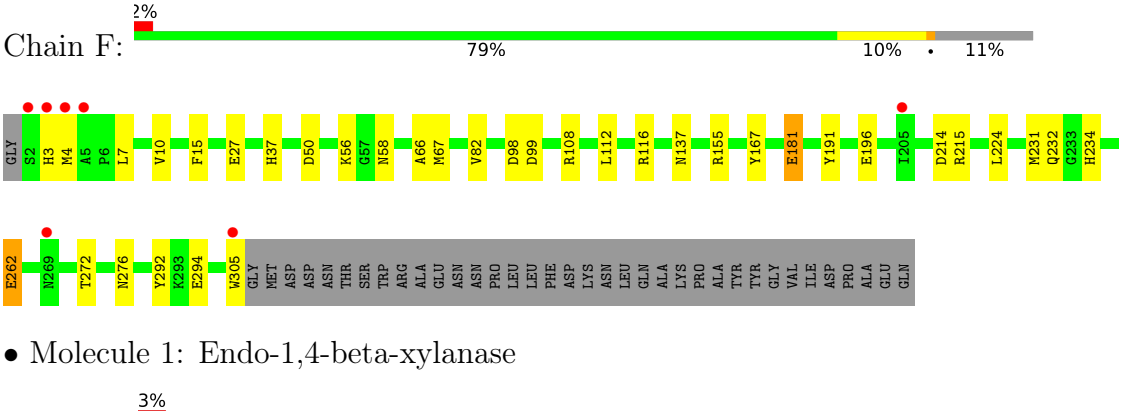
• Molecule 1: Endo-1,4-beta-xylanase



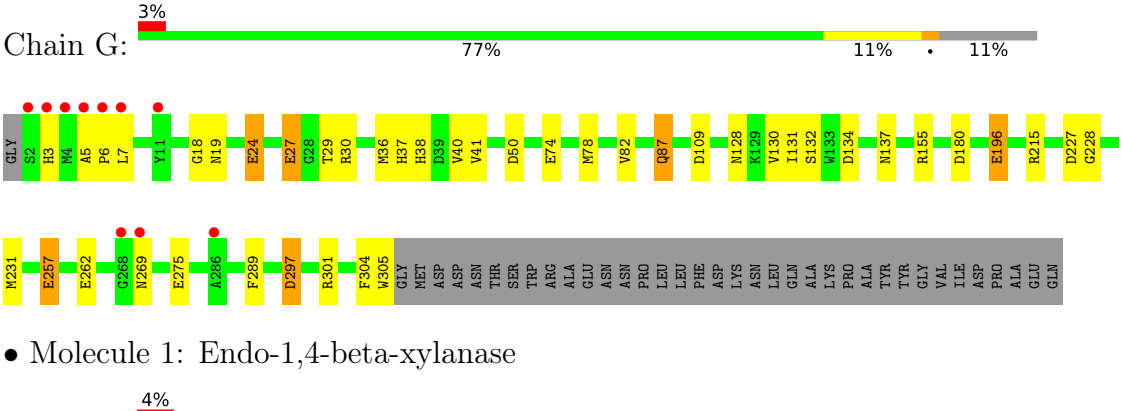
• Molecule 1: Endo-1,4-beta-xylanase



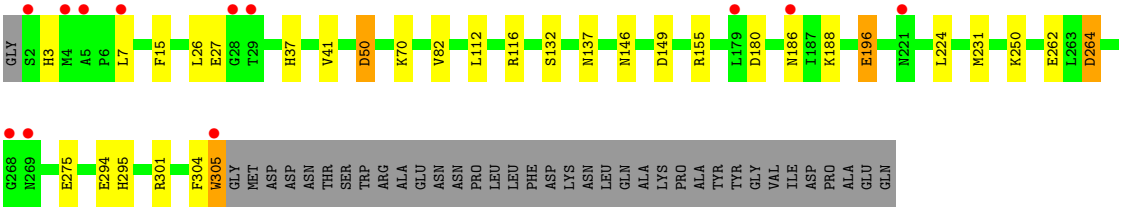
• Molecule 1: Endo-1,4-beta-xylanase



• Molecule 1: Endo-1,4-beta-xylanase



• Molecule 1: Endo-1,4-beta-xylanase


GLY
S2
H3
M4
A5
P6
L7
F15
L26
E27
G28
T29
H37
V41
D50
K70
V82
L112
R116
S132
N137
N146
D149
R155
L179
D180
N186
I187
K188
E196
N221
L224
M231
K250
E262
L263
D264
G268
N269
E275
E294
H295
R301
F304
W305
GLY
MET
ASP
ASP
ASN
THR
SER
TRP
ARG
ALA
GLU
ASN
ASN
PRO
LEU
LEU
PHE
ASP
LYS
ASN
LEU
GLN
ALA
LYS
PRO
ALA
TYR
TYR
GLY
VAL
ILE
ASP
PRO
ALA
GLU
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.07Å 93.17Å 182.95Å 90.00° 99.96° 90.00°	Depositor
Resolution (Å)	42.61 – 1.34 42.61 – 1.34	Depositor EDS
% Data completeness (in resolution range)	86.7 (42.61-1.34) 86.7 (42.61-1.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 1.34Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.142 , 0.185 0.141 , 0.184	Depositor DCC
R_{free} test set	26358 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	23733	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.42 % 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 3.1846e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, CL

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	1.33	7/2633 (0.3%)	1.17	8/3580 (0.2%)
1	B	1.33	9/2635 (0.3%)	1.16	17/3578 (0.5%)
1	C	1.30	4/2566 (0.2%)	1.17	15/3485 (0.4%)
1	D	1.31	7/2586 (0.3%)	1.10	5/3512 (0.1%)
1	E	1.31	10/2588 (0.4%)	1.12	10/3512 (0.3%)
1	F	1.34	5/2633 (0.2%)	1.17	12/3574 (0.3%)
1	G	1.34	9/2584 (0.3%)	1.15	14/3512 (0.4%)
1	H	1.28	3/2642 (0.1%)	1.09	6/3591 (0.2%)
All	All	1.32	54/20867 (0.3%)	1.14	87/28344 (0.3%)

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	A	0	1
1	H	0	1
All	All	0	2

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	TYR	CE1-CZ	7.60	1.48	1.38
1	E	41	VAL	CB-CG2	-7.59	1.36	1.52
1	F	292	TYR	CD1-CE1	7.33	1.50	1.39
1	B	250[A]	LYS	CE-NZ	7.16	1.67	1.49
1	B	250[B]	LYS	CE-NZ	7.16	1.67	1.49
1	D	11	TYR	CD2-CE2	7.05	1.50	1.39
1	H	41	VAL	CB-CG2	-6.85	1.38	1.52
1	A	177	GLU	CG-CD	6.52	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	24	GLU	CG-CD	6.50	1.61	1.51
1	E	262	GLU	CD-OE2	6.46	1.32	1.25
1	B	167	TYR	CG-CD2	6.21	1.47	1.39
1	B	120[A]	GLN	CD-NE2	6.20	1.48	1.32
1	B	120[B]	GLN	CD-NE2	6.20	1.48	1.32
1	A	250	LYS	CE-NZ	6.17	1.64	1.49
1	C	250	LYS	CE-NZ	6.13	1.64	1.49
1	D	160	TYR	CD1-CE1	6.08	1.48	1.39
1	E	292	TYR	CD1-CE1	6.06	1.48	1.39
1	D	155	ARG	CB-CG	-6.01	1.36	1.52
1	C	262	GLU	CD-OE2	5.98	1.32	1.25
1	E	181	GLU	CG-CD	5.86	1.60	1.51
1	C	235	TYR	CD1-CE1	5.84	1.48	1.39
1	A	58	ASN	CB-CG	5.79	1.64	1.51
1	D	285	TYR	CG-CD1	5.79	1.46	1.39
1	F	191	TYR	CD1-CE1	5.79	1.48	1.39
1	F	167	TYR	CG-CD2	5.75	1.46	1.39
1	E	177	GLU	CD-OE2	5.74	1.31	1.25
1	G	196[A]	GLU	CD-OE1	-5.71	1.19	1.25
1	G	196[B]	GLU	CD-OE1	-5.71	1.19	1.25
1	E	96	LYS	CE-NZ	5.71	1.63	1.49
1	C	41	VAL	CB-CG2	-5.70	1.40	1.52
1	G	27	GLU	CB-CG	-5.68	1.41	1.52
1	B	262	GLU	CD-OE2	5.67	1.31	1.25
1	D	150	TYR	CE2-CZ	5.66	1.46	1.38
1	G	304	PHE	CE1-CZ	5.57	1.48	1.37
