



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:25 AM UTC

PDB ID : 8BWF / pdb_00008bwf
Title : PTBP1 RRM1 bound to an allosteric inhibitor
Authors : Schmeing, S.; Vetter, I.; t Hart, P.; Gasper, R.
Deposited on : 2022-12-06
Resolution : 2.90 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

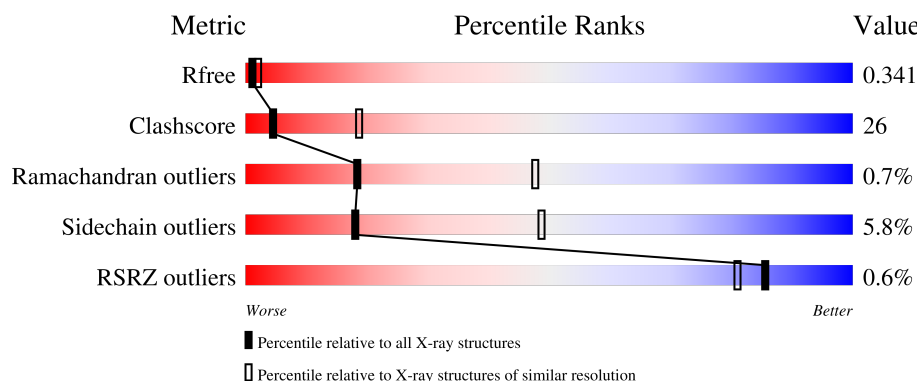
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



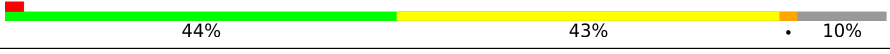
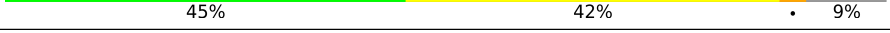
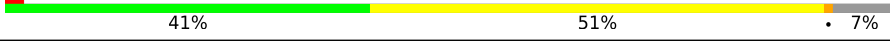
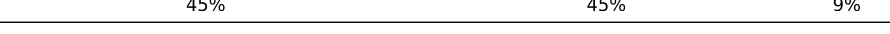
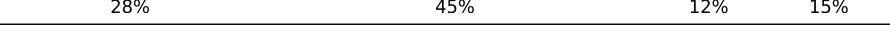
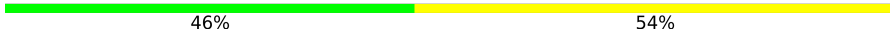
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	86	51% 37% 9%
1	B	86	49% 38% 10%
1	C	86	52% 36% 8%
1	D	86	45% 43% 10%
1	E	86	43% 43% 13%

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Mol	Chain	Length	Quality of chain
1	F	86	
1	G	86	
1	H	86	
1	I	86	
1	J	86	
1	K	86	
1	L	86	
1	M	86	
1	N	86	
1	O	86	
1	P	86	
2	a	13	
2	b	13	
2	c	13	
2	d	13	
2	e	13	
2	f	13	
2	g	13	
2	h	13	
2	i	13	
2	j	13	
2	k	13	
2	l	13	
2	m	13	
2	n	13	

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Mol	Chain	Length	Quality of chain
2	o	13	
2	p	13	

