



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:01 PM UTC

PDB ID : 5IFM / pdb_00005ifm
Title : Human NONO (p54nrb) Homodimer
Authors : Knott, G.J.; Bond, C.S.
Deposited on : 2016-02-26
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

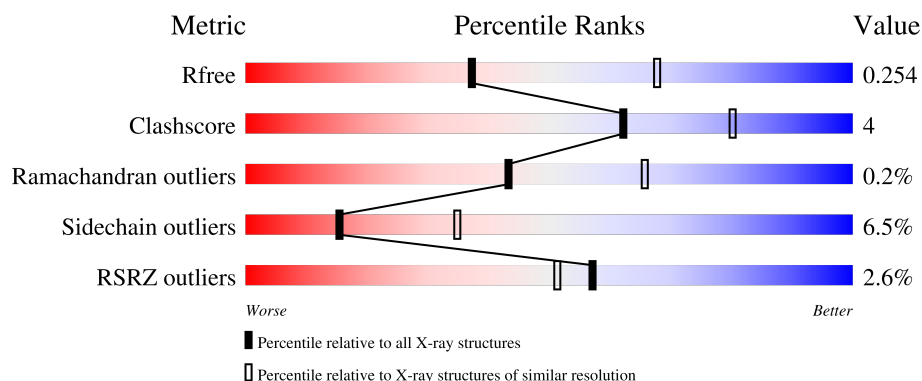
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

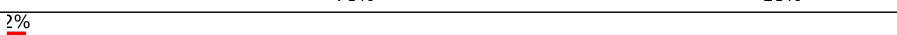
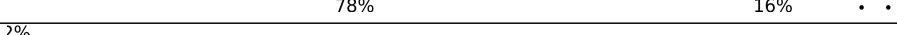
The reported resolution of this entry is 2.60 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	261	
1	B	261	
1	C	261	
1	D	261	
1	E	261	

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Mol	Chain	Length	Quality of chain
1	F	261	
1	G	261	
1	H	261	
1	I	261	
1	J	261	
1	K	261	
1	L	261	

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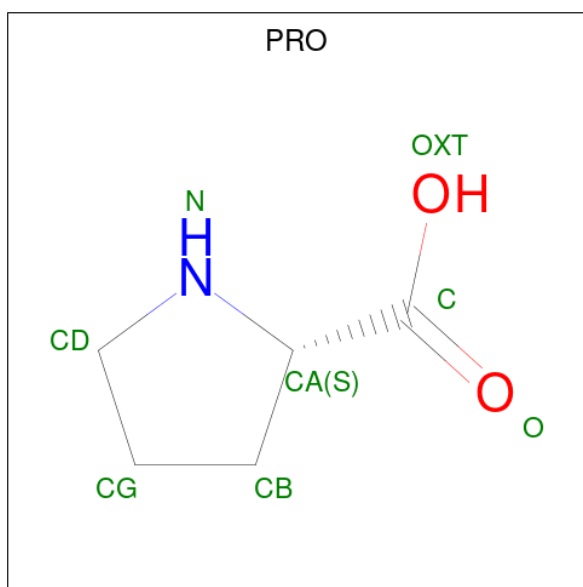
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Chain	Residue	Modelled	Actual	Comment	Reference
F	52	GLY	-	expression tag	UNP Q15233
G	52	GLY	-	expression tag	UNP Q15233
H	52	GLY	-	expression tag	UNP Q15233
I	52	GLY	-	expression tag	UNP Q15233
J	52	GLY	-	expression tag	UNP Q15233
K	52	GLY	-	expression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

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is PROLINE (CCD ID: PRO) (formula: C₅H₉NO₂).



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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is water.

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

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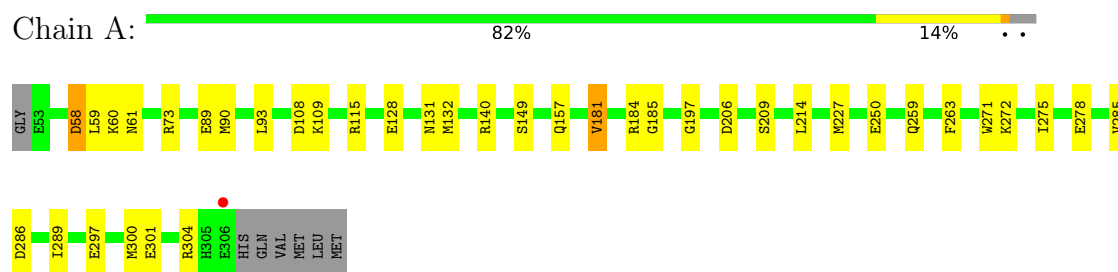
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	10	Total 10	O 10	0	0
6	I	5	Total 5	O 5	0	0
6	J	4	Total 4	O 4	0	0
6	K	7	Total 7	O 7	0	0
6	L	7	Total 7	O 7	0	0