1	E	294	GLU	CB-CG	5.56	1.62	1.52
1	A	223[A]	LYS	CE-NZ	5.54	1.62	1.49
1	A	223[B]	LYS	CE-NZ	5.54	1.62	1.49
1	H	196[A]	GLU	CD-OE1	-5.51	1.19	1.25
1	H	196[B]	GLU	CD-OE1	-5.51	1.19	1.25
1	E	235	TYR	CE1-CZ	5.45	1.45	1.38
1	D	150	TYR	CG-CD1	5.39	1.46	1.39
1	A	59	PHE	CE1-CZ	5.39	1.47	1.37
1	D	181	GLU	CG-CD	5.34	1.59	1.51
1	F	181	GLU	CG-CD	5.29	1.59	1.51
1	B	74	GLU	CB-CG	5.27	1.62	1.52
1	F	66	ALA	CA-CB	5.24	1.63	1.52
1	B	206	TYR	CE1-CZ	5.21	1.45	1.38
1	G	41	VAL	CB-CG2	-5.20	1.42	1.52
1	G	289	PHE	CB-CG	-5.17	1.42	1.51
1	E	186[A]	ASN	CB-CG	5.16	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	186[B]	ASN	CB-CG	5.16	1.62	1.51
1	G	74	GLU	CD-OE1	5.13	1.31	1.25
1	B	275	GLU	CB-CG	5.10	1.61	1.52
1	G	257	GLU	CD-OE2	5.10	1.31	1.25

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	301	ARG	NE-CZ-NH2	-13.16	113.72	120.30
1	G	301	ARG	NE-CZ-NH2	-11.78	114.41	120.30
1	C	215	ARG	NE-CZ-NH2	-11.45	114.58	120.30
1	D	155	ARG	NE-CZ-NH2	-10.88	114.86	120.30
1	B	301	ARG	NE-CZ-NH2	-10.39	115.11	120.30
1	G	215	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	C	301	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	A	215	ARG	NE-CZ-NH1	9.23	124.91	120.30
1	C	155	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	F	214	ASP	CB-CG-OD2	-9.15	110.06	118.30
1	B	155	ARG	NE-CZ-NH2	-9.01	115.80	120.30
1	F	215	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	H	301	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	G	180	ASP	CB-CG-OD1	8.32	125.78	118.30
1	G	227	ASP	CB-CG-OD1	-8.11	111.00	118.30
1	D	155	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	C	155	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	B	99	ASP	CB-CG-OD2	7.51	125.06	118.30
1	B	50	ASP	CB-CG-OD1	7.46	125.01	118.30
1	B	223	LYS	CD-CE-NZ	-7.31	94.89	111.70
1	A	155	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	G	180	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	G	134	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	C	250	LYS	CD-CE-NZ	6.99	127.77	111.70
1	A	262	GLU	OE1-CD-OE2	6.82	131.48	123.30
1	B	99	ASP	CB-CG-OD1	-6.80	112.18	118.30
1	C	124	LYS	CD-CE-NZ	-6.80	96.06	111.70
1	C	262	GLU	OE1-CD-OE2	6.78	131.44	123.30
1	F	108	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	C	50	ASP	CB-CG-OD1	6.59	124.23	118.30
1	G	24	GLU	CA-CB-CG	6.58	127.88	113.40
1	F	215	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	C	7	LEU	CB-CG-CD1	-6.52	99.92	111.00
1	E	109	ASP	CB-CG-OD1	6.34	124.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	215	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	H	264	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	B	7	LEU	CB-CG-CD2	-6.17	100.51	111.00
1	F	155	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	C	227	ASP	CB-CG-OD1	-6.15	112.76	118.30
1	H	155	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	G	155	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	E	78[A]	MET	CG-SD-CE	6.11	109.97	100.20
1	E	78[B]	MET	CG-SD-CE	6.11	109.97	100.20
1	D	129	LYS	CD-CE-NZ	-5.96	97.99	111.70
1	B	301	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	B	50	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	C	167	TYR	CB-CG-CD1	-5.81	117.51	121.00
