WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Sep 19, 2023 – 09:32 PM EDT

PDB ID	:	5IFM
Title	:	Human NONO (p54nrb) Homodimer
Authors	:	Knott, G.J.; Bond, C.S.
Deposited on	:	2016-02-26
Resolution	:	2.60 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

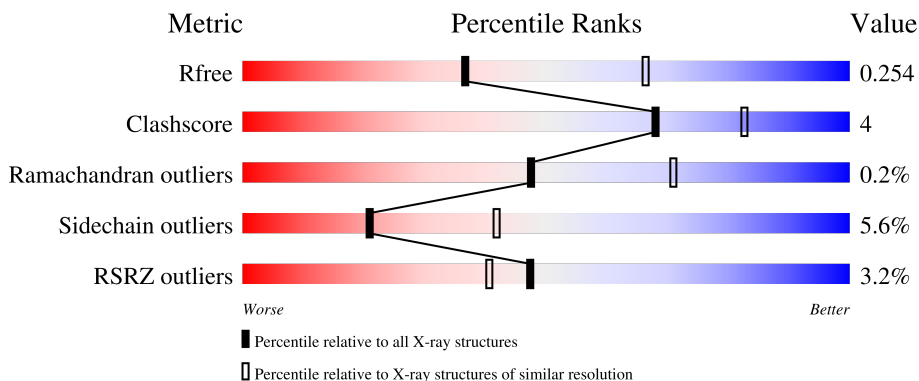|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Rfree		0.254
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		5.6%
RSRZ outliers		3.2%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	261	86% 11% ·
1	B	261	3% · 84% 15% ·
1	C	261	2% · 82% 15% ··
1	D	261	2% · 82% 14% ··
1	E	261	4% · 85% 13% ·

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Mol	Chain	Length	Quality of chain
1	F	261	2% 87% 10% ··
1	G	261	84% 12% ··
1	H	261	2% 84% 15% ·
1	I	261	6% 86% 10% ··
1	J	261	9% 89% 10% ··
1	K	261	5% 86% 12% ··
1	L	261	3% 85% 12% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	D	401	-	-	X	-
5	GOL	B	402	-	-	X	-
5	GOL	C	405	-	-	X	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 25317 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 Non-POU domain-containing octamer-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2065	1301	369	386	9			
1	B	259	Total	C	N	O	S	0	1	0
			2114	1333	380	390	11			
1	C	256	Total	C	N	O	S	0	1	0
			2090	1316	374	391	9			
1	D	257	Total	C	N	O	S	0	1	0
			2099	1320	379	391	9			
1	E	256	Total	C	N	O	S	0	0	0
			2084	1312	374	389	9			
1	F	255	Total	C	N	O	S	0	0	0
			2075	1307	373	386	9			
1	G	255	Total	C	N	O	S	0	1	0
			2084	1312	373	390	9			
1	H	257	Total	C	N	O	S	0	0	0
			2090	1317	375	388	10			
1	I	255	Total	C	N	O	S	0	0	0
			2075	1307	372	387	9			
1	J	259	Total	C	N	O	S	0	0	0
			2106	1328	377	390	11			
1	K	259	Total	C	N	O	S	0	0	0
			2106	1328	377	390	11			
1	L	255	Total	C	N	O	S	0	0	0
			2075	1307	372	387	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	GLY	-	expression tag	UNP Q15233
B	52	GLY	-	expression tag	UNP Q15233
C	52	GLY	-	expression tag	UNP Q15233
D	52	GLY	-	expression tag	UNP Q15233
E	52	GLY	-	expression tag	UNP Q15233

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Chain	Residue	Modelled	Actual	Comment	Reference
F	52	GLY	-	expression tag	UNP Q15233
G	52	GLY	-	expression tag	UNP Q15233
H	52	GLY	-	expression tag	UNP Q15233
I	52	GLY	-	expression tag	UNP Q15233
J	52	GLY	-	expression tag	UNP Q15233
K	52	GLY	-	expression tag	UNP Q15233
L	52	GLY	-	expression tag	UNP Q15233

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).

PRO
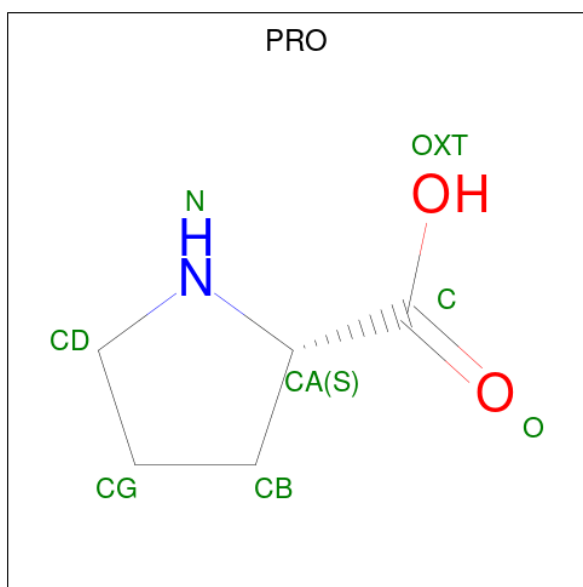
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 8	C 5	N 1	O 2	0	0
3	C	1	Total 8	C 5	N 1	O 2	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	K 1	0	0
4	B	1	Total 1	K 1	0	0
4	C	1	Total 1	K 1	0	0
4	D	1	Total 1	K 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 6	C 3	O 3	0	0
5	B	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	33	Total 33	O 33	0	0
6	B	26	Total 26	O 26	0	0
6	C	24	Total 24	O 24	0	0
6	D	37	Total 37	O 37	0	0
6	E	15	Total 15	O 15	0	0
6	F	7	Total 7	O 7	0	0
6	G	19	Total 19	O 19	0	0