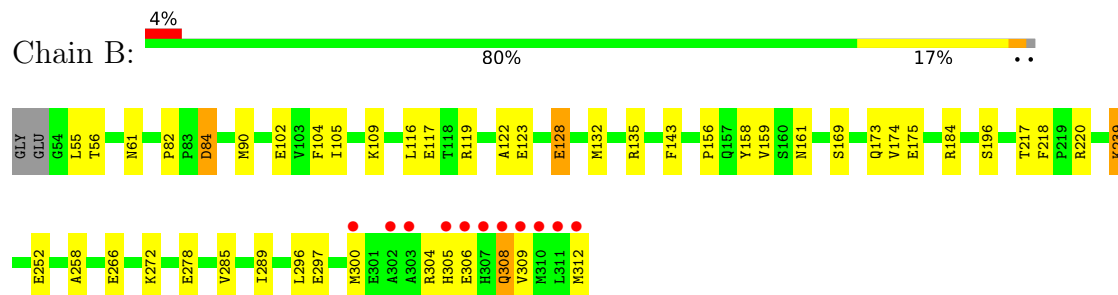
3 Residue-property plots [i](#)

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.

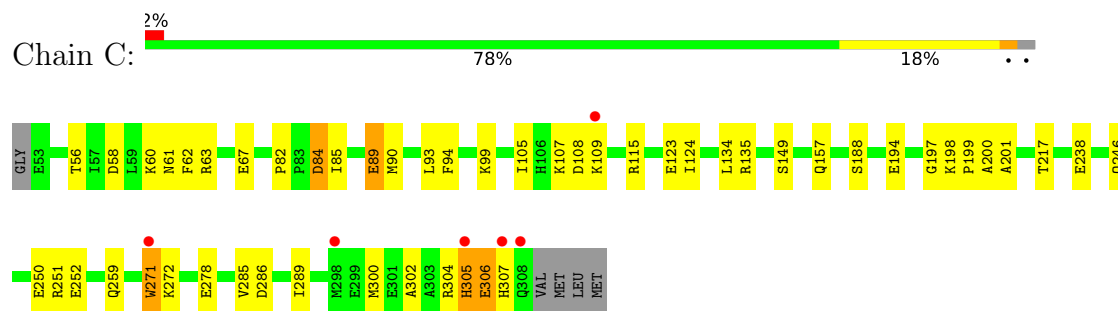
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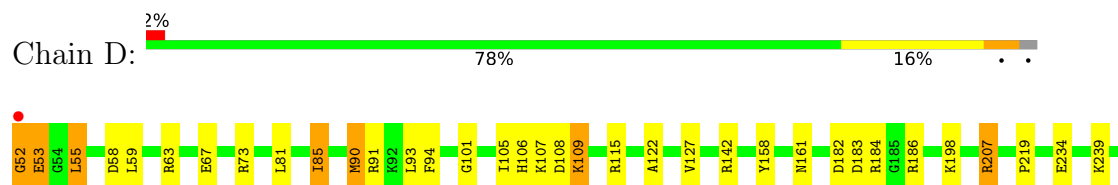
- Molecule 1: Non-POU domain-containing octamer-binding protein



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

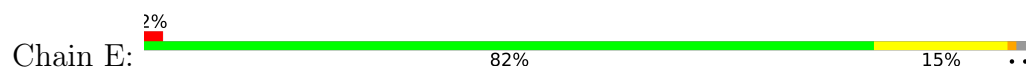


- Molecule 1: Non-POU domain-containing octamer-binding protein

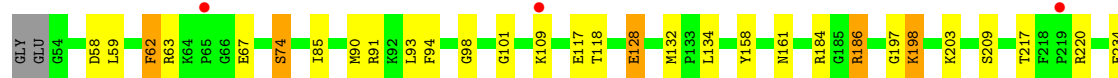
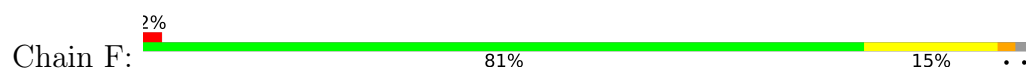




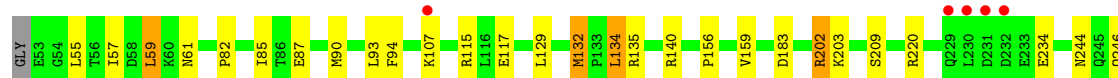
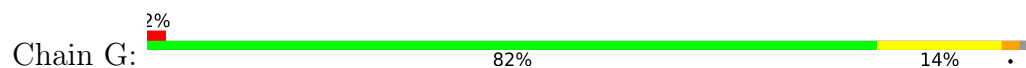
- Molecule 1: Non-POU domain-containing octamer-binding protein



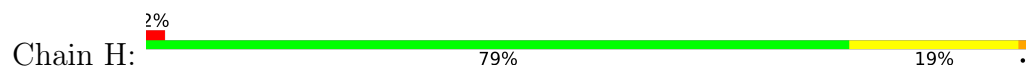
- Molecule 1: Non-POU domain-containing octamer-binding protein



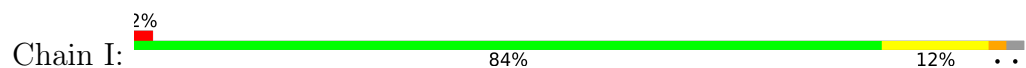
- Molecule 1: Non-POU domain-containing octamer-binding protein