1	A	215	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	F	50	ASP	CB-CG-OD1	5.77	123.49	118.30
1	E	301	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	F	155	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	197	ASP	CB-CG-OD1	5.65	123.38	118.30
1	E	223[A]	LYS	CD-CE-NZ	-5.62	98.76	111.70
1	E	223[B]	LYS	CD-CE-NZ	-5.62	98.76	111.70
1	F	292	TYR	CD1-CE1-CZ	-5.57	114.79	119.80
1	B	297	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	C	99	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	B	288	LEU	CB-CG-CD1	-5.47	101.70	111.00
1	E	96	LYS	CD-CE-NZ	5.45	124.23	111.70
1	A	134	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	E	214	ASP	CB-CG-OD1	5.40	123.16	118.30
1	G	50	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	245[A]	LYS	CD-CE-NZ	-5.35	99.40	111.70
1	B	245[B]	LYS	CD-CE-NZ	-5.35	99.40	111.70
1	B	30	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	G	297[A]	ASP	CB-CG-OD1	5.34	123.11	118.30
1	G	297[B]	ASP	CB-CG-OD1	5.34	123.11	118.30
1	G	109	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	H	180	ASP	CB-CG-OD1	5.26	123.04	118.30
1	F	56	LYS	CD-CE-NZ	-5.22	99.68	111.70
1	C	25	ASP	CB-CG-OD1	5.22	123.00	118.30
1	E	69	ASP	CB-CG-OD1	5.21	122.99	118.30
1	G	227	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	142	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	D	33	LEU	CB-CG-CD1	-5.18	102.19	111.00
1	E	227	ASP	CB-CG-OD2	5.16	122.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	262	GLU	OE1-CD-OE2	5.15	129.48	123.30
1	F	292	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	B	69	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	25	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	179	LEU	CB-CG-CD1	-5.06	102.40	111.00
1	B	292	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	F	214	ASP	CB-CG-OD1	5.04	122.84	118.30
1	H	50	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	C	223	LYS	CD-CE-NZ	-5.03	100.14	111.70
1	H	50	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	190	TYR	CB-CG-CD1	-5.01	118.00	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	ASN	Peptide
1	H	304	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2575	0	2475	45	0
1	B	2571	0	2483	31	0
1	C	2507	0	2412	34	0
1	D	2530	0	2424	29	1
1	E	2530	0	2438	37	1
1	F	2575	0	2467	27	0
1	G	2527	0	2422	33	0
1	H	2585	0	2480	31	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	1	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	431	0	0	11	1
4	B	447	0	0	14	0
4	C	453	0	0	14	0
4	D	400	0	0	15	0
4	E	407	0	0	14	1
4	F	429	0	0	11	0
4	G	392	0	0	9	0
4	H	353	0	0	9	1
All	All	23733	0	19601	258	3

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 (258) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270[B]:ASN:ND2	1:A:271[B]:TYR:H	0.93	1.40
1:A:270[B]:ASN:ND2	1:A:271[B]:TYR:N	1.71	1.35
1:A:224[B]:LEU:HD12	4:A:821:HOH:O	1.28	1.24
1:H:149[A]:ASP:OD1	4:H:852:HOH:O	1.58	1.21
1:B:224[B]:LEU:HD12	4:B:863:HOH:O	0.99	1.14
4:A:851:HOH:O	1:C:36[B]:MET:SD	2.06	1.13
1:B:224[A]:LEU:HA	4:B:752:HOH:O	1.45	1.13
1:A:268:GLY:O	1:A:270[B]:ASN:HB2	1.48	1.12
1:C:27:GLU:HB3	4:C:713:HOH:O	1.50	1.11
