



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:14 pm BST

PDB ID : 5AYY
Title : CRYSTAL STRUCTURE OF HUMAN QUINOLINATE PHOSPHORIBOSYLTRANSFERASE IN COMPLEX WITH THE REACTANT QUINOLINATE
Authors : Youn, H.S.; Kim, T.G.; Kim, M.K.; Kang, G.B.; Kang, J.Y.; Seo, Y.J.; Lee, J.G.; An, J.Y.; Park, K.R.; Lee, Y.; Im, Y.J.; Lee, J.H.; Fukuoka, S.I.; Eom, S.H.
Deposited on : 2015-09-14
Resolution : 3.09 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

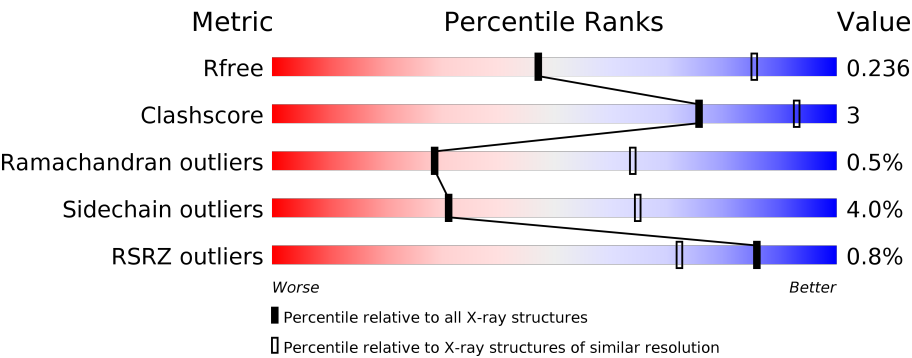
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 on 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	305	<div><div></div><div>86%7% • 5%</div></div>
1	B	305	<div>2%</div> <div><div></div><div>83%10% • 5%</div></div>
1	C	305	<div>%</div> <div><div></div><div>87%7% • 5%</div></div>
1	D	305	<div>%</div> <div><div></div><div>85%9% 5%</div></div>
1	E	305	<div>%</div> <div><div></div><div>85%9% 5%</div></div>
1	F	305	<div>%</div> <div><div></div><div>86%8% • 5%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	305	<div><div></div><div>83%10%5%</div></div>
1	H	305	<div><div></div><div>83%10%5%</div></div>
1	I	305	<div><div></div><div>87%7%5%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19117 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 Nicotinate-nucleotide pyrophosphorylase [carboxylating].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	B	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	C	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	D	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	E	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	F	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	G	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	H	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	I	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	LEU	-	expression tag	UNP V9HWJ5
A	299	GLU	-	expression tag	UNP V9HWJ5
A	300	HIS	-	expression tag	UNP V9HWJ5
A	301	HIS	-	expression tag	UNP V9HWJ5
A	302	HIS	-	expression tag	UNP V9HWJ5
A	303	HIS	-	expression tag	UNP V9HWJ5
A	304	HIS	-	expression tag	UNP V9HWJ5
A	305	HIS	-	expression tag	UNP V9HWJ5
B	298	LEU	-	expression tag	UNP V9HWJ5
B	299	GLU	-	expression tag	UNP V9HWJ5
B	300	HIS	-	expression tag	UNP V9HWJ5