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

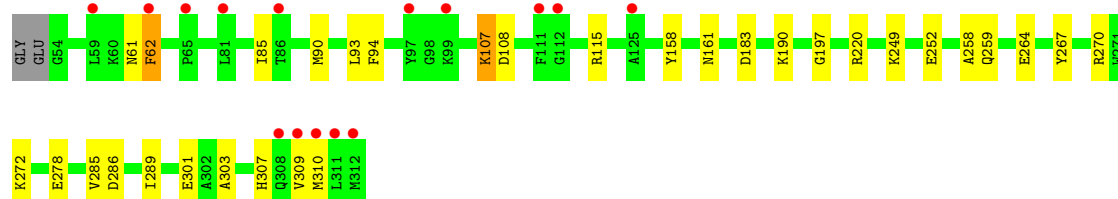
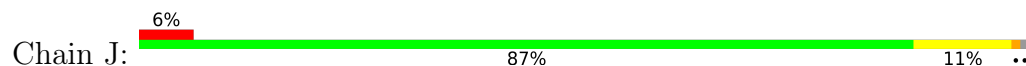


- Molecule 1: Non-POU domain-containing octamer-binding protein

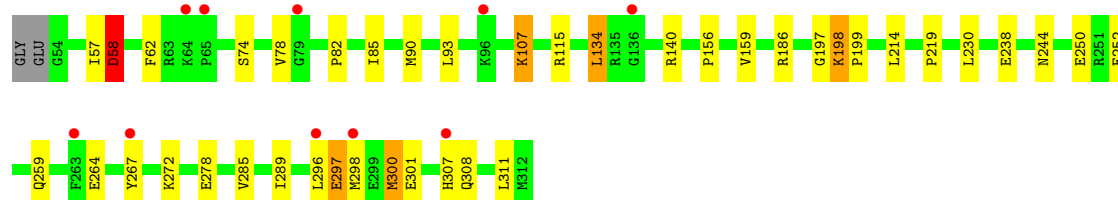
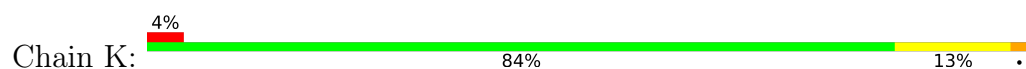




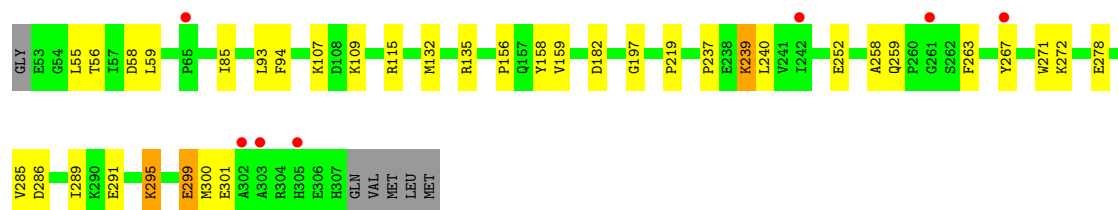
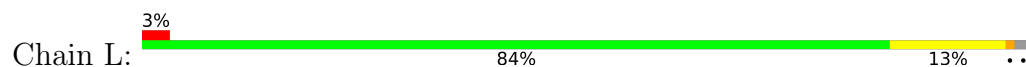
- Molecule 1: Non-POU domain-containing octamer-binding protein



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



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



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
$\langle I/\sigma(I) \rangle$ 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	5521 reflections (4.94%)	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)	0.32 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, K, GOL

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	0.86	0/2104	1.35	9/2823 (0.3%)
1	B	0.91	1/2157 (0.0%)	1.34	10/2893 (0.3%)
1	C	0.91	1/2133 (0.0%)	1.43	19/2862 (0.7%)
1	D	0.96	1/2139 (0.0%)	1.43	19/2869 (0.7%)
1	E	0.82	0/2124	1.38	11/2850 (0.4%)
1	F	0.82	0/2115	1.36	11/2838 (0.4%)
1	G	0.83	0/2124	1.36	5/2850 (0.2%)
1	H	0.83	0/2130	1.43	17/2858 (0.6%)
1	I	0.80	0/2115	1.36	8/2838 (0.3%)
1	J	0.78	0/2146	1.33	7/2879 (0.2%)
1	K	0.82	0/2146	1.38	13/2879 (0.5%)
1	L	0.83	0/2115	1.39	8/2838 (0.3%)
All	All	0.85	3/25548 (0.0%)	1.38	137/34277 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	304	ARG	C-N	5.89	1.41	1.33
1	D	300	MET	SD-CE	-5.59	1.65	1.79
1	B	82	PRO	CA-C	5.46	1.54	1.51