1:E:113[B]:ASP:OD2	1:G:27:GLU:OE2	1.69	1.09
1:A:270[B]:ASN:CG	1:A:271[B]:TYR:H	1.51	1.08
1:G:24:GLU:HG3	4:G:657:HOH:O	1.54	1.05
1:D:186[A]:ASN:ND2	4:D:897:HOH:O	1.89	1.04
1:F:305[A]:TRP:CE3	4:F:912:HOH:O	2.09	1.04
1:H:305[C]:TRP:CZ3	4:H:757:HOH:O	2.12	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186[B]:ASN:O	1:B:186[B]:ASN:ND2	1.93	1.01
1:A:270[B]:ASN:HD22	1:A:271[B]:TYR:N	1.42	1.01
1:F:305[A]:TRP:HE3	4:F:912:HOH:O	1.42	1.00
1:H:305[C]:TRP:HZ3	4:H:757:HOH:O	1.47	0.97
1:E:305:TRP:HE3	1:E:305:TRP:HA	1.28	0.97
1:E:305:TRP:HA	1:E:305:TRP:CE3	2.00	0.96
1:A:305:TRP:HA	1:A:305:TRP:CE3	1.99	0.96
1:A:305:TRP:HA	1:A:305:TRP:HE3	1.27	0.96
1:H:112[B]:LEU:HD21	1:H:116[B]:ARG:NH2	1.81	0.95
1:E:24:GLU:HG3	4:E:784:HOH:O	1.65	0.95
1:A:41[B]:VAL:HG11	1:A:71:VAL:HG11	1.48	0.93
1:E:68[C]:ILE:CD1	1:E:129:LYS:HD3	1.99	0.92
1:G:269:ASN:HB2	4:G:886:HOH:O	1.70	0.92
1:B:128[B]:ASN:OD1	4:B:945:HOH:O	1.87	0.92
1:D:27:GLU:HB3	4:D:778:HOH:O	1.68	0.92
1:H:250:LYS:HE2	4:H:844:HOH:O	1.72	0.90
1:G:305[B]:TRP:CZ3	4:G:842:HOH:O	2.26	0.89
1:B:186[B]:ASN:C	1:B:186[B]:ASN:HD22	1.79	0.85
1:F:27:GLU:HB3	4:F:795:HOH:O	1.77	0.85
1:G:78[B]:MET:O	1:G:130[B]:VAL:HG23	1.78	0.84
1:E:234[B]:HIS:HD2	4:E:717:HOH:O	1.61	0.83
1:H:305[B]:TRP:HA	4:H:833:HOH:O	1.79	0.82
1:C:232:GLN:OE1	1:C:234[B]:HIS:CE1	2.32	0.81
1:C:188:LYS:HE3	4:C:834:HOH:O	1.79	0.81
1:D:24:GLU:HG3	4:D:734:HOH:O	1.78	0.81
1:C:250:LYS:HD3	4:C:837:HOH:O	1.78	0.80
1:C:305[A]:TRP:CE3	1:C:305[A]:TRP:HA	2.16	0.80
1:C:305[A]:TRP:HA	1:C:305[A]:TRP:HE3	1.43	0.80
1:B:305[A]:TRP:HA	1:B:305[A]:TRP:CE3	2.17	0.80
1:A:41[B]:VAL:CG1	1:A:71:VAL:HG11	2.12	0.80
1:D:224:LEU:HA	4:D:748:HOH:O	1.80	0.80
1:D:32:GLU:OE2	4:D:771:HOH:O	1.99	0.80
1:C:305[B]:TRP:CZ2	4:C:806:HOH:O	2.34	0.79
1:G:128[B]:ASN:OD1	4:G:891:HOH:O	2.00	0.78
1:A:232:GLN:OE1	1:A:234[B]:HIS:CE1	2.37	0.78
1:F:224[B]:LEU:HA	4:F:671:HOH:O	1.82	0.78
1:A:245[B]:LYS:NZ	4:A:616:HOH:O	2.17	0.78
1:B:232:GLN:OE1	1:B:234[B]:HIS:CE1	2.37	0.77
1:G:297[B]:ASP:OD1	4:G:884:HOH:O	2.02	0.77
1:B:305[A]:TRP:HA	1:B:305[A]:TRP:HE3	1.49	0.77
1:E:112[B]:LEU:HD21	1:E:116[B]:ARG:NH2	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LEU:HA	4:C:852:HOH:O	1.84	0.77
1:H:27:GLU:HB2	4:H:742:HOH:O	1.84	0.76
1:A:41[B]:VAL:HG12	1:A:77:LYS:O	1.86	0.76
1:A:32[B]:GLU:OE2	4:A:931:HOH:O	2.04	0.76
1:E:82:VAL:HG21	1:E:137:ASN:HB2	1.68	0.76
1:A:223[B]:LYS:HG2	1:A:224[B]:LEU:H	1.52	0.75
1:C:250:LYS:CD	4:C:837:HOH:O	2.34	0.74
1:E:68[C]:ILE:HD11	1:E:129:LYS:HD3	1.67	0.74
1:H:294[B]:GLU:HG2	1:H:295:HIS:CE1	2.22	0.74
1:C:156:GLN:HB3	1:C:161[B]:GLN:NE2	2.02	0.73
1:G:305[B]:TRP:HZ3	4:G:842:HOH:O	1.66	0.73
1:B:24:GLU:HG3	4:B:740:HOH:O	1.87	0.73
1:F:67[B]:MET:HG3	4:F:532:HOH:O	1.89	0.72
1:A:41[B]:VAL:HG11	1:A:71:VAL:CG1	2.19	0.72
1:D:29[A]:THR:HG21	4:D:805:HOH:O	1.88	0.72
1:F:232:GLN:OE1	1:F:234[B]:HIS:CE1	2.42	0.72
1:F:58:ASN:HB2	4:F:727:HOH:O	1.89	0.71
1:D:69:ASP:OD1	4:D:760:HOH:O	2.09	0.71
1:D:112[A]:LEU:HD21	4:D:824:HOH:O	1.91	0.71
4:F:647:HOH:O	1:G:29:THR:HG21	1.93	0.69
1:C:156:GLN:HB3	1:C:161[B]:GLN:HE21	1.55	0.68
1:B:305[B]:TRP:CZ2	4:B:753:HOH:O	2.46	0.68
1:C:69:ASP:OD1	4:C:879:HOH:O	2.10	0.68