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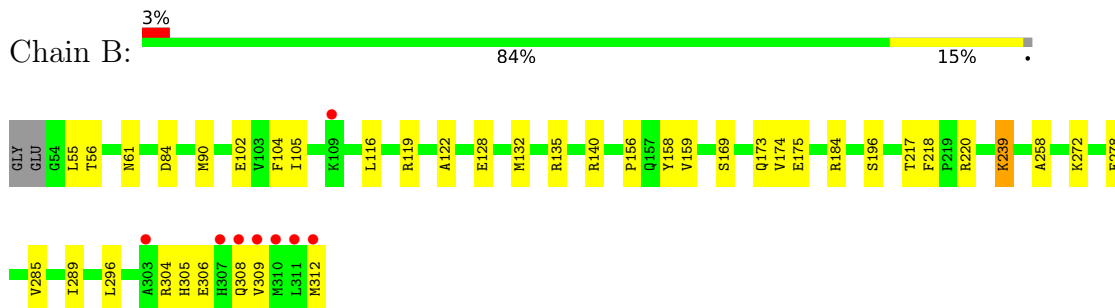| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	10	Total 10	O 10	0	0
6	I	5	Total 5	O 5	0	0
6	J	4	Total 4	O 4	0	0
6	K	7	Total 7	O 7	0	0
6	L	7	Total 7	O 7	0	0

3 Residue-property plots ⓘ

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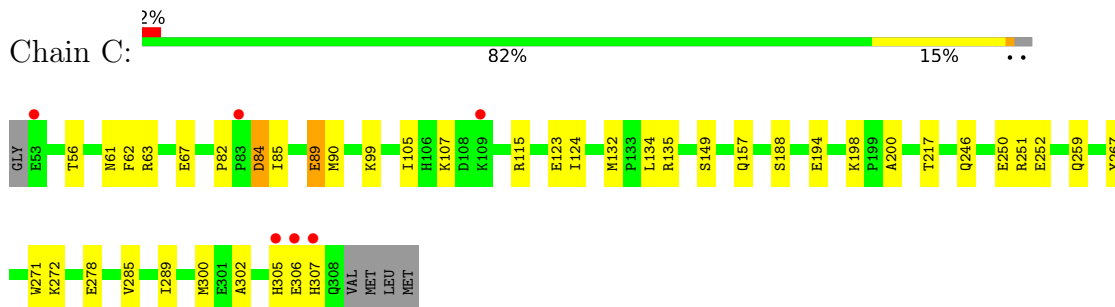
- Molecule 1: Non-POU domain-containing octamer-binding protein
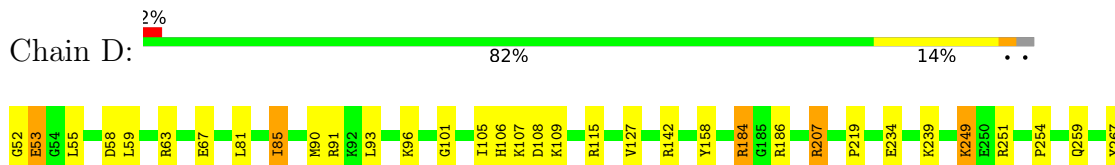
Chain A:

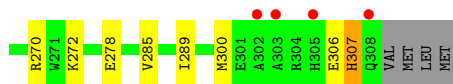- Molecule 1: Non-POU domain-containing octamer-binding protein

Chain B:

- Molecule 1: Non-POU domain-containing octamer-binding protein

Chain C:

- Molecule 1: Non-POU domain-containing octamer-binding protein

Chain D:

R270 W271 K272 E278 V285 I289 M300 E301 A302 A303 R304 H305 E306 H307 Q308 VAL MET LEU MET

• Molecule 1: Non-POU domain-containing octamer-binding protein

Chain E:

4%　85%　13%

GLY E53 D58 L59 R63 E67 R73 P82 P83 D84 M90 R91 K92 L93 F94 V103 R115 L134 R135 R140 S149 P156 Q157 Y158 V159 D183 E194 K198 R220 P221 Q246 E250 R251 E252 Q259 P260 G261 S262 F263 W271

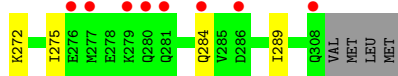K272 I275 E276 M277 E278 K279 Q280 Q281 Q284 V285 D286 I289 Q308 VAL MET LEU MET

• Molecule 1: Non-POU domain-containing octamer-binding protein

Chain F:

2%　87%　10%

GLY GLU G54 D58 L59 F62 R63 E67 I85 M90 R91 K92 L93 G101 E128 Y158 R184 G185 R186 K198 K203 S209 T217 F218 P219 R220 E250 R251 E252 Q259 F263 W271 K272 I275 E276 M277 E278 Q284 N288
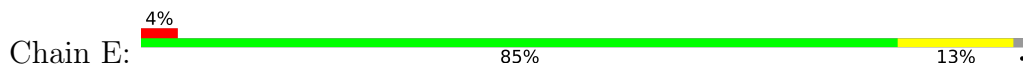
K295 R304 Q308 VAL MET LEU MET

• Molecule 1: Non-POU domain-containing octamer-binding protein

Chain G:

84%　12%

GLY E53 G54 L55 T56 I57 D58 L59 K60 N61 P82 I85 L93 K107 D108 K109 R115 M132 P133 L134 R135 R140 P156 V159 D183 R202 K203 S209 R220 E234 N244 Q245 Q246 F247 E250 R251 E252 Q259 M269 R270 W271 K272
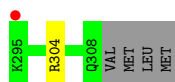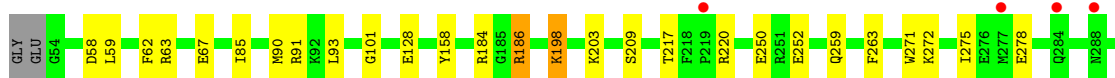
I275 E276 M277 I289 R293 R304 H307 GLN VAL MET LEU MET

• Molecule 1: Non-POU domain-containing octamer-binding protein

Chain H:

2%　84%　15%

GLY GLU G54 D58 L59 K60 G66 N80 I85 M90 L93 K96 K99 I105 D108 R115 R119 I124 A125 K126 V127 E128 L129 R140 V141 P156 Q157 Y158 V159 L163 R184 G185 R186 K203 T217 F218 P219 R220 E250 R251

E252 Q259 P260 G261 W271 I275 E276 M277 E278 Q284 E301 R304 H305 E306 H307 Q308 V309 M310 LEU MET

• Molecule 1: Non-POU domain-containing octamer-binding protein

Chain I:

6%　86%　10%

• Molecule 1: Non-POU domain-containing octamer-binding protein

Chain J:

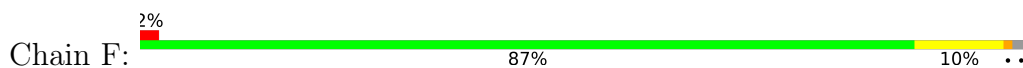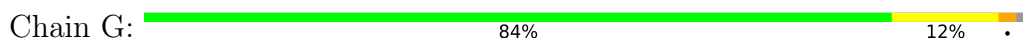
• Molecule 1: Non-POU domain-containing octamer-binding protein

Chain K:

• Molecule 1: Non-POU domain-containing octamer-binding protein

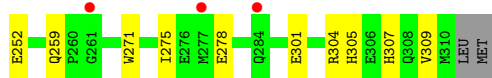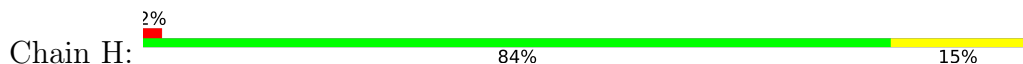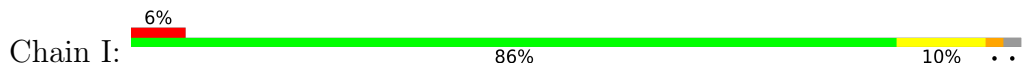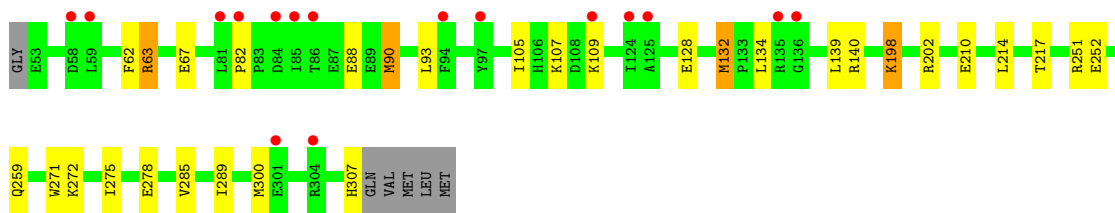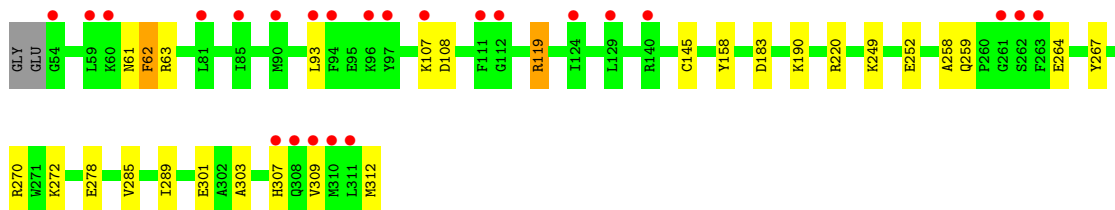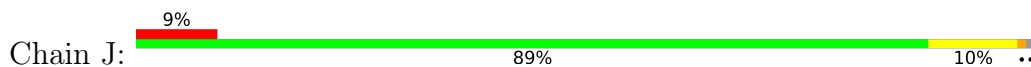Chain L:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.15Å 407.18Å 68.96Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	48.15 – 2.60 48.15 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.15-2.60) 98.8 (48.15-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.61Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.0	Depositor
R, R_{free}	0.197 , 0.234 0.213 , 0.254	Depositor DCC
R_{free} test set	5520 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.7	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.1	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	25317	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: GOL, K, 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	0.55	0/2104	0.73	0/2823
1	B	0.55	0/2157	0.74	0/2893
1	C	0.56	0/2133	0.76	0/2862
1	D	0.60	0/2139	0.78	0/2869
1	E	0.50	0/2124	0.70	0/2850
1	F	0.48	0/2115	0.69	0/2838
1	G	0.51	0/2124	0.70	0/2850
1	H	0.50	0/2130	0.73	0/2858
1	I	0.47	0/2115	0.69	0/2838
1	J	0.46	0/2146	0.68	1/2879 (0.0%)
1	K	0.47	0/2146	0.71	0/2879
1	L	0.49	0/2115	0.71	0/2838
All	All	0.51	0/25548	0.72	1/34277 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	119	ARG	CG-CD-NE	5.30	122.93	111.80

There are no chirality outliers.

There are no planarity outliers.

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2065	0	2064	23	0
1	B	2114	0	2124	35	0
1	C	2090	0	2085	32	0
1	D	2099	0	2094	32	0
1	E	2084	0	2079	20	0
1	F	2075	0	2073	15	0
1	G	2084	0	2076	21	0
1	H	2090	0	2091	23	0
1	I	2075	0	2071	18	0
1	J	2106	0	2111	13	0
1	K	2106	0	2111	17	0
1	L	2075	0	2071	17	0
2	A	1	0	0	1	0
2	C	2	0	0	1	0
2	D	1	0	0	2	0
2	E	1	0	0	1	0
2	F	2	0	0	1	0
2	G	1	0	0	1	0
2	H	1	0	0	1	0
2	L	1	0	0	0	0
3	A	8	0	7	2	0
3	C	8	0	7	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	12	0	16	8	0
5	C	12	0	16	7	0
5	D	6	0	8	2	0
6	A	33	0	0	1	0
6	B	26	0	0	0	0
6	C	24	0	0	1	0
6	D	37	0	0	0	0
6	E	15	0	0	1	0
6	F	7	0	0	0	0
6	G	19	0	0	0	0
6	H	10	0	0	0	0
6	I	5	0	0	0	0
6	J	4	0	0	0	0
6	K	7	0	0	0	0
6	L	7	0	0	0	0
All	All	25317	0	25104	191	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 4.