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	LYS	N-CA-C	7.52	122.49	113.16
1	K	58	ASP	CA-CB-CG	7.19	119.79	112.60
1	B	84	ASP	CA-CB-CG	6.87	119.47	112.60
1	D	109	LYS	N-CA-C	6.76	121.38	113.20
1	D	182	ASP	CA-C-N	6.73	130.21	120.38
1	D	182	ASP	C-N-CA	6.73	130.21	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	109	LYS	N-CA-C	6.57	120.88	112.34
1	K	197	GLY	CA-C-N	6.55	128.28	120.09
1	K	197	GLY	C-N-CA	6.55	128.28	120.09
1	A	109	LYS	N-CA-C	6.52	120.82	112.34
1	H	197	GLY	CA-C-N	6.50	128.21	120.09
1	H	197	GLY	C-N-CA	6.50	128.21	120.09
1	C	305	HIS	CA-C-N	6.45	128.82	120.44
1	C	305	HIS	C-N-CA	6.45	128.82	120.44
1	E	182	ASP	CA-C-N	6.40	129.15	120.38
1	E	182	ASP	C-N-CA	6.40	129.15	120.38
1	A	304	ARG	N-CA-C	6.37	119.60	110.24
1	C	305	HIS	CA-CB-CG	6.19	119.99	113.80
1	I	89	GLU	CA-C-N	6.16	128.44	120.44
1	I	89	GLU	C-N-CA	6.16	128.44	120.44
1	D	303	ALA	CA-C-N	6.08	128.34	120.44
1	D	303	ALA	C-N-CA	6.08	128.34	120.44
1	A	197	GLY	CA-C-N	6.07	127.68	120.09
1	A	197	GLY	C-N-CA	6.07	127.68	120.09
1	I	300	MET	N-CA-C	6.07	117.56	111.07
1	B	123	GLU	CB-CG-CD	6.00	122.81	112.60
1	E	202	ARG	CA-C-N	5.88	128.09	120.44
1	E	202	ARG	C-N-CA	5.88	128.09	120.44
1	F	238	GLU	CB-CG-CD	5.87	122.58	112.60
1	C	94	PHE	CA-C-N	5.85	128.40	120.38
1	C	94	PHE	C-N-CA	5.85	128.40	120.38
1	C	197	GLY	CA-C-N	5.82	127.37	120.09
1	C	197	GLY	C-N-CA	5.82	127.37	120.09
1	A	58	ASP	CA-CB-CG	5.82	118.42	112.60
1	D	244	ASN	CA-CB-CG	5.81	118.41	112.60
1	A	286	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	117	GLU	N-CA-C	5.81	117.28	111.07
1	D	183	ASP	CA-CB-CG	5.80	118.40	112.60
1	C	201	ALA	CA-C-N	5.80	127.98	120.44
1	C	201	ALA	C-N-CA	5.80	127.98	120.44
1	H	95	GLU	N-CA-C	-5.78	104.89	111.07
1	H	216	THR	CA-C-N	5.74	128.45	120.29
1	H	216	THR	C-N-CA	5.74	128.45	120.29
1	G	94	PHE	CA-C-N	5.73	128.23	120.38
1	G	94	PHE	C-N-CA	5.73	128.23	120.38
1	B	266	GLU	CB-CG-CD	5.71	122.31	112.60
1	H	234	GLU	CB-CG-CD	5.70	122.28	112.60
1	C	58	ASP	CA-CB-CG	5.67	118.27	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	GLU	CB-CG-CD	5.63	122.17	112.60
1	K	297	GLU	CA-C-N	5.63	128.09	120.44
1	K	297	GLU	C-N-CA	5.63	128.09	120.44
1	F	94	PHE	CA-C-N	5.60	128.05	120.38
1	F	94	PHE	C-N-CA	5.60	128.05	120.38
1	H	122	ALA	CA-C-N	5.60	128.24	120.29
1	H	122	ALA	C-N-CA	5.60	128.24	120.29
1	D	267	TYR	N-CA-C	5.59	118.31	111.82
1	D	286	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	308	GLN	CA-C-N	5.58	128.40	120.53
1	B	308	GLN	C-N-CA	5.58	128.40	120.53
1	L	94	PHE	CA-C-N	5.54	127.97	120.38
1	L	94	PHE	C-N-CA	5.54	127.97	120.38
1	H	161	ASN	CA-C-N	5.53	128.15	120.29
1	H	161	ASN	C-N-CA	5.53	128.15	120.29
1	G	87	GLU	CA-C-N	5.52	127.62	120.44
1	G	87	GLU	C-N-CA	5.52	127.62	120.44
1	E	117	GLU	N-CA-C	5.51	116.97	111.07
1	C	304	ARG	CA-C-N	5.51	127.92	120.65
1	C	304	ARG	C-N-CA	5.51	127.92	120.65
1	F	117	GLU	N-CA-C	5.51	116.97	111.07
1	F	197	GLY	CA-C-N	5.51	126.98	120.09
1	F	197	GLY	C-N-CA	5.51	126.98	120.09
1	E	262	SER	CA-C-N	5.49	127.64	120.28
1	E	262	SER	C-N-CA	5.49	127.64	120.28
1	J	94	PHE	CA-C-N	5.49	127.91	120.38
1	J	94	PHE	C-N-CA	5.49	127.91	120.38
1	D	94	PHE	CA-C-N	5.49	127.89	120.38
1	D	94	PHE	C-N-CA	5.49	127.89	120.38
1	B	143	PHE	CA-CB-CG	-5.47	108.33	113.80
1	G	117	GLU	N-CA-C	5.46	116.91	111.07
1	L	197	GLY	CA-C-N	5.45	126.91	120.09
1	L	197	GLY	C-N-CA	5.45	126.91	120.09
1	C	305	HIS	CB-CA-C	-5.43	102.59	110.96
1	K	244	ASN	CA-CB-CG	5.41	118.01	112.60
1	E	94	PHE	CA-C-N	5.39	127.50	120.28
1	E	94	PHE	C-N-CA	5.39	127.50	120.28
1	I	94	PHE	CA-C-N	5.36	127.73	120.38
1	I	94	PHE	C-N-CA	5.36	127.73	120.38
1	K	296	LEU	CA-C-N	5.34	127.98	120.28
1	K	296	LEU	C-N-CA	5.34	127.98	120.28
1	J	286	ASP	CA-CB-CG	5.34	117.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	52	GLY	CA-C-N	5.34	131.74	121.54
1	D	52	GLY	C-N-CA	5.34	131.74	121.54
1	J	161	ASN	CA-C-N	5.33	127.37	120.44
1	J	161	ASN	C-N-CA	5.33	127.37	120.44
1	D	55	LEU	N-CA-C	5.33	117.18	108.76
1	A	184	ARG	N-CA-C	-5.32	106.29	114.16
1	C	286	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	271	TRP	CA-C-N	5.26	127.33	120.28
1	C	271	TRP	C-N-CA	5.26	127.33	120.28
1	L	58	ASP	CA-CB-CG	5.26	117.86	112.60
1	E	286	ASP	CA-CB-CG	5.25	117.85	112.60
1	K	298	MET	CA-C-N	5.23	127.82	120.28
1	K	298	MET	C-N-CA	5.23	127.82	120.28
1	I	303	ALA	CA-C-N	5.22	127.23	120.44
1	I	303	ALA	C-N-CA	5.22	127.23	120.44
1	L	299	GLU	CA-C-N	5.21	127.53	120.65
1	L	299	GLU	C-N-CA	5.21	127.53	120.65
1	I	286	ASP	CA-CB-CG	5.20	117.80	112.60
1	H	263	PHE	CA-C-N	5.19	127.19	120.44
1	H	263	PHE	C-N-CA	5.19	127.19	120.44
1	H	238	GLU	CB-CG-CD	5.18	121.40	112.60
1	K	199	PRO	CA-C-N	5.17	127.21	120.28
1	K	199	PRO	C-N-CA	5.17	127.21	120.28
1	C	108	ASP	CA-CB-CG	5.16	117.76	112.60
1	D	307	HIS	CA-CB-CG	5.16	118.96	113.80
1	H	117	GLU	N-CA-C	5.15	116.59	110.97
1	E	183	ASP	CA-CB-CG	5.15	117.75	112.60
1	K	238	GLU	CB-CG-CD	5.15	121.35	112.60
1	B	161	ASN	CA-C-N	5.14	127.17	120.28
1	B	161	ASN	C-N-CA	5.14	127.17	120.28
1	F	234	GLU	CB-CG-CD	5.14	121.34	112.60
1	F	62	PHE	N-CA-C	-5.13	106.95	114.39
1	L	286	ASP	CA-CB-CG	5.12	117.72	112.60
1	F	161	ASN	CA-CB-CG	5.11	117.71	112.60
1	D	242	ILE	N-CA-CB	5.09	116.65	110.95
1	A	206	ASP	CA-CB-CG	5.08	117.69	112.60
1	D	122	ALA	CA-C-N	5.08	127.09	120.28
1	D	122	ALA	C-N-CA	5.08	127.09	120.28
1	J	197	GLY	CA-C-N	5.07	126.43	120.09
1	J	197	GLY	C-N-CA	5.07	126.43	120.09
1	D	161	ASN	CA-CB-CG	5.04	117.64	112.60
1	H	286	ASP	CA-CB-CG	5.04	117.64	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	306	GLU	CB-CG-CD	5.03	121.15	112.60
1	H	182	ASP	CA-C-N	5.03	127.72	120.38
1	H	182	ASP	C-N-CA	5.03	127.72	120.38
1	F	98	GLY	CA-C-N	5.02	127.99	120.87
1	F	98	GLY	C-N-CA	5.02	127.99	120.87