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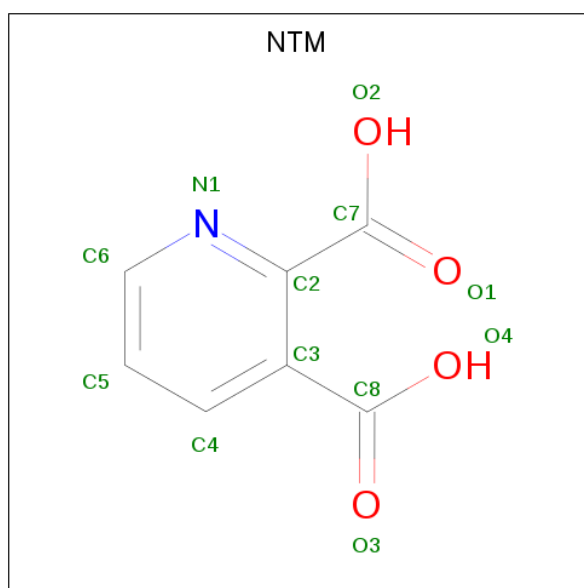
Chain	Residue	Modelled	Actual	Comment	Reference
B	301	HIS	-	expression tag	UNP V9HWJ5
B	302	HIS	-	expression tag	UNP V9HWJ5
B	303	HIS	-	expression tag	UNP V9HWJ5
B	304	HIS	-	expression tag	UNP V9HWJ5
B	305	HIS	-	expression tag	UNP V9HWJ5
C	298	LEU	-	expression tag	UNP V9HWJ5
C	299	GLU	-	expression tag	UNP V9HWJ5
C	300	HIS	-	expression tag	UNP V9HWJ5
C	301	HIS	-	expression tag	UNP V9HWJ5
C	302	HIS	-	expression tag	UNP V9HWJ5
C	303	HIS	-	expression tag	UNP V9HWJ5
C	304	HIS	-	expression tag	UNP V9HWJ5
C	305	HIS	-	expression tag	UNP V9HWJ5
D	298	LEU	-	expression tag	UNP V9HWJ5
D	299	GLU	-	expression tag	UNP V9HWJ5
D	300	HIS	-	expression tag	UNP V9HWJ5
D	301	HIS	-	expression tag	UNP V9HWJ5
D	302	HIS	-	expression tag	UNP V9HWJ5
D	303	HIS	-	expression tag	UNP V9HWJ5
D	304	HIS	-	expression tag	UNP V9HWJ5
D	305	HIS	-	expression tag	UNP V9HWJ5
E	298	LEU	-	expression tag	UNP V9HWJ5
E	299	GLU	-	expression tag	UNP V9HWJ5
E	300	HIS	-	expression tag	UNP V9HWJ5
E	301	HIS	-	expression tag	UNP V9HWJ5
E	302	HIS	-	expression tag	UNP V9HWJ5
E	303	HIS	-	expression tag	UNP V9HWJ5
E	304	HIS	-	expression tag	UNP V9HWJ5
E	305	HIS	-	expression tag	UNP V9HWJ5
F	298	LEU	-	expression tag	UNP V9HWJ5
F	299	GLU	-	expression tag	UNP V9HWJ5
F	300	HIS	-	expression tag	UNP V9HWJ5
F	301	HIS	-	expression tag	UNP V9HWJ5
F	302	HIS	-	expression tag	UNP V9HWJ5
F	303	HIS	-	expression tag	UNP V9HWJ5
F	304	HIS	-	expression tag	UNP V9HWJ5
F	305	HIS	-	expression tag	UNP V9HWJ5
G	298	LEU	-	expression tag	UNP V9HWJ5
G	299	GLU	-	expression tag	UNP V9HWJ5
G	300	HIS	-	expression tag	UNP V9HWJ5
G	301	HIS	-	expression tag	UNP V9HWJ5
G	302	HIS	-	expression tag	UNP V9HWJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	303	HIS	-	expression tag	UNP V9HWJ5
G	304	HIS	-	expression tag	UNP V9HWJ5
G	305	HIS	-	expression tag	UNP V9HWJ5
H	298	LEU	-	expression tag	UNP V9HWJ5
H	299	GLU	-	expression tag	UNP V9HWJ5
H	300	HIS	-	expression tag	UNP V9HWJ5
H	301	HIS	-	expression tag	UNP V9HWJ5
H	302	HIS	-	expression tag	UNP V9HWJ5
H	303	HIS	-	expression tag	UNP V9HWJ5
H	304	HIS	-	expression tag	UNP V9HWJ5
H	305	HIS	-	expression tag	UNP V9HWJ5
I	298	LEU	-	expression tag	UNP V9HWJ5
I	299	GLU	-	expression tag	UNP V9HWJ5
I	300	HIS	-	expression tag	UNP V9HWJ5
I	301	HIS	-	expression tag	UNP V9HWJ5
I	302	HIS	-	expression tag	UNP V9HWJ5
I	303	HIS	-	expression tag	UNP V9HWJ5
I	304	HIS	-	expression tag	UNP V9HWJ5
I	305	HIS	-	expression tag	UNP V9HWJ5

- Molecule 2 is QUINOLINIC ACID (three-letter code: NTM) (formula: $C_7H_5NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	7	1	4		
2	B	1	Total	C	N	O	0	0
			12	7	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			12	7	1	4		
2	D	1	Total	C	N	O	0	0
			12	7	1	4		
2	E	1	Total	C	N	O	0	0
			12	7	1	4		
2	F	1	Total	C	N	O	0	0
			12	7	1	4		
2	G	1	Total	C	N	O	0	0
			12	7	1	4		
2	H	1	Total	C	N	O	0	0
			12	7	1	4		
2	I	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 3 is water.

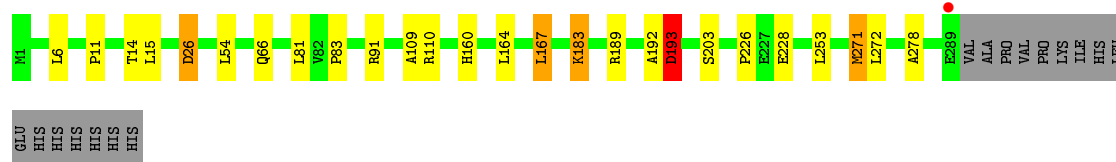
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	1	Total	O	0	0
			1	1		
3	C	5	Total	O	0	0
			5	5		
3	D	7	Total	O	0	0
			7	7		
3	E	6	Total	O	0	0
			6	6		
3	F	3	Total	O	0	0
			3	3		
3	G	1	Total	O	0	0
			1	1		
3	H	9	Total	O	0	0
			9	9		
3	I	4	Total	O	0	0
			4	4		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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.