1:B:224[B]:LEU:CD1	4:B:863:HOH:O	1.81	0.68
1:D:32:GLU:OE1	4:D:742:HOH:O	2.11	0.68
1:E:3:HIS:CE1	1:E:7[A]:LEU:HD11	2.29	0.67
1:F:305[A]:TRP:HB2	4:F:912:HOH:O	1.95	0.67
1:D:32:GLU:O	1:D:36[B]:MET:HG2	1.94	0.67
1:F:112:LEU:HD21	1:F:116[B]:ARG:NH2	2.10	0.66
1:F:272:THR:HG22	4:F:793:HOH:O	1.94	0.66
1:G:269:ASN:CB	4:G:886:HOH:O	2.36	0.66
1:C:82:VAL:HG21	1:C:137[B]:ASN:HB2	1.78	0.66
1:D:3:HIS:CE1	1:D:7[A]:LEU:HD11	2.31	0.65
1:A:305:TRP:CE3	1:A:305:TRP:CA	2.77	0.65
1:A:223[B]:LYS:HG2	1:A:224[B]:LEU:N	2.10	0.65
1:A:234[B]:HIS:CE1	4:A:824:HOH:O	2.49	0.65
1:C:36[B]:MET:O	1:C:36[B]:MET:HG3	1.94	0.65
1:D:272:THR:N	4:D:834:HOH:O	2.29	0.65
1:F:82:VAL:HG21	1:F:137:ASN:HB2	1.79	0.64
1:G:130[B]:VAL:HG22	1:G:131:ILE:N	2.12	0.64
1:H:82:VAL:HG21	1:H:137:ASN:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLY:O	1:A:270[B]:ASN:CB	2.37	0.64
1:B:82:VAL:HG21	1:B:137:ASN:HB2	1.80	0.64
1:G:82:VAL:HG21	1:G:137:ASN:HB2	1.81	0.63
1:A:272[A]:THR:O	1:A:273[A]:LEU:CB	2.46	0.63
1:A:270[B]:ASN:CG	1:A:271[B]:TYR:N	2.26	0.62
1:D:234[B]:HIS:HD2	4:D:801:HOH:O	1.80	0.62
1:C:112[A]:LEU:HD21	4:C:826:HOH:O	2.00	0.62
1:D:82:VAL:HG21	1:D:137:ASN:HB2	1.82	0.62
1:A:270[B]:ASN:ND2	1:A:271[B]:TYR:CA	2.63	0.62
1:H:112[B]:LEU:HD21	1:H:116[B]:ARG:CZ	2.28	0.62
1:A:68[B]:ILE:HD12	1:A:126:PHE:CE1	2.35	0.61
1:C:250:LYS:NZ	4:C:837:HOH:O	2.33	0.61
1:D:234[B]:HIS:HE1	1:D:262:GLU:OE1	1.83	0.61
1:H:3:HIS:CE1	1:H:7[A]:LEU:HD11	2.35	0.61
1:E:113[B]:ASP:OD2	1:G:27:GLU:CD	2.38	0.60
1:C:250:LYS:CE	4:C:837:HOH:O	2.50	0.60
1:B:156:GLN:NE2	4:B:862:HOH:O	2.31	0.60
1:G:130[B]:VAL:HG22	1:G:132:SER:H	1.67	0.59
1:H:224:LEU:HA	4:H:732:HOH:O	2.00	0.59
1:C:186:ASN:CG	4:C:735:HOH:O	2.39	0.59
1:E:2:SER:N	4:E:677:HOH:O	2.34	0.59
1:A:128:ASN:HB2	4:A:899:HOH:O	2.02	0.59
1:A:272[B]:THR:CG2	1:A:277:LEU:HB2	2.32	0.59
1:B:29[B]:THR:HG22	4:B:916:HOH:O	2.02	0.59
1:C:262:GLU:HA	1:C:305[B]:TRP:CD1	2.39	0.58
1:E:250[B]:LYS:NZ	4:E:756:HOH:O	2.30	0.58
1:C:82:VAL:HG21	1:C:137[A]:ASN:HB2	1.84	0.57
1:A:82:VAL:HG21	1:A:137:ASN:HB2	1.87	0.57
1:E:68[C]:ILE:HD13	1:E:129:LYS:HD3	1.83	0.57
1:F:4:MET:HB2	1:G:7[C]:LEU:HD11	1.87	0.57
1:F:181:GLU:HG3	4:F:736:HOH:O	2.04	0.57
1:D:305[A]:TRP:HA	1:D:305[A]:TRP:CE3	2.40	0.56
1:E:305:TRP:CE3	1:E:305:TRP:CA	2.81	0.56
1:A:272[B]:THR:HG23	1:A:277:LEU:HB2	1.88	0.56
1:G:78[B]:MET:O	1:G:130[B]:VAL:CG2	2.52	0.56
1:F:294[A]:GLU:HG3	4:F:841:HOH:O	2.05	0.56
1:B:68[B]:ILE:HD12	1:B:126:PHE:CE1	2.41	0.56
1:A:305:TRP:C	4:A:833:HOH:O	2.44	0.55
1:E:234[B]:HIS:HE1	1:E:262:GLU:OE1	1.89	0.55
1:E:250[B]:LYS:HD2	4:E:756:HOH:O	2.06	0.55
1:B:128[B]:ASN:ND2	4:B:945:HOH:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:GLU:HG3	4:D:758:HOH:O	2.07	0.55
1:C:232:GLN:OE1	1:C:234[B]:HIS:NE2	2.40	0.55
1:A:2:SER:N	4:A:802:HOH:O	2.40	0.54
1:E:161[B]:GLN:OE1	4:E:904:HOH:O	2.18	0.54
1:H:112[B]:LEU:CD2	1:H:116[B]:ARG:CZ	2.85	0.54
1:A:234[B]:HIS:HE1	4:A:824:HOH:O	1.85	0.54
1:D:232:GLN:OE1	1:D:234[B]:HIS:NE2	2.41	0.54
1:H:112[B]:LEU:HG	1:H:116[B]:ARG:CZ	2.38	0.54
1:D:96:LYS:NZ	4:D:792:HOH:O	2.40	0.54
1:H:26:LEU:HD13	1:H:70[B]:LYS:HG2	1.90	0.54
1:E:96:LYS:HE2	4:E:676:HOH:O	2.08	0.53