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
3	SO4	K	201	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11682 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 Polypyrimidine tract-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	78	Total	C	N	O	S	0	0	0
			614	395	104	112	3			
1	B	77	Total	C	N	O	S	0	0	0
			604	389	101	111	3			
1	C	79	Total	C	N	O	S	0	0	0
			618	397	105	113	3			
1	D	77	Total	C	N	O	S	0	0	0
			609	391	104	111	3			
1	E	75	Total	C	N	O	S	0	0	0
			590	379	99	109	3			
1	F	79	Total	C	N	O	S	0	0	0
			618	397	105	113	3			
1	G	80	Total	C	N	O	S	0	0	0
			632	406	107	116	3			
1	H	77	Total	C	N	O	S	0	0	0
			607	390	103	111	3			
1	I	77	Total	C	N	O	S	0	1	0
			608	391	102	112	3			
1	J	78	Total	C	N	O	S	0	0	0
			611	392	104	112	3			
1	K	83	Total	C	N	O	S	0	0	0
			656	422	111	120	3			
1	L	77	Total	C	N	O	S	0	0	0
			609	391	104	111	3			
1	M	77	Total	C	N	O	S	0	0	0
			604	387	103	111	3			
1	N	80	Total	C	N	O	S	0	0	0
			636	409	108	116	3			
1	O	78	Total	C	N	O	S	0	0	0
			616	396	105	112	3			
1	P	73	Total	C	N	O	S	0	0	0
			576	372	96	105	3			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	GLY	-	expression tag	UNP P26599
A	56	PRO	-	expression tag	UNP P26599
B	55	GLY	-	expression tag	UNP P26599
B	56	PRO	-	expression tag	UNP P26599
C	55	GLY	-	expression tag	UNP P26599
C	56	PRO	-	expression tag	UNP P26599
D	55	GLY	-	expression tag	UNP P26599
D	56	PRO	-	expression tag	UNP P26599
E	55	GLY	-	expression tag	UNP P26599
E	56	PRO	-	expression tag	UNP P26599
F	55	GLY	-	expression tag	UNP P26599
F	56	PRO	-	expression tag	UNP P26599
G	55	GLY	-	expression tag	UNP P26599
G	56	PRO	-	expression tag	UNP P26599
H	55	GLY	-	expression tag	UNP P26599
H	56	PRO	-	expression tag	UNP P26599
I	55	GLY	-	expression tag	UNP P26599
I	56	PRO	-	expression tag	UNP P26599
J	55	GLY	-	expression tag	UNP P26599
J	56	PRO	-	expression tag	UNP P26599
K	55	GLY	-	expression tag	UNP P26599
K	56	PRO	-	expression tag	UNP P26599
L	55	GLY	-	expression tag	UNP P26599
L	56	PRO	-	expression tag	UNP P26599
M	55	GLY	-	expression tag	UNP P26599
M	56	PRO	-	expression tag	UNP P26599
N	55	GLY	-	expression tag	UNP P26599
N	56	PRO	-	expression tag	UNP P26599
O	55	GLY	-	expression tag	UNP P26599
O	56	PRO	-	expression tag	UNP P26599
P	55	GLY	-	expression tag	UNP P26599
P	56	PRO	-	expression tag	UNP P26599

- Molecule 2 is a protein called Ligand.

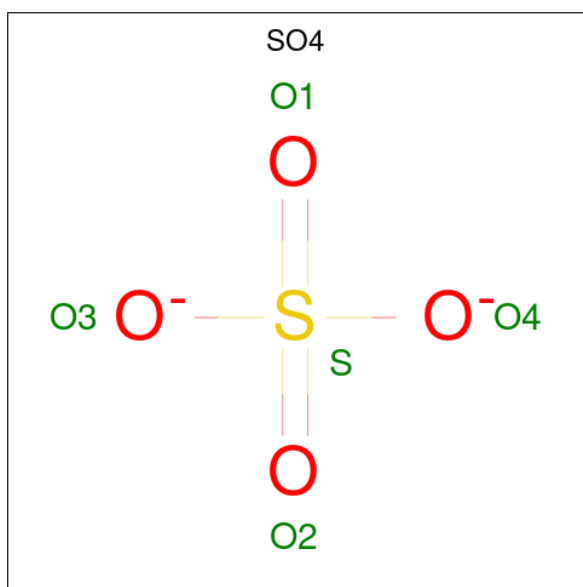
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	a	13	Total 109	C 70	N 21	O 18	0	0	0
2	b	13	Total 109	C 70	N 21	O 18	0	0	0
2	c	13	Total 109	C 70	N 21	O 18	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	d	13	Total	C	N	O	0	0	0
			109	70	21	18			
2	e	13	Total	C	N	O	0	0	0
			109	70	21	18			
2	f	13	Total	C	N	O	0	0	0
			109	70	21	18			
2	g	13	Total	C	N	O	0	0	0
			109	70	21	18			
2	h	13	Total	C	N	O	0	0	0
			109	70	21	18			
2	i	13	Total	C	N	O	0	0	0
			109	70	21	18			
2	j	13	Total	C	N	O	0	0	0
			109	70	21	18			
2	k	13	Total	C	N	O	0	0	0
			109	70	21	18			
2	l	13	Total	C	N	O	0	0	0
			109	70	21	18			
2	m	13	Total	C	N	O	0	0	0
			109	70	21	18			
2	n	13	Total	C	N	O	0	0	0
			109	70	21	18			
2	o	13	Total	C	N	O	0	0	0
			109	70	21	18			
2	p	13	Total	C	N	O	0	0	0
			109	70	21	18			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