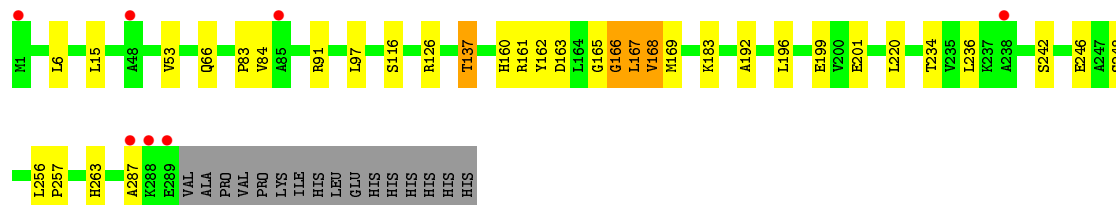
- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain A: 




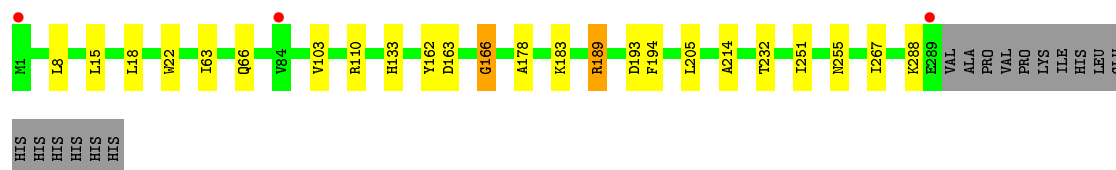
- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain B: 




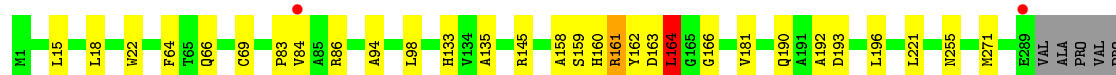
- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain C: 




- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain D: 



LYS
ILE
HIS
LEU
GLU
HIS
HIS
HIS
HIS
HIS


- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain E: 

M1 D2 A3 L6 P11 T14 D26 W47 Q66 Q70 R86 W130 A135 F144 V147 H160 G166 L167 V185 R189 A192 L196 E199 V200 L218 F240 V243 T252 I267 S268 M271 E289 VAL ALA

PRO VAL PRO PRO LYS ILE HIS LEU GLU HIS HIS HIS HIS HIS HIS


- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain F: 

M1 L6 L15 A44 L54 Q66 L81 S112 R138 R161 Y162 D163 L164 L167 V168 K183 A184 V185 R189 L196 K197 V198 D217 L220 L236 E246 L279 K284 L285 K288 E289 VAL ALA PRO VAL PRO LYS ILE HIS LEU

GLU HIS HIS HIS HIS HIS HIS


- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain G: 

M1 D2 L18 A44 W47 A55 Q56 Q57 W73 P83 R86 W87 A88 W130 T131 G132 H133 R138 V154 H160 R161 Y162 D163 L164 G165 G166 L167 K183 D193 L196 C202 S203 S204 L205 A208 V219 L220 L221 L229 L236

M271 L285 E289 VAL ALA PRO VAL PRO LYS ILE HIS LEU GLU HIS HIS HIS HIS HIS HIS


- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain H: 

M1 D2 A3 I6 L15 L18 R24 Q43 A44 W47 Q66 P83 W84 A85 R86 E89 W90 P91 E101 R110 G111 S112 F144 H160 R161 L164 G165 L166 L167 V168 R189 A192 D193 E199 L205 A214 L220 E246 A247

S248 L279 L283 K284 L285 E289 VAL ALA PRO PRO LYS ILE HIS LEU GLU HIS HIS HIS HIS HIS HIS

- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain I: 

M1 D2 A3 L6 L15 L18 W22 A39 L54 L81 W84 A109 R110 A118 V122 F144 V147 G165 G166 K171 D172 R186 D193 D254 A278 E289 VAL ALA PRO PRO VAL PRO LYS ILE HIS LEU GLU HIS HIS HIS HIS

HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.25Å 174.25Å 211.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.43 – 3.09 45.43 – 3.09	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.43-3.09) 98.9 (45.43-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.99 (at 3.12Å)	Xtriage
Refinement program	REFMAC 6.5.0	Depositor
R, R_{free}	0.185 , 0.239 0.180 , 0.236	Depositor DCC
R_{free} test set	3421 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19117	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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 26.58 % 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 2.5660e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.62	0/2151	0.83	2/2931 (0.1%)
1	B	0.58	0/2151	0.87	4/2931 (0.1%)
1	C	0.60	0/2151	0.81	0/2931
1	D	0.60	0/2151	0.82	2/2931 (0.1%)
1	E	0.58	0/2151	0.79	0/2931
1	F	0.58	0/2151	0.83	3/2931 (0.1%)
1	G	0.60	0/2151	0.90	8/2931 (0.3%)
1	H	0.62	0/2151	0.80	0/2931
1	I	0.61	0/2151	0.83	0/2931
All	All	0.60	0/19359	0.83	19/26379 (0.1%)