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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2065	0	2064	23	0
1	B	2114	0	2124	37	0
1	C	2090	0	2085	33	0
1	D	2099	0	2094	33	0
1	E	2084	0	2079	25	0
1	F	2075	0	2073	20	0
1	G	2084	0	2076	22	0
1	H	2090	0	2091	25	0
1	I	2075	0	2071	20	0
1	J	2106	0	2111	14	0
1	K	2106	0	2111	17	0
1	L	2075	0	2071	18	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	208	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 (208) 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:B:296:LEU:HG	1:B:300:MET:HE2	1.65	0.78
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:304:ARG:HH12	1:H:250:GLU:CD	2.01	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: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: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:D:219:PRO:HG2	1:D:300:MET:HE2	1.86	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:E:90:MET:HE2	1:E:103:VAL:HG13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:297:GLU:HA	1:B:300:MET:HE3	1.88	0.56
1:C:124:ILE:HG23	1:D:59:LEU:HD13	1.88	0.55
1:G:129:LEU:HD23	1:G:132:MET:HE3	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:E:90:MET:HE3	1:E:114:ILE:HB	1.89	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:D:207[A]:ARG:HG2	1:D:207[A]:ARG:HH11	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:D:307:HIS:C	1:D:307:HIS:CD2	2.85	0.54
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
1:C:199:PRO:HB3	1:H:310:MET:HE2	1.90	0.53
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:132:MET:HE2	1:I:134:LEU:HD23	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:132:MET:HE1	1:E:134:LEU:HD23	1.94	0.50
1:G:300:MET:HE1	1:H:271:TRP:HB2	1.92	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:E:271:TRP:HB2	1:F:300:MET:HE1	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
1:C:271:TRP:HE1	1:D:300:MET:HE1	1.78	0.48
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:B:304:ARG:C	1:B:306:GLU:H	2.22	0.47
1:G:57:ILE:HG23	1:H:96:LYS:HG2	1.96	0.47
1:F:198:LYS:HB3	1:J:310:MET:HE1	1.95	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:C:271:TRP:NE1	1:D:300:MET:HE1	2.30	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
1:A:271:TRP:HE1	1:A:275:ILE:HD11	1.80	0.46
1:E:300:MET:HE1	1:F:271:TRP:HB2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:219:PRO:HD2	1:I:300:MET:HE1	1.99	0.44
1:L:300:MET:HE3	1:L:301:GLU:HG2	1.99	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:F:74:SER:HB3	1:F:118:THR:C	2.43	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: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: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
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:D:307:HIS:C	1:D:307:HIS:HD2	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:J:62:PHE:CD1	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:A:297:GLU:HA	1:A:300:MET:HE3	2.02	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: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:C:84:ASP:CG	1:C:135:ARG:HH12	2.28	0.40
1:F:132:MET:HE1	1:F:134:LEU:HD13	2.02	0.40
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 [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	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%)	16	34
1	D	256/261 (98%)	248 (97%)	6 (2%)	2 (1%)	16	34
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%)	30	51
1	K	257/261 (98%)	249 (97%)	7 (3%)	1 (0%)	30	51
1	L	253/261 (97%)	244 (96%)	9 (4%)	0	100	100
All	All	3057/3132 (98%)	2962 (97%)	89 (3%)	6 (0%)	43	66