All (191) 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:K:285:VAL:HG21	1:L:285:VAL:HG21	1.43	0.98
1:B:84:ASP:HB2	1:B:135:ARG:HH22	1.31	0.95
1:C:61:ASN:HA	5:C:405:GOL:H32	1.55	0.88
1:I:285:VAL:HG21	1:J:285:VAL:HG21	1.57	0.84
1:L:156:PRO:HD2	1:L:159:VAL:HG21	1.58	0.84
1:B:169:SER:HB2	5:B:402:GOL:H11	1.61	0.83
1:H:217:THR:HG22	1:H:304:ARG:HD2	1.61	0.81
1:F:198:LYS:HB2	1:J:309:VAL:HG11	1.63	0.79
1:H:93:LEU:HD22	1:H:129:LEU:HD11	1.63	0.79
1:B:239:LYS:HE3	1:B:239:LYS:HA	1.65	0.79
1:C:200:ALA:HB2	5:C:404:GOL:H12	1.65	0.77
1:B:173:GLN:HA	5:B:402:GOL:H12	1.66	0.77
1:A:285:VAL:HG21	1:B:285:VAL:HG21	1.64	0.77
1:C:285:VAL:HG21	1:D:285:VAL:HG21	1.67	0.75
1:G:234:GLU:HB2	2:G:401:CL:CL	2.25	0.74
1:B:102:GLU:HB2	5:B:401:GOL:H12	1.71	0.72
1:C:62:PHE:H	5:C:405:GOL:H12	1.54	0.71
1:C:157:GLN:H	3:C:403:PRO:HD2	1.55	0.70
1:C:200:ALA:CB	5:C:404:GOL:H12	2.21	0.70
1:G:82:PRO:HG3	1:G:134:LEU:HD12	1.73	0.69
1:C:278:GLU:HG2	1:D:289:ILE:HG12	1.75	0.69
1:K:82:PRO:HG3	1:K:134:LEU:HD12	1.74	0.69
1:E:271:TRP:NE1	1:E:275:ILE:HD11	2.08	0.69
1:A:271:TRP:NE1	1:A:275:ILE:HD11	2.08	0.68
1:I:82:PRO:HG3	1:I:134:LEU:HD12	1.76	0.67
1:F:91:ARG:NH2	1:F:101:GLY:O	2.27	0.67
1:H:271:TRP:NE1	1:H:275:ILE:HD11	2.10	0.67
1:C:289:ILE:HG12	1:D:278:GLU:HG2	1.76	0.66
1:C:62:PHE:N	5:C:405:GOL:H12	2.10	0.66
1:F:271:TRP:NE1	1:F:275:ILE:HD11	2.11	0.66
1:C:82:PRO:HG3	1:C:134:LEU:HD12	1.76	0.66
1:B:84:ASP:HB2	1:B:135:ARG:NH2	2.08	0.65
1:E:140:ARG:NH1	2:E:401:CL:CL	2.67	0.65
1:C:198:LYS:HD2	1:H:309:VAL:HA	1.78	0.64
1:L:239:LYS:HE3	1:L:239:LYS:H	1.60	0.64
1:I:271:TRP:NE1	1:I:275:ILE:HD11	2.11	0.64
1:E:82:PRO:HG3	1:E:134:LEU:HD12	1.79	0.64
1:G:304:ARG:HH12	1:H:250:GLU:CD	2.01	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:271:TRP:NE1	1:G:275:ILE:HD11	2.14	0.63
1:C:61:ASN:O	1:D:52:GLY:HA3	1.99	0.62
1:A:250:GLU:HG3	1:B:158:TYR:CD2	2.35	0.61
1:D:142:ARG:NH1	2:D:401:CL:CL	2.70	0.61
1:K:219:PRO:HG2	1:K:300:MET:SD	2.40	0.61
1:E:250:GLU:HG3	1:F:158:TYR:CD2	2.36	0.60
1:A:271:TRP:CZ2	1:B:220:ARG:HD2	2.36	0.60
1:C:271:TRP:HE1	1:D:300:MET:HE3	1.66	0.60
1:K:278:GLU:HG2	1:L:289:ILE:HG12	1.84	0.59
1:A:140:ARG:NH1	2:A:401:CL:CL	2.73	0.58
1:D:63:ARG:HD2	1:D:67:GLU:O	2.03	0.58
1:F:217:THR:HG22	1:F:304:ARG:HD3	1.83	0.58
1:A:289:ILE:HG12	1:B:278:GLU:HG2	1.86	0.58
1:D:184:ARG:HE	1:D:186:ARG:HH11	1.50	0.58
1:B:309:VAL:HG22	1:E:198:LYS:HD2	1.85	0.57
1:G:250:GLU:HG3	1:H:158:TYR:CD2	2.39	0.57
5:C:405:GOL:H2	1:D:127:VAL:CG1	2.35	0.56
1:I:289:ILE:HG12	1:J:278:GLU:HG2	1.87	0.56
1:K:289:ILE:HG12	1:L:278:GLU:HG2	1.87	0.56
1:I:278:GLU:HG2	1:J:289:ILE:HG12	1.88	0.56
1:D:234:GLU:HB3	2:D:401:CL:CL	2.43	0.56
1:E:158:TYR:CD2	1:F:250:GLU:HG3	2.41	0.56
1:C:124:ILE:HG23	1:D:59:LEU:HD13	1.88	0.55
1:E:59:LEU:HD23	1:F:128:GLU:OE2	2.06	0.55
1:D:254:PRO:HA	5:D:402:GOL:H32	1.88	0.55
1:A:60:LYS:N	1:B:128:GLU:OE1	2.35	0.55
1:C:271:TRP:HE1	1:D:300:MET:CE	2.20	0.55
1:C:246:GLN:HG3	1:H:184:ARG:HG2	1.88	0.55
1:C:251:ARG:HB2	1:G:109:LYS:HZ3	1.72	0.55
1:D:207[A]:ARG:HH11	1:D:207[A]:ARG:HG2	1.72	0.55