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	B	0	1
1	C	0	2
1	D	0	3
1	F	0	1
1	G	0	3
1	H	0	2
1	I	0	1
All	All	0	14

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	LEU	N-CA-C	10.33	138.88	111.00
1	B	287	ALA	CB-CA-C	10.21	125.41	110.10
1	G	161	ARG	N-CA-CB	8.73	126.31	110.60
1	F	189	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	G	161	ARG	N-CA-C	-7.36	91.14	111.00
1	G	160	HIS	CB-CA-C	-7.04	96.32	110.40
1	A	167	LEU	CA-CB-CG	6.94	131.26	115.30
1	F	138	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	G	193	ASP	N-CA-C	6.28	127.95	111.00
1	G	160	HIS	N-CA-C	6.07	127.39	111.00
1	B	162	TYR	CB-CA-C	-6.00	98.40	110.40
1	D	145	ARG	NE-CZ-NH2	5.81	123.20	120.30
1	B	163	ASP	N-CA-CB	5.66	120.80	110.60
1	G	164	LEU	CA-CB-CG	5.51	127.97	115.30
1	G	167	LEU	CA-CB-CG	5.47	127.88	115.30
1	F	189	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	G	138	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	86	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	A	26	ASP	CB-CG-OD1	5.10	122.89	118.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	PRO	Peptide
1	B	165	GLY	Peptide
1	C	162	TYR	Peptide
1	C	189	ARG	Sidechain
1	D	162	TYR	Peptide
1	D	221	LEU	Peptide
1	D	83	PRO	Peptide
1	F	162	TYR	Peptide
1	G	160	HIS	Mainchain
1	G	166	GLY	Peptide
1	G	83	PRO	Peptide
1	H	165	GLY	Peptide
1	H	83	PRO	Peptide
1	I	165	GLY	Peptide

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	2108	0	2131	12	0
1	B	2108	0	2131	17	0
1	C	2108	0	2131	17	0
1	D	2108	0	2131	16	0
1	E	2108	0	2131	14	0
1	F	2108	0	2131	10	0
1	G	2108	0	2131	19	0
1	H	2108	0	2131	16	0
1	I	2108	0	2131	8	0
2	A	12	0	3	1	0
2	B	12	0	3	2	0
2	C	12	0	3	0	0
2	D	12	0	3	1	0
2	E	12	0	3	0	0
2	F	12	0	3	0	0
2	G	12	0	3	0	0
2	H	12	0	3	0	0
2	I	12	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	5	0	0	0	0
3	D	7	0	0	2	0
3	E	6	0	0	1	0
3	F	3	0	0	0	0
3	G	1	0	0	0	0
3	H	9	0	0	1	0
3	I	4	0	0	0	0
All	All	19117	0	19206	120	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 3.