1:F:99[B]:ASP:OD2	1:H:146[B]:ASN:ND2	2.42	0.53
1:B:44:GLY:HA2	1:B:305[B]:TRP:CH2	2.43	0.52
1:E:199:GLN:NE2	4:E:756:HOH:O	2.41	0.52
1:D:112[B]:LEU:HD21	1:D:170[B]:GLN:HG3	1.92	0.52
1:E:68[C]:ILE:CD1	1:E:129:LYS:CD	2.84	0.52
1:H:186:ASN:OD1	1:H:188[B]:LYS:NZ	2.43	0.52
1:C:186:ASN:OD1	1:C:186:ASN:C	2.48	0.51
1:B:232:GLN:OE1	1:B:234[B]:HIS:NE2	2.44	0.51
1:B:20:ALA:HB2	1:B:305[B]:TRP:CD1	2.46	0.51
1:F:262:GLU:HG2	1:F:305[A]:TRP:CE3	2.45	0.51
1:H:294[B]:GLU:HG2	1:H:295:HIS:ND1	2.26	0.51
1:F:276:ASN:OD1	1:G:30:ARG:NH2	2.43	0.51
1:E:68[C]:ILE:HD11	1:E:129:LYS:CD	2.38	0.51
1:F:112:LEU:HG	1:F:116[B]:ARG:CZ	2.41	0.50
1:A:24:GLU:HG3	4:A:720:HOH:O	2.10	0.50
1:A:270[A]:ASN:N	1:A:270[A]:ASN:OD1	2.44	0.50
1:C:27:GLU:HG3	4:C:616:HOH:O	2.12	0.50
1:E:112[B]:LEU:HG	1:E:116[B]:ARG:CZ	2.42	0.50
1:D:234[B]:HIS:CE1	1:D:262:GLU:OE1	2.64	0.50
1:E:96:LYS:CE	4:E:676:HOH:O	2.60	0.50
1:G:3:HIS:CE1	1:G:7[A]:LEU:HD11	2.46	0.50
1:C:186:ASN:OD1	1:C:186:ASN:O	2.30	0.49
1:F:3:HIS:HB2	1:F:37:HIS:CE1	2.46	0.49
1:G:196[A]:GLU:OE2	1:G:231:MET:HG2	2.12	0.49
1:C:264[B]:ASP:OD1	1:C:264[B]:ASP:O	2.29	0.49
1:H:196[A]:GLU:OE2	1:H:231:MET:HG2	2.13	0.49
1:A:41[B]:VAL:HG13	1:A:41[B]:VAL:O	2.12	0.49
1:A:272[A]:THR:O	1:A:273[A]:LEU:HB3	2.13	0.49
1:D:29[B]:THR:HG21	4:D:805:HOH:O	2.11	0.49
1:A:3:HIS:CE1	1:A:7[A]:LEU:HD11	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245[B]:LYS:HG3	1:B:291:LEU:HD11	1.95	0.48
1:B:305[A]:TRP:CE3	1:B:305[A]:TRP:CA	2.93	0.48
1:E:112[B]:LEU:HD21	1:E:116[B]:ARG:HH22	1.77	0.48
1:F:3:HIS:CE1	1:F:7[A]:LEU:HD11	2.48	0.48
1:F:10:VAL:HG11	1:G:5:ALA:HB2	1.95	0.48
1:B:128[B]:ASN:CG	4:B:945:HOH:O	2.40	0.47
1:D:232:GLN:OE1	1:D:234[B]:HIS:CE1	2.66	0.47
1:E:223[B]:LYS:NZ	4:E:883:HOH:O	2.18	0.47
1:E:156[B]:GLN:HG3	3:E:403:CL:CL	2.52	0.47
1:B:68[B]:ILE:HD12	1:B:126:PHE:CD1	2.49	0.47
1:D:18:GLY:HA2	1:D:40:VAL:O	2.15	0.46
1:E:2:SER:CA	4:E:677:HOH:O	2.64	0.46
1:E:3:HIS:HB2	1:E:37:HIS:CE1	2.50	0.46
1:E:224:LEU:HA	4:E:712:HOH:O	2.13	0.46
1:G:19[B]:ASN:HB2	1:G:38:HIS:CD2	2.50	0.46
1:H:112[B]:LEU:HG	1:H:116[B]:ARG:NH1	2.29	0.46
1:F:10:VAL:HG11	1:G:5:ALA:CB	2.46	0.46
1:H:50:ASP:OD2	4:H:853:HOH:O	2.21	0.45
1:F:99[B]:ASP:OD2	1:H:146[B]:ASN:CG	2.55	0.45
1:B:186[B]:ASN:ND2	1:B:186[B]:ASN:C	2.54	0.45
1:A:232:GLN:OE1	1:A:234[B]:HIS:NE2	2.50	0.45
1:A:272[A]:THR:O	1:A:273[A]:LEU:HB2	2.16	0.45
1:B:96:LYS:NZ	4:B:744:HOH:O	2.38	0.45
1:C:264[B]:ASP:OD1	1:C:264[B]:ASP:C	2.54	0.45
1:H:112[B]:LEU:CG	1:H:116[B]:ARG:CZ	2.95	0.45
1:F:3:HIS:NE2	1:F:7[A]:LEU:HD11	2.32	0.44
1:G:262:GLU:HA	1:G:305[B]:TRP:HB2	1.99	0.44
1:H:264:ASP:HB2	1:H:305[B]:TRP:C	2.37	0.44
1:D:196[B]:GLU:HG3	1:D:231:MET:CE	2.47	0.44
1:G:196[B]:GLU:H	1:G:196[B]:GLU:CD	2.19	0.44
1:C:305[B]:TRP:CE2	4:C:806:HOH:O	2.66	0.44
1:D:8:LYS:HE2	1:D:36[A]:MET:O	2.17	0.44
1:E:294:GLU:HG3	4:E:734:HOH:O	2.17	0.44
1:A:196[B]:GLU:HG3	1:A:231:MET:CE	2.48	0.43
1:B:196[A]:GLU:OE2	1:B:231:MET:HG2	2.18	0.43
1:C:305[A]:TRP:CE3	1:C:305[A]:TRP:CA	2.92	0.43
1:C:69:ASP:CG	4:C:879:HOH:O	2.56	0.43
1:G:3:HIS:HB2	1:G:37:HIS:CE1	2.53	0.43
1:G:87[B]:GLN:NE2	4:G:683:HOH:O	2.45	0.43
1:F:98:ASP:HB2	1:H:149[A]:ASP:OD2	2.18	0.43