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%)	213 (96%)	9 (4%)	27	54
1	B	228/228 (100%)	222 (97%)	6 (3%)	40	68
1	C	225/228 (99%)	212 (94%)	13 (6%)	18	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	225/228 (99%)	206 (92%)	19 (8%)	10	23
1	E	224/228 (98%)	214 (96%)	10 (4%)	24	50
1	F	223/228 (98%)	206 (92%)	17 (8%)	12	27
1	G	224/228 (98%)	205 (92%)	19 (8%)	10	22
1	H	225/228 (99%)	206 (92%)	19 (8%)	10	23
1	I	223/228 (98%)	207 (93%)	16 (7%)	13	30
1	J	227/228 (100%)	212 (93%)	15 (7%)	15	34
1	K	227/228 (100%)	207 (91%)	20 (9%)	9	21
1	L	223/228 (98%)	209 (94%)	14 (6%)	16	36
All	All	2696/2736 (98%)	2519 (93%)	177 (7%)	15	34

All (177) 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	131	ASN
1	A	132	MET
1	A	181	VAL
1	A	259	GLN
1	A	263	PHE
1	A	272	LYS
1	B	119	ARG
1	B	128	GLU
1	B	132	MET
1	B	239	LYS
1	B	252	GLU
1	B	305	HIS
1	C	60	LYS
1	C	84	ASP
1	C	89	GLU
1	C	93	LEU
1	C	99	LYS
1	C	123[A]	GLU
1	C	123[B]	GLU
1	C	188	SER
1	C	238	GLU
1	C	252	GLU

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Mol	Chain	Res	Type
1	C	259	GLN
1	C	272	LYS
1	C	307	HIS
1	D	53	GLU
1	D	55	LEU
1	D	73	ARG
1	D	85	ILE
1	D	90	MET
1	D	93	LEU
1	D	109	LYS
1	D	115	ARG
1	D	198	LYS
1	D	207[A]	ARG
1	D	207[B]	ARG
1	D	239	LYS
1	D	249	LYS
1	D	252	GLU
1	D	259	GLN
1	D	264	GLU
1	D	270	ARG
1	D	272	LYS
1	D	307	HIS
1	E	58	ASP
1	E	85	ILE
1	E	93	LEU
1	E	115	ARG
1	E	134	LEU
1	E	198	LYS
1	E	252	GLU
1	E	259	GLN
1	E	263	PHE
1	E	272	LYS
1	F	58	ASP
1	F	74	SER
1	F	85	ILE
1	F	90	MET
1	F	93	LEU
1	F	109	LYS
1	F	128	GLU
1	F	186	ARG
1	F	198	LYS
1	F	203	LYS