All (120) 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:H:189:ARG:NH1	1:H:214:ALA:O	1.69	1.25
1:D:193:ASP:OD1	1:G:133:HIS:ND1	2.19	0.76
1:C:189:ARG:CB	1:C:189:ARG:HH21	1.99	0.75
1:H:189:ARG:CZ	1:H:214:ALA:O	2.37	0.72
1:B:167:LEU:O	1:B:168:VAL:C	2.31	0.69
1:C:189:ARG:HH21	1:C:189:ARG:HB2	1.59	0.66
1:C:193:ASP:OD2	1:C:194:PHE:N	2.25	0.66
1:B:234:THR:HG22	1:B:263:HIS:CD2	2.31	0.65
1:D:193:ASP:OD1	1:G:133:HIS:CE1	2.52	0.63
1:A:26:ASP:O	1:G:163:ASP:O	2.18	0.62
1:A:183:LYS:H	1:A:183:LYS:HD2	1.64	0.61
1:B:137:THR:HG22	2:B:401:NTM:C6	2.31	0.61
1:F:185:VAL:O	1:F:189:ARG:HG2	2.00	0.61
1:C:193:ASP:OD2	1:C:194:PHE:HD1	1.86	0.59
1:A:271:MET:HG3	1:A:272:LEU:N	2.17	0.59
1:D:193:ASP:HB3	3:D:507:HOH:O	2.00	0.59
1:C:189:ARG:HB3	1:C:189:ARG:NH2	2.18	0.59
1:C:193:ASP:OD2	1:C:194:PHE:CD1	2.57	0.57
1:E:11:PRO:HG2	1:E:14:THR:OG1	2.04	0.57
1:E:160:HIS:HB3	3:E:501:HOH:O	2.05	0.57
1:B:192:ALA:HB1	1:B:196:LEU:HB2	1.86	0.57
1:D:84:VAL:O	1:D:84:VAL:HG12	2.04	0.57
1:B:83:PRO:O	1:B:84:VAL:HG22	2.05	0.57
1:D:190:GLN:NE2	1:G:1:MET:HB2	2.20	0.56
1:E:47:TRP:CZ3	1:E:86:ARG:HB2	2.42	0.54
1:H:112:SER:HB3	1:H:279:LEU:HD12	1.88	0.54
1:B:166:GLY:O	1:B:167:LEU:HB2	2.06	0.54
1:C:18:LEU:HG	1:C:22:TRP:CZ2	2.42	0.54
1:D:64:PHE:HB3	1:D:69:CYS:HB2	1.90	0.54
1:B:234:THR:HA	1:B:263:HIS:HD2	1.73	0.54
1:E:185:VAL:HG22	1:E:200:VAL:HG21	1.90	0.53
1:F:168:VAL:HB	1:F:198:VAL:HG22	1.90	0.53
1:G:44:ALA:HB2	1:G:285:LEU:HD23	1.90	0.53
1:D:163:ASP:O	1:D:164:LEU:HB2	2.09	0.53
1:C:189:ARG:CB	1:C:189:ARG:NH2	2.69	0.52
1:G:130:TRP:CZ2	1:G:132:GLY:HA3	2.44	0.52
1:H:44:ALA:HB2	1:H:285:LEU:HD23	1.91	0.52
1:A:160:HIS:CE1	2:A:401:NTM:H4	2.44	0.52
1:A:109:ALA:HB1	1:A:278:ALA:HB1	1.92	0.51
1:F:44:ALA:HA	1:F:285:LEU:HA	1.91	0.51
1:C:205:LEU:HB2	1:C:232:THR:HG23	1.92	0.51
1:G:163:ASP:O	1:G:164:LEU:CB	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:MET:HG2	1:G:2:ASP:H	1.76	0.51
1:B:53:VAL:HG23	1:B:116:SER:HA	1.93	0.50
1:G:1:MET:CG	1:G:2:ASP:H	2.25	0.50
1:B:201:GLU:HG2	1:B:220:LEU:HD22	1.93	0.50
1:A:192:ALA:O	1:A:193:ASP:C	2.49	0.49
1:D:160:HIS:HB3	3:D:501:HOH:O	2.11	0.49
1:B:160:HIS:HE1	1:B:246:GLU:OE1	1.96	0.49
1:C:178:ALA:O	1:C:183:LYS:NZ	2.43	0.49
1:I:54:LEU:HB2	1:I:81:LEU:HD21	1.95	0.49
1:A:183:LYS:CD	1:A:183:LYS:H	2.26	0.49
1:I:171:LYS:O	1:I:172:ASP:C	2.50	0.49
1:H:101:GLU:HG3	1:H:283:LEU:HD23	1.94	0.48
1:B:160:HIS:CD2	2:B:401:NTM:H4	2.48	0.48
1:E:240:PHE:O	1:E:243:VAL:HG12	2.13	0.48
1:F:112:SER:HB3	1:F:279:LEU:HD12	1.96	0.48
1:I:18:LEU:HG	1:I:22:TRP:CZ2	2.49	0.48
1:E:144:PHE:CZ	1:E:147:VAL:HG11	2.48	0.48
1:F:54:LEU:HB2	1:F:81:LEU:HD21	1.95	0.48
1:H:161:ARG:NH2	1:H:164:LEU:HD12	2.29	0.47
1:G:47:TRP:CZ3	1:G:86:ARG:HB2	2.49	0.47
1:A:14:THR:HG22	1:H:24:ARG:HE	1.79	0.47
1:H:3:ALA:HA	1:H:6:LEU:HD22	1.96	0.47
1:B:234:THR:HG22	1:B:263:HIS:HD2	1.78	0.47
1:A:253:LEU:N	1:A:271:MET:HE3	2.30	0.46