1:B:224[B]:LEU:HA	4:B:752:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:250:LYS:CE	4:H:844:HOH:O	2.48	0.43
1:G:269:ASN:ND2	4:G:886:HOH:O	2.43	0.43
1:D:3:HIS:HB2	1:D:37:HIS:CE1	2.54	0.43
1:B:3:HIS:CE1	1:B:7:LEU:HD11	2.54	0.43
1:F:7[C]:LEU:HA	1:F:7[C]:LEU:HD12	1.64	0.43
1:A:3:HIS:HB2	1:A:37:HIS:CE1	2.54	0.43
1:G:262:GLU:HG2	1:G:305[B]:TRP:CE3	2.54	0.42
1:A:272[B]:THR:HG21	1:A:277:LEU:HB2	1.99	0.42
1:C:196[A]:GLU:OE2	1:C:231:MET:HG2	2.19	0.42
1:B:305[A]:TRP:CD1	4:B:913:HOH:O	2.70	0.42
1:C:81:HIS:HE1	1:C:137[A]:ASN:ND2	2.17	0.42
1:B:305[B]:TRP:CE2	4:B:753:HOH:O	2.70	0.42
1:H:112[B]:LEU:HD21	1:H:116[B]:ARG:HH22	1.74	0.42
1:F:196[A]:GLU:OE2	1:F:231:MET:HG2	2.20	0.42
1:G:130[B]:VAL:HG21	1:G:132:SER:O	2.20	0.42
1:H:262:GLU:HG2	1:H:305[C]:TRP:CE3	2.55	0.42
1:H:3:HIS:HB2	1:H:37:HIS:CE1	2.55	0.42
1:A:68[B]:ILE:HD12	1:A:126:PHE:CD1	2.55	0.42
1:G:18:GLY:HA2	1:G:40:VAL:O	2.20	0.42
1:D:27:GLU:HG3	4:D:568:HOH:O	2.20	0.42
1:B:18:GLY:HA2	1:B:40:VAL:O	2.20	0.41
1:G:228:GLY:HA2	1:G:257:GLU:O	2.21	0.41
1:H:132:SER:HB3	1:H:188[B]:LYS:HB2	2.03	0.41
1:A:18:GLY:HA2	1:A:40:VAL:O	2.21	0.41
1:A:232:GLN:HB3	1:A:234[B]:HIS:CD2	2.56	0.41
1:A:294:GLU:HG3	4:A:642:HOH:O	2.21	0.41
1:E:2:SER:HA	4:E:677:HOH:O	2.20	0.41
1:E:196[A]:GLU:OE2	1:E:231:MET:HG2	2.21	0.41
1:E:234[B]:HIS:CE1	1:E:262:GLU:OE1	2.71	0.40
1:G:6:PRO:HG3	1:G:36:MET:HE2	2.03	0.40
1:C:20:ALA:HB2	1:C:305[B]:TRP:CD1	2.56	0.40
1:E:112[B]:LEU:HD21	1:E:116[B]:ARG:CZ	2.50	0.40
1:E:232:GLN:OE1	1:E:234[B]:HIS:NE2	2.54	0.40
1:E:267:ALA:HB1	1:E:272:THR:HG21	2.03	0.40
1:C:196[B]:GLU:OE2	1:C:231:MET:HB3	2.21	0.40
1:H:149[A]:ASP:OD1	1:H:149[A]:ASP:C	2.59	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:724:HOH:O	4:E:706:HOH:O[1_655]	2.09	0.11
1:E:30:ARG:NH2	1:H:275[B]:GLU:OE1[2_546]	2.10	0.10
1:D:128[B]:ASN:OD1	4:H:745:HOH:O[2_646]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	321/341 (94%)	313 (98%)	5 (2%)	3 (1%)	17 3
1	B	320/341 (94%)	317 (99%)	3 (1%)	0	100 100
1	C	311/341 (91%)	307 (99%)	4 (1%)	0	100 100
1	D	312/341 (92%)	305 (98%)	7 (2%)	0	100 100
1	E	314/341 (92%)	307 (98%)	7 (2%)	0	100 100
1	F	319/341 (94%)	311 (98%)	8 (2%)	0	100 100
1	G	314/341 (92%)	309 (98%)	5 (2%)	0	100 100
1	H	321/341 (94%)	313 (98%)	8 (2%)	0	100 100
All	All	2532/2728 (93%)	2482 (98%)	47 (2%)	3 (0%)	51 22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270[A]	ASN
1	A	270[B]	ASN
1	A	269	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/288 (96%)	273 (99%)	4 (1%)	67	34
1	B	277/288 (96%)	273 (99%)	4 (1%)	67	34
1	C	269/288 (93%)	263 (98%)	6 (2%)	52	17
1	D	272/288 (94%)	270 (99%)	2 (1%)	84	62
1	E	272/288 (94%)	269 (99%)	3 (1%)	73	44
1	F	276/288 (96%)	275 (100%)	1 (0%)	91	79
1	G	271/288 (94%)	268 (99%)	3 (1%)	73	44
1	H	278/288 (96%)	275 (99%)	3 (1%)	73	44
All	All	2192/2304 (95%)	2166 (99%)	26 (1%)	73	40

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	PHE
1	A	270[A]	ASN
1	A	270[B]	ASN
1	A	305	TRP
1	B	15	PHE
1	B	99	ASP
1	B	272	THR
1	B	273	LEU
1	C	15	PHE
1	C	99	ASP
1	C	272	THR
1	C	273	LEU
1	C	305[A]	TRP
1	C	305[B]	TRP
1	D	15	PHE
1	D	221	ASN
1	E	15	PHE
1	E	277	LEU
1	E	305	TRP
1	F	15	PHE
1	G	87[A]	GLN
1	G	87[B]	GLN
1	G	275	GLU
1	H	15	PHE