1:A:278:GLU:HG2	1:B:289:ILE:HG12	1.89	0.55
1:G:293:ARG:HG2	1:H:271:TRP:CH2	2.42	0.55
1:A:61:ASN:HB3	1:B:128:GLU:HA	1.89	0.54
1:G:59:LEU:HD21	1:H:124:ILE:HG23	1.90	0.54
1:I:300:MET:HB3	1:J:267:TYR:CD1	2.42	0.54
1:K:230:LEU:HD23	1:L:182:ASP:HA	1.90	0.54
1:E:271:TRP:CZ2	1:F:220:ARG:HD2	2.43	0.54
2:F:402:CL:CL	1:I:140:ARG:NH1	2.78	0.54
1:H:129:LEU:HB3	1:H:141:VAL:HG21	1.89	0.54
1:A:89:GLU:O	1:A:93:LEU:HG	2.08	0.53
1:D:251:ARG:HB3	5:D:402:GOL:H11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:GLU:HG3	1:D:158:TYR:CD2	2.43	0.53
1:A:181:VAL:HG13	1:A:185:GLY:HA2	1.91	0.53
1:I:271:TRP:CZ2	1:J:220:ARG:HD2	2.44	0.53
1:D:207[A]:ARG:HH11	1:D:207[A]:ARG:CG	2.23	0.52
1:I:90:MET:HG3	1:I:105:ILE:HD11	1.90	0.52
1:A:157:GLN:H	3:A:402:PRO:HD2	1.75	0.51
1:E:220:ARG:HD2	1:F:271:TRP:CZ2	2.45	0.51
1:I:251:ARG:NH1	1:J:158:TYR:O	2.44	0.51
1:C:89:GLU:OE1	1:C:135:ARG:NH2	2.44	0.51
1:C:300:MET:HB3	1:D:267:TYR:CD1	2.46	0.51
1:B:184:ARG:HD3	1:E:246:GLN:HG3	1.92	0.50
1:B:218:PHE:HA	1:B:304:ARG:HD3	1.92	0.50
1:I:128:GLU:HA	1:J:61:ASN:HB3	1.91	0.50
1:D:106:HIS:CE1	1:D:108:ASP:HB3	2.47	0.50
1:G:134:LEU:HD13	1:G:135:ARG:HD3	1.94	0.50
1:D:307:HIS:CD2	1:D:307:HIS:C	2.85	0.50
1:H:159:VAL:HA	1:H:163:LEU:HD23	1.94	0.50
1:K:58:ASP:HB3	1:L:56:THR:HG22	1.94	0.50
1:C:267:TYR:HB3	1:D:300:MET:HE2	1.94	0.49
1:B:308:GLN:HE21	1:B:312:MET:HG3	1.77	0.49
1:B:116:LEU:HD12	1:B:122:ALA:HA	1.95	0.49
1:E:90:MET:O	1:E:94:PHE:HD1	1.94	0.49
1:G:220:ARG:HD2	1:H:271:TRP:CZ2	2.48	0.49
2:C:402:CL:CL	1:G:140:ARG:NH1	2.83	0.48
1:I:63:ARG:NH1	1:I:67:GLU:O	2.43	0.48
1:G:289:ILE:HG12	1:H:278:GLU:HG2	1.95	0.48
1:G:57:ILE:HG23	1:H:96:LYS:HG2	1.96	0.47
1:L:237:PRO:HD2	1:L:240:LEU:HD12	1.95	0.47
1:A:59:LEU:HB2	1:B:55:LEU:O	2.15	0.47
1:D:207[A]:ARG:HG2	1:D:207[A]:ARG:NH1	2.30	0.47
1:E:91:ARG:HG2	1:E:103:VAL:HG21	1.96	0.47
1:B:174:VAL:HB	5:B:402:GOL:H32	1.97	0.47
1:K:297:GLU:HG3	1:L:271:TRP:HZ2	1.80	0.46
1:G:271:TRP:CZ2	1:H:220:ARG:HD2	2.51	0.46
1:A:58:ASP:HA	1:B:56:THR:HG22	1.96	0.46
1:B:174:VAL:H	5:B:402:GOL:H12	1.79	0.46
1:F:184:ARG:HB3	1:F:186:ARG:HD2	1.97	0.46
1:D:63:ARG:HG3	1:D:67:GLU:HB3	1.96	0.46
1:K:214:LEU:HD11	1:L:258:ALA:HB2	1.98	0.46
1:E:271:TRP:HE1	1:E:275:ILE:HD11	1.80	0.46
1:G:59:LEU:HA	1:H:128:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TRP:HE1	1:A:275:ILE:HD11	1.80	0.46
1:B:169:SER:CB	5:B:402:GOL:H31	2.46	0.46
1:B:169:SER:CB	5:B:402:GOL:H11	2.40	0.45
1:C:84:ASP:OD1	1:C:135:ARG:NH1	2.49	0.45
1:G:156:PRO:HD2	1:G:159:VAL:HG21	1.98	0.45
1:B:90:MET:HG3	1:B:105:ILE:HD11	1.99	0.45
1:B:217:THR:HG22	1:B:304:ARG:HD2	1.99	0.45
1:K:264:GLU:HB2	1:L:219:PRO:HB3	1.98	0.45
1:C:217:THR:HG21	1:D:249:LYS:O	2.17	0.45
1:C:90:MET:HG3	1:C:105:ILE:HD11	1.99	0.45
1:H:271:TRP:HE1	1:H:275:ILE:HD11	1.82	0.45
1:C:302:ALA:O	1:C:305:HIS:HB2	2.17	0.44
1:I:214:LEU:HD11	1:J:258:ALA:HB2	1.98	0.44
1:F:59:LEU:HG	1:F:62:PHE:HD2	1.83	0.44
1:A:73:ARG:HG3	6:A:522:HOH:O	2.16	0.44
1:F:198:LYS:HG3	1:J:309:VAL:HG21	2.00	0.44
1:H:218:PHE:HE1	1:H:301:GLU:HG2	1.83	0.44
1:A:214:LEU:HD11	1:B:258:ALA:HB2	2.00	0.44