1:H:168:VAL:HG21	1:H:192:ALA:HB2	1.97	0.46
1:E:26:ASP:O	1:F:164:LEU:HB3	2.16	0.46
1:G:162:TYR:HD2	1:G:163:ASP:HB3	1.80	0.46
1:A:11:PRO:HG2	1:A:14:THR:OG1	2.16	0.45
1:D:18:LEU:HG	1:D:22:TRP:CZ2	2.51	0.45
1:A:253:LEU:H	1:A:271:MET:CE	2.30	0.45
1:C:251:ILE:HD12	1:C:267:ILE:HG23	1.99	0.45
1:H:220:LEU:HD21	1:H:248:SER:HB3	1.97	0.45
1:D:133:HIS:CE1	1:G:193:ASP:OD1	2.70	0.45
1:B:167:LEU:O	1:B:169:MET:N	2.49	0.45
1:B:199:GLU:OE2	1:B:246:GLU:OE1	2.35	0.44
1:D:161:ARG:NH1	2:D:401:NTM:O4	2.50	0.44
1:I:3:ALA:HA	1:I:6:LEU:HD22	1.99	0.44
1:G:55:ALA:HB2	1:G:154:VAL:HG11	1.99	0.44
1:G:208:ALA:HB1	1:G:219:VAL:HG11	1.99	0.44
1:G:202:CYS:SG	1:G:208:ALA:HA	2.57	0.44
1:E:192:ALA:HB1	1:E:196:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ILE:HD13	1:C:103:VAL:HG12	2.01	0.43
1:H:199:GLU:OE2	1:H:246:GLU:OE1	2.36	0.43
1:B:161:ARG:HB2	1:B:166:GLY:O	2.19	0.43
1:D:192:ALA:HB1	1:D:196:LEU:HB2	2.00	0.43
1:F:220:LEU:HD12	1:F:246:GLU:CD	2.39	0.43
1:I:144:PHE:CZ	1:I:147:VAL:HG11	2.54	0.43
1:D:255:ASN:OD1	1:D:255:ASN:C	2.56	0.43
1:E:135:ALA:O	1:E:268:SER:HA	2.19	0.43
1:E:130:TRP:CH2	1:E:267:ILE:HD12	2.54	0.43
1:I:109:ALA:HB1	1:I:278:ALA:HB1	2.01	0.42
1:G:57:GLN:HG2	1:G:73:TRP:CZ2	2.54	0.42
1:E:166:GLY:O	1:E:167:LEU:HB2	2.19	0.42
1:C:8:LEU:HD22	1:I:39:ALA:HB2	2.01	0.42
1:F:288:LYS:HG2	1:F:289:GLU:N	2.35	0.42
1:F:189:ARG:HH11	1:F:198:VAL:HB	1.84	0.42
1:C:189:ARG:NH2	1:C:214:ALA:O	2.53	0.42
1:E:3:ALA:HA	1:E:6:LEU:HD22	2.02	0.42
1:G:221:LEU:HD12	1:G:229:LEU:HD12	2.01	0.42
1:H:89:GLU:OE1	1:H:91:ARG:NH1	2.51	0.42
1:G:73:TRP:CE3	1:G:88:ALA:HB2	2.55	0.42
1:C:133:HIS:CE1	1:H:193:ASP:OD1	2.73	0.41
1:B:256:LEU:HB3	1:B:257:PRO:HD3	2.02	0.41
1:B:168:VAL:HG21	1:B:192:ALA:HB2	2.02	0.41
1:E:199:GLU:HA	1:E:218:LEU:O	2.19	0.41
1:D:94:ALA:O	1:D:98:LEU:HG	2.21	0.41
1:D:135:ALA:HA	1:D:158:ALA:O	2.21	0.41
1:I:118:ALA:O	1:I:122:VAL:HG23	2.20	0.41
1:G:160:HIS:ND1	1:G:160:HIS:C	2.74	0.41
1:F:189:ARG:NH1	1:F:217:ASP:OD1	2.54	0.41
1:A:54:LEU:HB2	1:A:81:LEU:HD21	2.03	0.41
1:H:43:GLN:HG2	1:H:91:ARG:HE	1.85	0.41
1:D:159:SER:C	1:D:160:HIS:O	2.60	0.40
1:E:252:THR:HA	1:E:271:MET:HE2	2.03	0.40
1:H:160:HIS:HB3	3:H:502:HOH:O	2.21	0.40
1:C:163:ASP:HB3	1:C:166:GLY:H	1.87	0.40
1:C:255:ASN:OD1	1:C:255:ASN:C	2.60	0.40
1:H:47:TRP:CZ3	1:H:86:ARG:HB2	2.56	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	287/305 (94%)	276 (96%)	10 (4%)	1 (0%)	41	73
1	B	287/305 (94%)	264 (92%)	21 (7%)	2 (1%)	22	57
1	C	287/305 (94%)	273 (95%)	13 (4%)	1 (0%)	41	73
1	D	287/305 (94%)	269 (94%)	16 (6%)	2 (1%)	22	57
1	E	287/305 (94%)	275 (96%)	11 (4%)	1 (0%)	41	73
1	F	287/305 (94%)	269 (94%)	16 (6%)	2 (1%)	22	57
1	G	287/305 (94%)	275 (96%)	11 (4%)	1 (0%)	41	73
1	H	287/305 (94%)	274 (96%)	12 (4%)	1 (0%)	41	73
1	I	287/305 (94%)	275 (96%)	9 (3%)	3 (1%)	15	49
All	All	2583/2745 (94%)	2450 (95%)	119 (5%)	14 (0%)	29	64