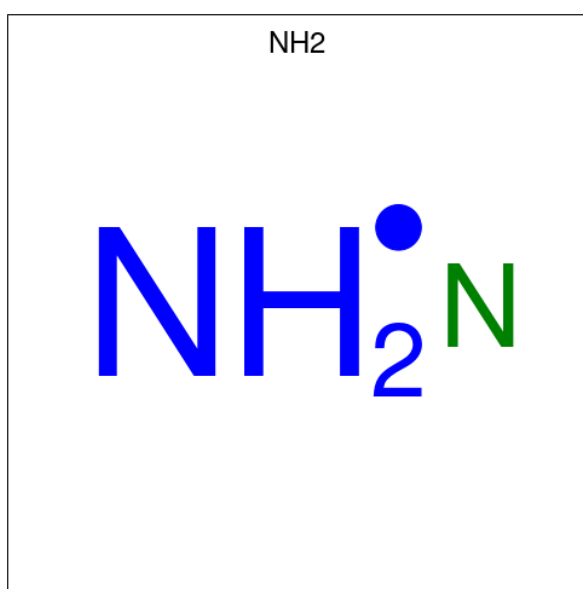
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	g	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is AMINO GROUP (CCD ID: NH2) (formula: H₂N).



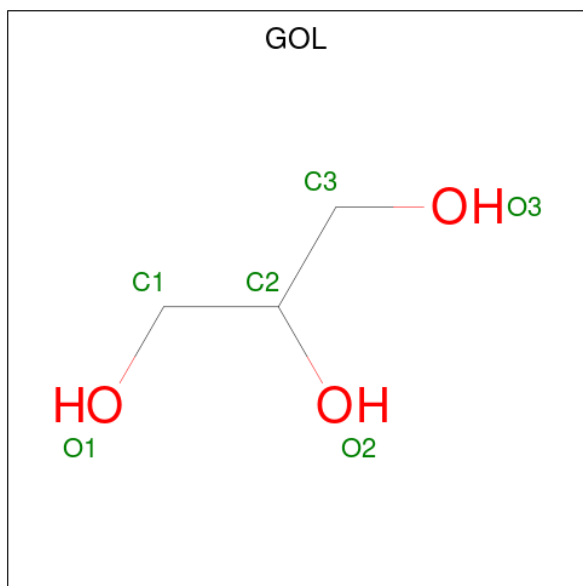
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	a	1	Total	N	0	0
			1	1		
4	b	1	Total	N	0	0
			1	1		
4	c	1	Total	N	0	0
			1	1		
4	d	1	Total	N	0	0
			1	1		
4	e	1	Total	N	0	0
			1	1		
4	f	1	Total	N	0	0
			1	1		
4	g	1	Total	N	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	h	1	Total N 1 1	0	0
4	i	1	Total N 1 1	0	0
4	j	1	Total N 1 1	0	0
4	k	1	Total N 1 1	0	0
4	l	1	Total N 1 1	0	0
4	m	1	Total N 1 1	0	0
4	n	1	Total N 1 1	0	0
4	o	1	Total N 1 1	0	0
4	p	1	Total N 1 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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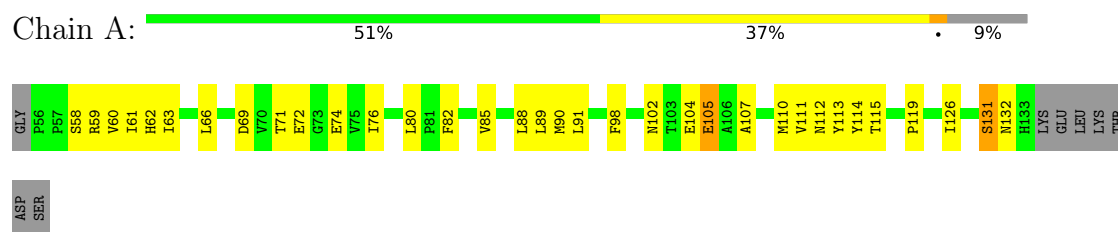
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	I	1	Total	C	O	0	0
			6	3	3		
5	i	1	Total	C	O	0	0
			6	3	3		