1:D:90:MET:HG3	1:D:105:ILE:HD11	1.99	0.44
1:K:300:MET:HG2	1:L:267:TYR:CD2	2.52	0.44
1:A:271:TRP:HE3	1:B:296:LEU:HD23	1.81	0.43
1:E:84:ASP:OD1	1:E:135:ARG:NH2	2.50	0.43
1:I:63:ARG:HG2	1:I:67:GLU:HB3	2.00	0.43
1:E:289:ILE:HG12	1:F:278:GLU:HG2	2.01	0.43
1:K:156:PRO:HD2	1:K:159:VAL:HG21	2.01	0.43
1:A:128:GLU:HA	1:B:61:ASN:HB3	2.01	0.43
1:G:251:ARG:NH1	1:H:158:TYR:O	2.51	0.43
1:E:156:PRO:HD2	1:E:159:VAL:HG21	2.00	0.43
1:J:303:ALA:O	1:J:307:HIS:ND1	2.49	0.43
1:C:115:ARG:HD2	6:C:516:HOH:O	2.19	0.43
1:B:304:ARG:C	1:B:306:GLU:H	2.22	0.43
1:E:73:ARG:HG3	6:E:511:HOH:O	2.19	0.43
1:L:156:PRO:HD2	1:L:159:VAL:CG2	2.40	0.43
1:B:175:GLU:OE2	1:B:196:SER:HA	2.18	0.42
1:D:219:PRO:HG2	1:D:300:MET:HE2	1.99	0.42
1:E:149:SER:CB	1:E:194:GLU:HG2	2.49	0.42
1:H:156:PRO:HD2	1:H:159:VAL:HG21	2.02	0.42
1:K:57:ILE:HD12	1:L:59:LEU:HD13	2.00	0.42
1:C:56:THR:HG22	1:D:58:ASP:HA	2.00	0.42
1:C:251:ARG:NH1	1:D:158:TYR:O	2.50	0.42
1:E:63:ARG:HG2	1:E:67:GLU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:ASN:HB3	1:H:128:GLU:HA	2.01	0.41
1:I:217:THR:HG21	1:J:249:LYS:O	2.20	0.41
1:I:132:MET:HG2	1:I:139:LEU:HD12	2.02	0.41
1:K:267:TYR:OH	1:L:299:GLU:HG3	2.20	0.41
1:B:104:PHE:CE2	1:C:306:GLU:HG2	2.56	0.41
1:D:81:LEU:HD22	1:D:85:ILE:HD13	2.02	0.41
1:J:62:PHE:CD1	1:J:62:PHE:N	2.88	0.41
1:B:156:PRO:HD2	1:B:159:VAL:HG21	2.03	0.41
1:A:209:SER:O	1:B:272:LYS:NZ	2.53	0.41
1:C:63:ARG:HG2	1:C:67:GLU:HB3	2.03	0.41
1:C:149:SER:CB	1:C:194:GLU:HG2	2.51	0.41
2:H:401:CL:CL	1:K:140:ARG:NH1	2.91	0.41
1:A:157:GLN:HB2	3:A:402:PRO:HG2	2.03	0.41
1:A:297:GLU:HA	1:A:300:MET:HE3	2.03	0.41
1:D:91:ARG:NH2	1:D:101:GLY:O	2.54	0.41
1:G:244:ASN:O	1:G:247:PHE:HB3	2.21	0.41
1:H:184:ARG:HB2	1:H:186:ARG:HD2	2.02	0.40
1:A:149:SER:HB3	1:A:227:MET:HB2	2.03	0.40
1:C:200:ALA:HB3	5:C:404:GOL:H12	2.01	0.40
1:D:184:ARG:HG3	1:G:246:GLN:HG3	2.03	0.40
1:D:306:GLU:HA	1:G:202:ARG:HD3	2.02	0.40
1:K:250:GLU:HG3	1:L:158:TYR:CD2	2.56	0.40
1:L:291:GLU:O	1:L:295:LYS:HD3	2.21	0.40
1:I:271:TRP:HE1	1:I:275:ILE:HD11	1.84	0.40
1:K:198:LYS:H	1:K:198:LYS:HG3	1.49	0.40
1:B:169:SER:HB2	5:B:402:GOL:H31	2.03	0.40
1:E:221:PRO:HD2	1:F:271:TRP:CD1	2.57	0.40
1:F:63:ARG:HG2	1:F:67:GLU:HB3	2.04	0.40
1:H:90:MET:HG3	1:H:105:ILE:HD11	2.03	0.40
1:I:198:LYS:H	1:I:198:LYS:HG3	1.61	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	252/261 (97%)	242 (96%)	10 (4%)	0	100	100
1	B	258/261 (99%)	249 (96%)	9 (4%)	0	100	100
1	C	255/261 (98%)	248 (97%)	5 (2%)	2 (1%)	19	39
1	D	256/261 (98%)	248 (97%)	6 (2%)	2 (1%)	19	39
1	E	254/261 (97%)	249 (98%)	5 (2%)	0	100	100
1	F	253/261 (97%)	246 (97%)	7 (3%)	0	100	100
1	G	254/261 (97%)	246 (97%)	8 (3%)	0	100	100
1	H	255/261 (98%)	246 (96%)	9 (4%)	0	100	100
1	I	253/261 (97%)	245 (97%)	8 (3%)	0	100	100
1	J	257/261 (98%)	250 (97%)	6 (2%)	1 (0%)	34	57
1	K	257/261 (98%)	249 (97%)	7 (3%)	1 (0%)	34	57
1	L	253/261 (97%)	244 (96%)	9 (4%)	0	100	100
All	All	3057/3132 (98%)	2962 (97%)	89 (3%)	6 (0%)	47	71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	85	ILE
1	D	53	GLU
1	J	107	LYS
1	C	107	LYS
1	D	107	LYS
1	K	107	LYS