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Mol	Chain	Res	Type
1	H	305[B]	TRP
1	H	305[C]	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	156	GLN
1	D	221	ASN
1	E	199	GLN
1	E	298	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 21 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	304/341 (89%)	0.00	8 (2%)	56	62	13, 19, 29, 54	5 (1%)
1	B	304/341 (89%)	-0.02	8 (2%)	56	62	13, 18, 27, 55	5 (1%)
1	C	302/341 (88%)	-0.28	5 (1%)	70	74	13, 18, 29, 54	7 (2%)
1	D	301/341 (88%)	-0.25	5 (1%)	70	74	14, 20, 31, 56	7 (2%)
1	E	301/341 (88%)	-0.13	6 (1%)	65	70	13, 18, 30, 67	6 (1%)
1	F	304/341 (89%)	-0.18	7 (2%)	60	66	14, 20, 30, 46	5 (1%)
1	G	304/341 (89%)	-0.07	10 (3%)	46	52	15, 22, 32, 46	7 (2%)
1	H	304/341 (89%)	-0.05	12 (3%)	39	45	16, 22, 33, 46	6 (1%)
All	All	2424/2728 (88%)	-0.12	61 (2%)	57	63	13, 20, 31, 67	48 (1%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271	TYR	8.7
1	A	271[A]	TYR	6.9
1	D	273	LEU	5.9
1	A	269	ASN	5.7
1	E	305	TRP	5.2
1	F	2	SER	5.1
1	B	269	ASN	5.0
1	F	4	MET	4.8
1	B	305[A]	TRP	4.7
1	C	1	GLY	4.6
1	A	305	TRP	4.5
1	E	2	SER	4.5
1	H	305[B]	TRP	4.3
1	H	5	ALA	3.8
1	B	273	LEU	3.8
1	C	272	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	269	ASN	3.7
1	A	273[A]	LEU	3.7
1	H	269[A]	ASN	3.6
1	G	5	ALA	3.6
1	G	2	SER	3.5
1	C	305[A]	TRP	3.5
1	E	268	GLY	3.5
1	E	272	THR	3.3
1	H	268	GLY	3.3
1	G	6	PRO	3.3
1	A	270[A]	ASN	3.3
1	D	275	GLU	3.3
1	B	270	ASN	3.2
1	F	5	ALA	3.2
1	G	4	MET	3.1
1	E	275	GLU	3.1
1	G	3	HIS	3.0
1	G	7[A]	LEU	2.9
1	D	305[A]	TRP	2.9
1	F	3	HIS	2.8
1	C	268	GLY	2.8
1	H	2	SER	2.8
1	B	272	THR	2.8
1	H	7[A]	LEU	2.8
1	F	205	ILE	2.7
1	C	275	GLU	2.7
1	G	268	GLY	2.7
1	H	221	ASN	2.6
1	G	11	TYR	2.5
1	H	4	MET	2.5
1	A	275	GLU	2.5
1	G	286	ALA	2.4
1	F	305[A]	TRP	2.4
1	H	29[A]	THR	2.4
1	H	28	GLY	2.3
1	H	179	LEU	2.3
1	B	275	GLU	2.3
1	E	273	LEU	2.2
1	H	186	ASN	2.1
1	D	238	ASN	2.1
1	D	240	ASN	2.1
1	A	27[A]	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	276	ASN	2.0
1	A	154	LEU	2.0
1	G	269	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 monosaccharides 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, 95^{th} 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	MG	C	401[A]	1/1	0.97	0.17	14,14,14,14	1
2	MG	C	401[B]	1/1	0.97	0.17	25,25,25,25	1
2	MG	E	404	1/1	0.98	0.06	33,33,33,33	0
2	MG	B	403	1/1	0.99	0.04	23,23,23,23	0
2	MG	D	401	1/1	0.99	0.04	21,21,21,21	0
2	MG	A	403	1/1	0.99	0.06	27,27,27,27	0
2	MG	F	401	1/1	0.99	0.06	20,20,20,20	0
2	MG	G	401	1/1	0.99	0.08	27,27,27,27	0
3	CL	E	403	1/1	0.99	0.08	38,38,38,38	0
2	MG	B	401	1/1	1.00	0.04	19,19,19,19	0
2	MG	E	401	1/1	1.00	0.04	20,20,20,20	0
2	MG	H	401	1/1	1.00	0.10	25,25,25,25	0
3	CL	A	402[A]	1/1	1.00	0.06	15,15,15,15	1
3	CL	B	402[A]	1/1	1.00	0.06	14,14,14,14	1
3	CL	C	402[A]	1/1	1.00	0.04	17,17,17,17	1
3	CL	D	402[A]	1/1	1.00	0.04	22,22,22,22	1
3	CL	E	402[A]	1/1	1.00	0.04	16,16,16,16	1
2	MG	A	401	1/1	1.00	0.06	18,18,18,18	0
3	CL	F	402[A]	1/1	1.00	0.04	18,18,18,18	1
3	CL	G	402[A]	1/1	1.00	0.05	18,18,18,18	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	H	402[A]	1/1	1.00	0.05	18,18,18,18	1

6.5 Other polymers (i)

There are no such residues in this entry.