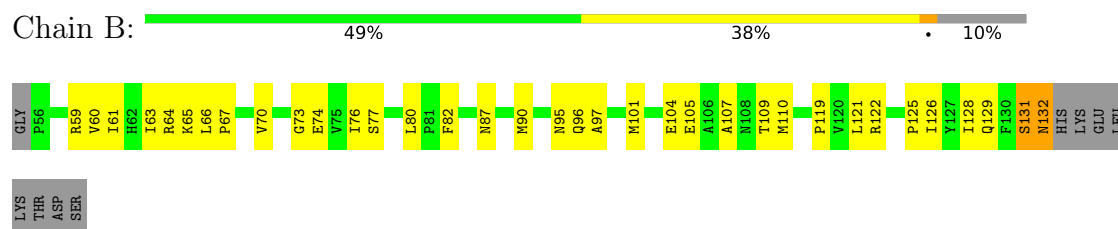
3 Residue-property plots

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.

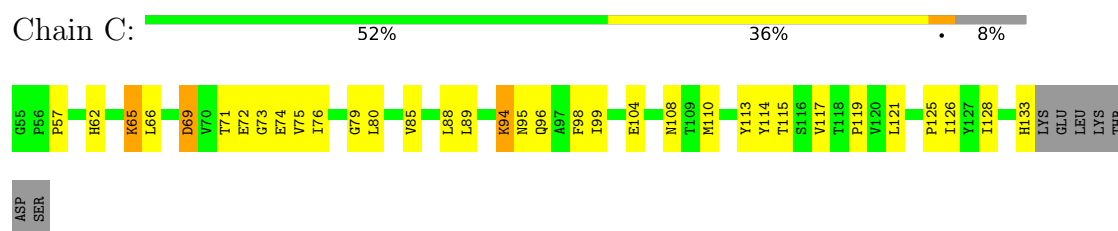
• Molecule 1: Polypyrimidine tract-binding protein 1



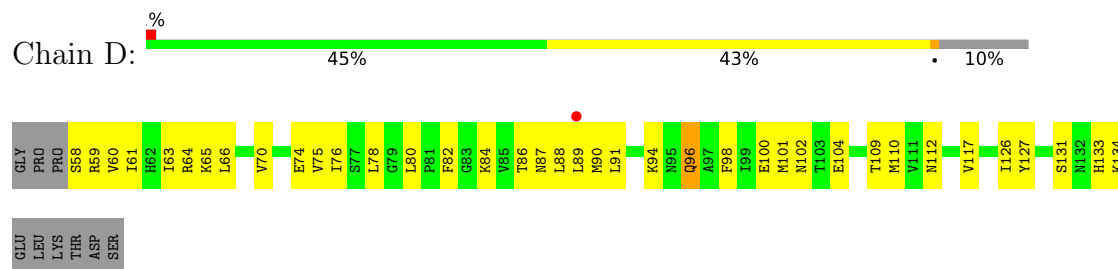
• Molecule 1: Polypyrimidine tract-binding protein 1



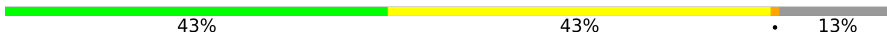
• Molecule 1: Polypyrimidine tract-binding protein 1