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	222/228 (97%)	216 (97%)	6 (3%)	44	71

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	228/228 (100%)	223 (98%)	5 (2%)	52	76
1	C	225/228 (99%)	214 (95%)	11 (5%)	25	48
1	D	225/228 (99%)	209 (93%)	16 (7%)	14	29
1	E	224/228 (98%)	215 (96%)	9 (4%)	31	57
1	F	223/228 (98%)	211 (95%)	12 (5%)	22	44
1	G	224/228 (98%)	206 (92%)	18 (8%)	12	24
1	H	225/228 (99%)	211 (94%)	14 (6%)	18	37
1	I	223/228 (98%)	208 (93%)	15 (7%)	16	33
1	J	227/228 (100%)	212 (93%)	15 (7%)	16	33
1	K	227/228 (100%)	211 (93%)	16 (7%)	15	30
1	L	223/228 (98%)	208 (93%)	15 (7%)	16	33
All	All	2696/2736 (98%)	2544 (94%)	152 (6%)	21	42

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	MET
1	A	108	ASP
1	A	115	ARG
1	A	132	MET
1	A	263	PHE
1	A	272	LYS
1	B	119	ARG
1	B	132	MET
1	B	140	ARG
1	B	239	LYS
1	B	305	HIS
1	C	84	ASP
1	C	89	GLU
1	C	99	LYS
1	C	123[A]	GLU
1	C	123[B]	GLU
1	C	132	MET
1	C	188	SER
1	C	252	GLU
1	C	259	GLN
1	C	272	LYS
1	C	307	HIS

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Mol	Chain	Res	Type
1	D	53	GLU
1	D	55	LEU
1	D	85	ILE
1	D	93	LEU
1	D	96	LYS
1	D	109	LYS
1	D	115	ARG
1	D	184	ARG
1	D	207[A]	ARG
1	D	207[B]	ARG
1	D	239	LYS
1	D	249	LYS
1	D	259	GLN
1	D	270	ARG
1	D	272	LYS
1	D	307	HIS
1	E	58	ASP
1	E	93	LEU
1	E	115	ARG
1	E	183	ASP
1	E	252	GLU
1	E	259	GLN
1	E	263	PHE
1	E	272	LYS
1	E	284	GLN
1	F	58	ASP
1	F	85	ILE
1	F	90	MET
1	F	93	LEU
1	F	186	ARG
1	F	198	LYS
1	F	203	LYS
1	F	209	SER
1	F	252	GLU
1	F	259	GLN
1	F	263	PHE
1	F	272	LYS
1	G	55	LEU
1	G	59	LEU
1	G	85	ILE
1	G	93	LEU
1	G	107	LYS

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Mol	Chain	Res	Type
1	G	115	ARG
1	G	132	MET
1	G	134	LEU
1	G	140	ARG
1	G	183	ASP
1	G	202	ARG
1	G	203	LYS
1	G	209	SER
1	G	252	GLU
1	G	259	GLN
1	G	269	MET
1	G	272	LYS
1	G	304	ARG
1	H	58	ASP
1	H	60	LYS
1	H	80	ASN
1	H	85	ILE
1	H	108	ASP
1	H	115	ARG
1	H	119	ARG
1	H	126	LYS
1	H	140	ARG
1	H	203	LYS
1	H	252	GLU
1	H	259	GLN
1	H	305	HIS
1	H	307	HIS
1	I	62	PHE
1	I	63	ARG
1	I	88	GLU
1	I	90	MET
1	I	93	LEU
1	I	107	LYS
1	I	109	LYS
1	I	132	MET
1	I	198	LYS
1	I	202	ARG
1	I	210	GLU
1	I	252	GLU
1	I	259	GLN
1	I	272	LYS
1	I	307	HIS

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Mol	Chain	Res	Type
1	J	62	PHE
1	J	63	ARG
1	J	93	LEU
1	J	108	ASP
1	J	119	ARG
1	J	145	CYS
1	J	183	ASP
1	J	190	LYS
1	J	252	GLU
1	J	259	GLN
1	J	264	GLU
1	J	270	ARG
1	J	272	LYS
1	J	301	GLU
1	J	312	MET
1	K	58	ASP
1	K	62	PHE
1	K	64	LYS
1	K	74	SER
1	K	85	ILE
1	K	93	LEU
1	K	109	LYS
1	K	186	ARG
1	K	198	LYS
1	K	252	GLU
1	K	259	GLN
1	K	272	LYS
1	K	301	GLU
1	K	307	HIS
1	K	308	GLN
1	K	311	LEU
1	L	55	LEU
1	L	85	ILE
1	L	93	LEU
1	L	107	LYS
1	L	109	LYS
1	L	115	ARG
1	L	132	MET
1	L	135	ARG
1	L	140	ARG
1	L	184	ARG
1	L	239	LYS

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Mol	Chain	Res	Type
1	L	252	GLU
1	L	259	GLN
1	L	263	PHE
1	L	272	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	308	GLN
1	D	280	GLN
1	D	307	HIS
1	D	308	GLN
1	H	307	HIS
1	L	154	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 14 are monoatomic - leaving 7 for Mogul analysis.

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
3	PRO	A	402	-	8,8,8	0.93	0	10,10,10	1.16	1 (10%)
5	GOL	B	401	-	5,5,5	0.38	0	5,5,5	0.89	0
3	PRO	C	403	-	8,8,8	0.86	0	10,10,10	1.02	0
5	GOL	B	402	-	5,5,5	0.30	0	5,5,5	0.49	0
5	GOL	C	405	-	5,5,5	0.25	0	5,5,5	1.01	0
5	GOL	C	404	-	5,5,5	0.31	0	5,5,5	0.68	0
5	GOL	D	402	-	5,5,5	0.26	0	5,5,5	0.44	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
3	PRO	A	402	-	-	2/4/11/11	0/1/1/1
5	GOL	B	401	-	-	2/4/4/4	-
3	PRO	C	403	-	-	2/4/11/11	0/1/1/1
5	GOL	B	402	-	-	2/4/4/4	-
5	GOL	C	405	-	-	2/4/4/4	-
5	GOL	C	404	-	-	3/4/4/4	-
5	GOL	D	402	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	PRO	C-CA-N	2.03	114.73	106.73