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	168	VAL
1	C	166	GLY
1	D	166	GLY
1	E	167	LEU
1	D	164	LEU
1	I	166	GLY
1	F	167	LEU
1	G	160	HIS
1	H	167	LEU
1	A	193	ASP
1	B	166	GLY
1	I	193	ASP
1	F	161	ARG
1	I	165	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	212/227 (93%)	198 (93%)	14 (7%)	16	47
1	B	212/227 (93%)	201 (95%)	11 (5%)	23	55
1	C	212/227 (93%)	208 (98%)	4 (2%)	57	81
1	D	212/227 (93%)	206 (97%)	6 (3%)	43	73
1	E	212/227 (93%)	209 (99%)	3 (1%)	67	86
1	F	212/227 (93%)	202 (95%)	10 (5%)	26	59
1	G	212/227 (93%)	203 (96%)	9 (4%)	30	62
1	H	212/227 (93%)	200 (94%)	12 (6%)	20	52
1	I	212/227 (93%)	204 (96%)	8 (4%)	33	66
All	All	1908/2043 (93%)	1831 (96%)	77 (4%)	31	65

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	15	LEU
1	A	66	GLN
1	A	91	ARG
1	A	110	ARG
1	A	164	LEU
1	A	167	LEU
1	A	183	LYS
1	A	189	ARG
1	A	193	ASP
1	A	203	SER
1	A	226	PRO
1	A	228	GLU
1	A	271	MET
1	B	6	LEU
1	B	15	LEU
1	B	66	GLN
1	B	91	ARG

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Mol	Chain	Res	Type
1	B	97	LEU
1	B	126	ARG
1	B	137	THR
1	B	183	LYS
1	B	236	LEU
1	B	242	SER
1	B	248	SER
1	C	15	LEU
1	C	66	GLN
1	C	110	ARG
1	C	288	LYS
1	D	15	LEU
1	D	66	GLN
1	D	161	ARG
1	D	164	LEU
1	D	181	VAL
1	D	271	MET
1	E	66	GLN
1	E	70	GLN
1	E	189	ARG
1	F	1	MET
1	F	6	LEU
1	F	15	LEU
1	F	66	GLN
1	F	183	LYS
1	F	196	LEU
1	F	236	LEU
1	F	284	LYS
1	F	285	LEU
1	F	289	GLU
1	G	1	MET
1	G	18	LEU
1	G	167	LEU
1	G	183	LYS
1	G	196	LEU
1	G	203	SER
1	G	205	LEU
1	G	236	LEU
1	G	271	MET
1	H	6	LEU
1	H	15	LEU
1	H	18	LEU

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Mol	Chain	Res	Type
1	H	66	GLN
1	H	84	VAL
1	H	91	ARG
1	H	110	ARG
1	H	144	PHE
1	H	161	ARG
1	H	167	LEU
1	H	193	ASP
1	H	205	LEU
1	I	6	LEU
1	I	15	LEU
1	I	84	VAL
1	I	110	ARG
1	I	186	ARG
1	I	193	ASP
1	I	254	ASP
1	I	289	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	GLN
1	B	160	HIS
1	B	263	HIS
1	C	133	HIS
1	D	190	GLN
1	G	239	GLN
1	I	95	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

9 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	NTM	A	401	-	7,12,12	2.32	2 (28%)	8,16,16	2.53	3 (37%)
2	NTM	G	401	-	7,12,12	3.25	2 (28%)	8,16,16	1.29	1 (12%)
2	NTM	C	401	-	7,12,12	2.62	2 (28%)	8,16,16	1.53	2 (25%)
2	NTM	E	401	-	7,12,12	2.94	2 (28%)	8,16,16	2.00	2 (25%)
2	NTM	H	401	-	7,12,12	2.56	1 (14%)	8,16,16	1.46	1 (12%)
2	NTM	F	401	-	7,12,12	3.70	2 (28%)	8,16,16	1.78	2 (25%)
2	NTM	D	401	-	7,12,12	2.57	1 (14%)	8,16,16	1.54	1 (12%)
2	NTM	B	401	-	7,12,12	3.22	2 (28%)	8,16,16	1.76	2 (25%)
2	NTM	I	401	-	7,12,12	3.67	2 (28%)	8,16,16	1.98	3 (37%)