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Mol	Chain	Res	Type
1	F	209	SER
1	F	252	GLU
1	F	259	GLN
1	F	263	PHE
1	F	272	LYS
1	F	290	LYS
1	F	295	LYS
1	G	55	LEU
1	G	59	LEU
1	G	85	ILE
1	G	90	MET
1	G	93	LEU
1	G	107	LYS
1	G	115	ARG
1	G	132	MET
1	G	134	LEU
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	295	LYS
1	G	304	ARG
1	H	58	ASP
1	H	60	LYS
1	H	80	ASN
1	H	85	ILE
1	H	90	MET
1	H	108	ASP
1	H	109	LYS
1	H	115	ARG
1	H	119	ARG
1	H	126	LYS
1	H	129	LEU
1	H	132	MET
1	H	140	ARG
1	H	186	ARG
1	H	203	LYS
1	H	252	GLU

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Mol	Chain	Res	Type
1	H	259	GLN
1	H	295	LYS
1	H	307	HIS
1	I	62	PHE
1	I	63	ARG
1	I	85	ILE
1	I	88	GLU
1	I	90	MET
1	I	93	LEU
1	I	107	LYS
1	I	115	ARG
1	I	132	MET
1	I	198	LYS
1	I	210	GLU
1	I	252	GLU
1	I	259	GLN
1	I	272	LYS
1	I	301	GLU
1	I	307	HIS
1	J	62	PHE
1	J	85	ILE
1	J	90	MET
1	J	93	LEU
1	J	107	LYS
1	J	108	ASP
1	J	115	ARG
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	K	58	ASP
1	K	62	PHE
1	K	74	SER
1	K	78	VAL
1	K	85	ILE
1	K	90	MET
1	K	93	LEU
1	K	107	LYS

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Mol	Chain	Res	Type
1	K	115	ARG
1	K	134	LEU
1	K	186	ARG
1	K	198	LYS
1	K	252	GLU
1	K	259	GLN
1	K	272	LYS
1	K	300	MET
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	239	LYS
1	L	252	GLU
1	L	259	GLN
1	L	263	PHE
1	L	272	LYS
1	L	295	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	B	308	GLN
1	C	173	GLN
1	C	253	GLN
1	D	280	GLN
1	D	307	HIS
1	D	308	GLN
1	E	61	ASN
1	F	173	GLN
1	G	61	ASN
1	H	307	HIS
1	I	61	ASN

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Mol	Chain	Res	Type
1	J	61	ASN
1	L	154	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
5	GOL	D	402	-	5,5,5	0.25	0	5,5,5	0.44	0
5	GOL	C	404	-	5,5,5	0.31	0	5,5,5	0.70	0
3	PRO	C	403	-	8,8,8	0.89	0	10,10,10	1.01	0
5	GOL	B	401	-	5,5,5	0.39	0	5,5,5	0.92	0
5	GOL	C	405	-	5,5,5	0.25	0	5,5,5	1.05	0
3	PRO	A	402	-	8,8,8	0.96	0	10,10,10	1.16	1 (10%)
5	GOL	B	402	-	5,5,5	0.30	0	5,5,5	0.50	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
5	GOL	D	402	-	-	4/4/4/4	-
5	GOL	C	404	-	-	4/4/4/4	-
3	PRO	C	403	-	-	2/4/11/11	0/1/1/1
5	GOL	B	401	-	-	2/4/4/4	-
5	GOL	C	405	-	-	2/4/4/4	-
3	PRO	A	402	-	-	2/4/11/11	0/1/1/1
5	GOL	B	402	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	PRO	C-CA-N	2.02	114.73	106.84

There are no chirality outliers.