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	402	GOL	O1-C1-C2-C3
5	C	405	GOL	C1-C2-C3-O3
5	D	402	GOL	O1-C1-C2-C3
5	D	402	GOL	C1-C2-C3-O3
5	C	405	GOL	O2-C2-C3-O3
5	C	404	GOL	C1-C2-C3-O3
3	A	402	PRO	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
5	B	402	GOL	O1-C1-C2-O2
5	D	402	GOL	O1-C1-C2-O2
5	D	402	GOL	O2-C2-C3-O3
3	A	402	PRO	O-C-CA-N
3	C	403	PRO	OXT-C-CA-N
5	C	404	GOL	O1-C1-C2-C3
5	C	404	GOL	O2-C2-C3-O3
3	C	403	PRO	O-C-CA-N
5	B	401	GOL	O1-C1-C2-C3
5	B	401	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	PRO	2	0
5	B	401	GOL	1	0
3	C	403	PRO	1	0
5	B	402	GOL	7	0
5	C	405	GOL	4	0
5	C	404	GOL	3	0
5	D	402	GOL	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	254/261 (97%)	-0.13	1 (0%)	92	91	22, 50, 81, 113	0
1	B	259/261 (99%)	-0.08	8 (3%)	49	42	23, 49, 96, 148	0
1	C	256/261 (98%)	-0.09	6 (2%)	60	54	22, 46, 86, 132	0
1	D	257/261 (98%)	-0.22	4 (1%)	72	68	25, 46, 100, 148	0
1	E	256/261 (98%)	-0.03	10 (3%)	39	32	28, 63, 116, 138	0
1	F	255/261 (97%)	-0.04	5 (1%)	65	60	35, 64, 119, 140	0
1	G	255/261 (97%)	-0.17	1 (0%)	92	91	25, 55, 103, 129	0
1	H	257/261 (98%)	-0.07	5 (1%)	66	62	35, 63, 103, 126	0
1	I	255/261 (97%)	0.24	16 (6%)	20	15	41, 71, 123, 136	0
1	J	259/261 (99%)	0.44	24 (9%)	8	6	45, 80, 143, 165	0
1	K	259/261 (99%)	0.17	12 (4%)	32	26	37, 66, 108, 124	0
1	L	255/261 (97%)	0.02	8 (3%)	49	42	38, 72, 109, 141	0
All	All	3077/3132 (98%)	0.00	100 (3%)	47	40	22, 60, 115, 165	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	81	LEU	6.8
1	J	309	VAL	6.3
1	L	305	HIS	5.4
1	B	307	HIS	5.1
1	L	303	ALA	5.0
1	I	85	ILE	4.9
1	J	308	GLN	4.6
1	B	310	MET	4.6
1	K	84	ASP	4.5
1	C	305	HIS	4.1
1	B	309	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	K	298	MET	4.1
1	E	280	GLN	4.1
1	K	85	ILE	3.9
1	I	81	LEU	3.9
1	J	310	MET	3.9
1	I	59	LEU	3.8
1	J	311	LEU	3.7
1	K	136	GLY	3.7
1	C	83	PRO	3.7
1	J	97	TYR	3.6
1	J	85	ILE	3.6
1	D	302	ALA	3.6
1	J	54	GLY	3.5
1	L	302	ALA	3.5
1	L	306	GLU	3.5
1	K	82	PRO	3.4
1	I	97	TYR	3.4
1	K	65	PRO	3.4
1	D	305	HIS	3.3
1	C	53	GLU	3.3
1	B	312	MET	3.2
1	I	58	ASP	3.2
1	B	311	LEU	3.2
1	D	308	GLN	3.2
1	H	261	GLY	3.1
1	B	308	GLN	3.0
1	J	107	LYS	3.0
1	J	261	GLY	2.9
1	J	90	MET	2.9
1	I	304	ARG	2.8
1	E	261	GLY	2.8
1	F	284	GLN	2.8
1	H	284	GLN	2.7
1	B	303	ALA	2.7
1	J	307	HIS	2.7
1	J	59	LEU	2.7
1	K	81	LEU	2.7
1	L	307	HIS	2.7
1	E	281	GLN	2.7
1	E	276	GLU	2.7
1	I	94	PHE	2.6
1	E	277	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	267	TYR	2.6
1	E	279	LYS	2.6
1	G	277	MET	2.6
1	J	124	ILE	2.6
1	K	300	MET	2.6
1	K	267	TYR	2.6
1	J	111	PHE	2.6
1	J	112	GLY	2.6
1	D	303	ALA	2.5
1	J	129	LEU	2.5
1	I	82	PRO	2.5
1	I	109	LYS	2.5
1	J	96	LYS	2.5
1	J	94	PHE	2.5
1	E	284	GLN	2.4
1	K	137	LYS	2.4
1	H	277	MET	2.4
1	J	263	PHE	2.4
1	I	136	GLY	2.4
1	F	295	LYS	2.4
1	L	300	MET	2.4
1	J	93	LEU	2.4
1	J	140	ARG	2.3
1	H	66	GLY	2.3
1	C	307	HIS	2.3
1	E	53	GLU	2.3
1	I	135	ARG	2.3
1	E	308	GLN	2.2
1	E	286	ASP	2.2
1	B	109	LYS	2.2
1	I	301	GLU	2.2
1	F	219	PRO	2.2
1	L	53	GLU	2.1
1	I	124	ILE	2.1
1	I	84	ASP	2.1
1	F	277	MET	2.1
1	J	262	SER	2.1
1	I	125	ALA	2.1
1	J	60	LYS	2.0
1	C	109	LYS	2.0
1	F	288	ASN	2.0
1	H	99	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	86	THR	2.0
1	K	310	MET	2.0
1	A	81	LEU	2.0
1	C	306	GLU	2.0
1	K	64	LYS	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	K	C	406	1/1	0.76	0.20	76,76,76,76	0
2	CL	F	402	1/1	0.80	0.15	79,79,79,79	0
5	GOL	B	401	6/6	0.80	0.30	38,41,46,50	0
5	GOL	B	402	6/6	0.81	0.36	48,55,58,59	0
5	GOL	C	404	6/6	0.81	0.26	49,51,57,61	0
5	GOL	D	402	6/6	0.81	0.34	56,69,71,72	0
2	CL	L	401	1/1	0.82	0.18	73,73,73,73	0
4	K	A	403	1/1	0.86	0.15	73,73,73,73	0
5	GOL	C	405	6/6	0.89	0.22	30,42,46,47	0
3	PRO	C	403	8/8	0.89	0.22	64,67,107,128	0
4	K	D	403	1/1	0.90	0.16	71,71,71,71	0
3	PRO	A	402	8/8	0.91	0.29	45,47,62,82	0
4	K	B	403	1/1	0.92	0.17	71,71,71,71	0
2	CL	D	401	1/1	0.92	0.22	90,90,90,90	0
2	CL	C	401	1/1	0.93	0.13	56,56,56,56	0
2	CL	F	401	1/1	0.94	0.26	64,64,64,64	0
2	CL	C	402	1/1	0.94	0.20	59,59,59,59	0
2	CL	A	401	1/1	0.96	0.25	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	G	401	1/1	0.96	0.13	70,70,70,70	0
2	CL	H	401	1/1	0.96	0.09	63,63,63,63	0
2	CL	E	401	1/1	0.99	0.14	52,52,52,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.