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	NTM	A	401	-	-	0/0/8/8	0/1/1/1
2	NTM	G	401	-	-	0/0/8/8	0/1/1/1
2	NTM	C	401	-	-	0/0/8/8	0/1/1/1
2	NTM	E	401	-	-	0/0/8/8	0/1/1/1
2	NTM	H	401	-	-	0/0/8/8	0/1/1/1
2	NTM	F	401	-	-	0/0/8/8	0/1/1/1
2	NTM	D	401	-	-	0/0/8/8	0/1/1/1
2	NTM	B	401	-	-	0/0/8/8	0/1/1/1
2	NTM	I	401	-	-	0/0/8/8	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	401	NTM	C3-C2	8.54	1.51	1.41
2	F	401	NTM	C3-C2	8.43	1.51	1.41
2	E	401	NTM	C3-C2	7.24	1.50	1.41
2	G	401	NTM	C3-C2	6.74	1.49	1.41
2	D	401	NTM	C3-C2	6.59	1.49	1.41
2	H	401	NTM	C3-C2	6.53	1.49	1.41
2	C	401	NTM	C3-C2	6.34	1.49	1.41
2	B	401	NTM	C3-C2	6.29	1.49	1.41
2	B	401	NTM	C3-C8	5.64	1.52	1.47
2	A	401	NTM	C3-C2	5.57	1.48	1.41
2	G	401	NTM	C3-C8	5.25	1.52	1.47
2	F	401	NTM	C3-C8	4.63	1.51	1.47
2	I	401	NTM	C3-C8	4.53	1.51	1.47
2	E	401	NTM	C3-C8	2.67	1.50	1.47
2	C	401	NTM	C3-C8	2.46	1.49	1.47
2	A	401	NTM	C3-C8	2.40	1.49	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NTM	C3-C2-N1	-5.89	117.16	122.02
2	E	401	NTM	C3-C2-N1	-4.43	118.36	122.02
2	I	401	NTM	C3-C2-N1	-4.13	118.61	122.02
2	C	401	NTM	C3-C2-N1	-3.33	119.27	122.02
2	B	401	NTM	C3-C2-C7	-3.03	118.24	123.56
2	F	401	NTM	C3-C2-N1	-3.01	119.54	122.02
2	G	401	NTM	C3-C2-N1	-2.82	119.69	122.02
2	A	401	NTM	C4-C3-C2	2.75	119.71	117.43
2	A	401	NTM	C6-N1-C2	2.63	121.96	116.81
2	D	401	NTM	C3-C2-N1	-2.63	119.85	122.02
2	B	401	NTM	C4-C3-C2	-2.62	115.25	117.43
2	H	401	NTM	C4-C3-C8	-2.51	116.46	120.20
2	F	401	NTM	C6-N1-C2	2.43	121.57	116.81
2	I	401	NTM	C6-N1-C2	2.33	121.36	116.81
2	E	401	NTM	C6-N1-C2	2.31	121.32	116.81
2	I	401	NTM	C4-C3-C8	-2.20	116.92	120.20
2	C	401	NTM	C6-N1-C2	2.16	121.03	116.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NTM	1	0
2	D	401	NTM	1	0
2	B	401	NTM	2	0

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	289/305 (94%)	-0.42	1 (0%) 94 88	32, 45, 70, 140	0
1	B	289/305 (94%)	-0.10	7 (2%) 59 37	48, 80, 113, 136	0
1	C	289/305 (94%)	-0.48	3 (1%) 82 67	29, 52, 83, 136	0
1	D	289/305 (94%)	-0.51	2 (0%) 87 75	31, 48, 71, 120	0
1	E	289/305 (94%)	-0.42	2 (0%) 87 75	37, 53, 77, 123	0
1	F	289/305 (94%)	-0.29	2 (0%) 87 75	40, 57, 81, 125	0
1	G	289/305 (94%)	-0.52	1 (0%) 94 88	32, 45, 65, 114	0
1	H	289/305 (94%)	-0.57	1 (0%) 94 88	29, 43, 62, 108	0
1	I	289/305 (94%)	-0.54	1 (0%) 94 88	30, 44, 69, 120	0
All	All	2601/2745 (94%)	-0.43	20 (0%) 86 72	29, 50, 91, 140	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	5.0
1	A	289	GLU	4.7
1	B	289	GLU	4.2
1	F	289	GLU	3.8
1	C	289	GLU	3.8
1	G	289	GLU	3.2
1	E	289	GLU	3.1
1	B	1	MET	3.0
1	B	288	LYS	2.8
1	F	1	MET	2.8
1	I	289	GLU	2.8
1	B	238	ALA	2.6
1	B	85	ALA	2.6
1	B	48	ALA	2.4
1	B	287	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	84	VAL	2.2
1	E	1	MET	2.2
1	C	84	VAL	2.2
1	H	289	GLU	2.1
1	D	289	GLU	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 carbohydrates 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(\AA^2)	Q<0.9
2	NTM	B	401	12/12	0.90	0.22	58,73,76,78	5
2	NTM	F	401	12/12	0.91	0.28	45,56,71,82	6
2	NTM	A	401	12/12	0.91	0.23	35,48,66,72	5
2	NTM	G	401	12/12	0.95	0.25	37,46,63,65	5
2	NTM	E	401	12/12	0.95	0.18	58,63,72,75	3
2	NTM	I	401	12/12	0.96	0.15	60,65,70,72	0
2	NTM	H	401	12/12	0.97	0.16	32,33,34,35	4
2	NTM	D	401	12/12	0.97	0.18	28,29,29,31	4
2	NTM	C	401	12/12	0.98	0.15	43,45,50,53	2

6.5 Other polymers [i](#)

There are no such residues in this entry.