All (18) 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
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	OXT-C-CA-N
3	A	402	PRO	O-C-CA-N
3	C	403	PRO	OXT-C-CA-N
5	C	404	GOL	O2-C2-C3-O3
5	B	401	GOL	O1-C1-C2-C3
5	C	404	GOL	O1-C1-C2-C3
5	B	401	GOL	O1-C1-C2-O2
3	C	403	PRO	O-C-CA-N
5	C	404	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
5	D	402	GOL	2	0
5	C	404	GOL	3	0
3	C	403	PRO	1	0
5	B	401	GOL	1	0
5	C	405	GOL	4	0
3	A	402	PRO	2	0
5	B	402	GOL	7	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	254/261 (97%)	-0.08	1 (0%) 88 86	22, 50, 81, 113	0
1	B	259/261 (99%)	0.14	11 (4%) 40 35	20, 49, 96, 148	1 (0%)
1	C	256/261 (98%)	-0.09	6 (2%) 61 55	20, 46, 86, 132	1 (0%)
1	D	257/261 (98%)	-0.09	5 (1%) 66 61	16, 46, 100, 148	1 (0%)
1	E	256/261 (98%)	0.18	5 (1%) 65 60	28, 63, 116, 138	0
1	F	255/261 (97%)	0.21	4 (1%) 70 66	35, 64, 119, 140	0
1	G	255/261 (97%)	0.08	6 (2%) 59 54	20, 55, 103, 129	1 (0%)
1	H	257/261 (98%)	0.20	5 (1%) 66 61	35, 63, 103, 126	0
1	I	255/261 (97%)	0.36	4 (1%) 70 66	41, 71, 123, 136	0
1	J	259/261 (99%)	0.68	15 (5%) 29 23	45, 80, 143, 165	0
1	K	259/261 (99%)	0.43	10 (3%) 43 38	37, 66, 108, 124	0
1	L	255/261 (97%)	0.33	7 (2%) 56 50	38, 72, 109, 141	0
All	All	3077/3132 (98%)	0.20	79 (2%) 57 51	16, 60, 115, 165	4 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	309	VAL	5.0
1	B	311	LEU	4.8
1	B	310	MET	4.7
1	B	307	HIS	4.6
1	J	311	LEU	4.2
1	B	309	VAL	4.1
1	B	312	MET	4.0
1	J	97	TYR	3.8
1	K	267	TYR	3.6
1	J	81	LEU	3.6
1	L	302	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	305	HIS	3.4
1	J	99	LYS	3.3
1	J	62	PHE	3.1
1	G	230	LEU	3.1
1	J	65	PRO	3.0
1	K	65	PRO	2.9
1	D	305	HIS	2.9
1	K	64	LYS	2.8
1	K	263	PHE	2.8
1	H	308	GLN	2.8
1	G	107	LYS	2.8
1	J	308	GLN	2.8
1	L	305	HIS	2.8
1	E	308	GLN	2.7
1	E	261	GLY	2.7
1	B	303	ALA	2.6
1	B	308	GLN	2.5
1	F	308	GLN	2.5
1	A	306	GLU	2.5
1	J	125	ALA	2.5
1	I	81	LEU	2.4
1	I	85	ILE	2.4
1	B	305	HIS	2.4
1	F	65	PRO	2.4
1	C	308	GLN	2.4
1	G	229	GLN	2.4
1	H	309	VAL	2.4
1	J	59	LEU	2.3
1	E	306	GLU	2.3
1	J	312	MET	2.3
1	C	307	HIS	2.3
1	D	307	HIS	2.3
1	B	306	GLU	2.3
1	L	261	GLY	2.3
1	K	307	HIS	2.2
1	D	52	GLY	2.2
1	H	249	LYS	2.2
1	G	232	ASP	2.2
1	F	109	LYS	2.2
1	D	303	ALA	2.2
1	D	308	GLN	2.2
1	K	96	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	298	MET	2.2
1	C	109	LYS	2.2
1	H	307	HIS	2.2
1	L	65	PRO	2.1
1	B	300	MET	2.1
1	K	136	GLY	2.1
1	L	303	ALA	2.1
1	E	252	GLU	2.1
1	K	296	LEU	2.1
1	L	267	TYR	2.1
1	B	302	ALA	2.1
1	J	310	MET	2.1
1	J	111	PHE	2.1
1	I	93	LEU	2.1
1	G	307	HIS	2.1
1	H	305	HIS	2.1
1	J	112	GLY	2.1
1	K	79	GLY	2.1
1	E	109	LYS	2.0
1	J	86	THR	2.0
1	G	231	ASP	2.0
1	C	271	TRP	2.0
1	K	298	MET	2.0
1	F	219	PRO	2.0
1	L	242	ILE	2.0
1	I	97	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PRO	C	403	8/8	0.77	0.17	64,67,107,128	0
5	GOL	C	404	6/6	0.80	0.19	49,51,57,61	0
5	GOL	B	402	6/6	0.85	0.20	48,55,58,59	0
2	CL	L	401	1/1	0.88	0.11	73,73,73,73	0
5	GOL	B	401	6/6	0.88	0.22	38,41,46,50	0
5	GOL	D	402	6/6	0.88	0.17	56,69,71,72	0
3	PRO	A	402	8/8	0.89	0.17	45,47,62,82	0
4	K	C	406	1/1	0.89	0.12	76,76,76,76	0
4	K	A	403	1/1	0.90	0.10	73,73,73,73	0
5	GOL	C	405	6/6	0.90	0.17	30,42,46,47	0
4	K	D	403	1/1	0.90	0.10	71,71,71,71	0
2	CL	D	401	1/1	0.91	0.13	90,90,90,90	0
4	K	B	403	1/1	0.93	0.10	71,71,71,71	0
2	CL	H	401	1/1	0.93	0.08	63,63,63,63	0
2	CL	G	401	1/1	0.94	0.10	70,70,70,70	0
2	CL	F	402	1/1	0.94	0.11	79,79,79,79	0
2	CL	F	401	1/1	0.95	0.14	64,64,64,64	0
2	CL	C	402	1/1	0.96	0.07	59,59,59,59	0
2	CL	C	401	1/1	0.96	0.08	56,56,56,56	0
2	CL	A	401	1/1	0.97	0.09	48,48,48,48	0
2	CL	E	401	1/1	0.98	0.06	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.