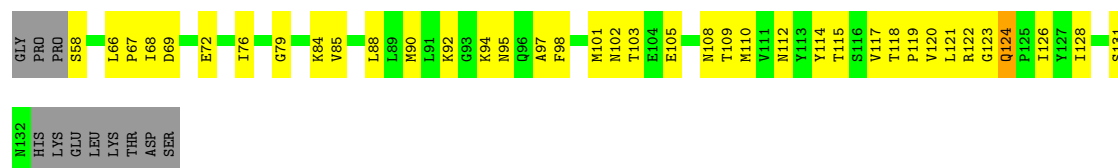


• Molecule 1: Polypyrimidine tract-binding protein 1

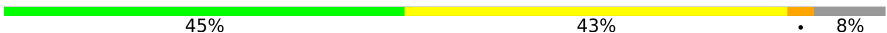


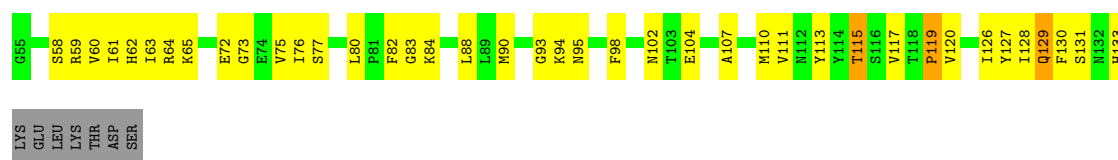
- Molecule 1: Polypyrimidine tract-binding protein 1

Chain E: 



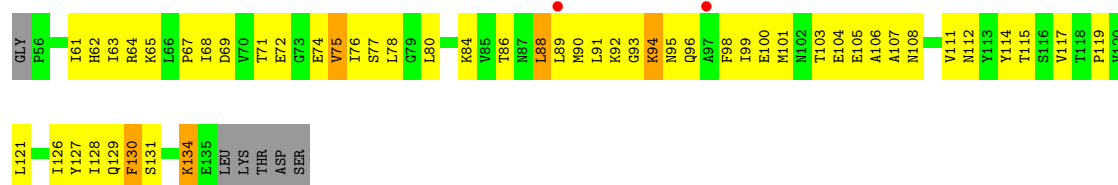
- Molecule 1: Polypyrimidine tract-binding protein 1

Chain F: 



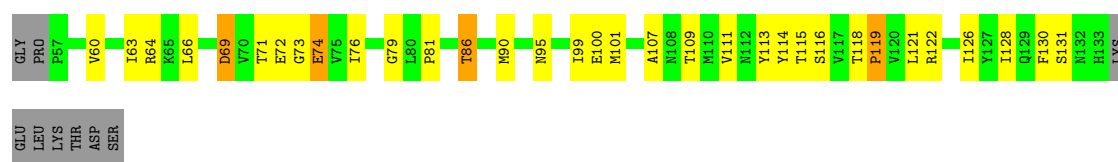
- Molecule 1: Polypyrimidine tract-binding protein 1

Chain G: 

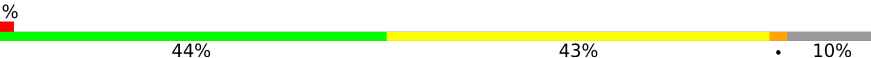


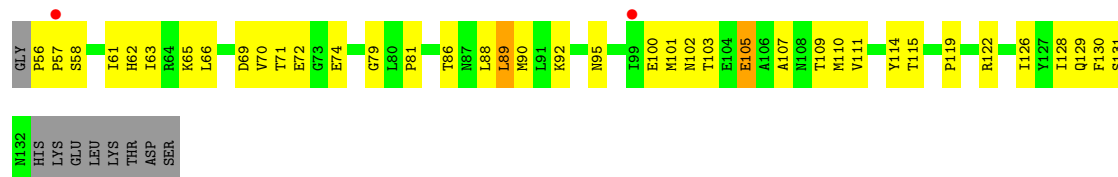
- Molecule 1: Polypyrimidine tract-binding protein 1

Chain H: 

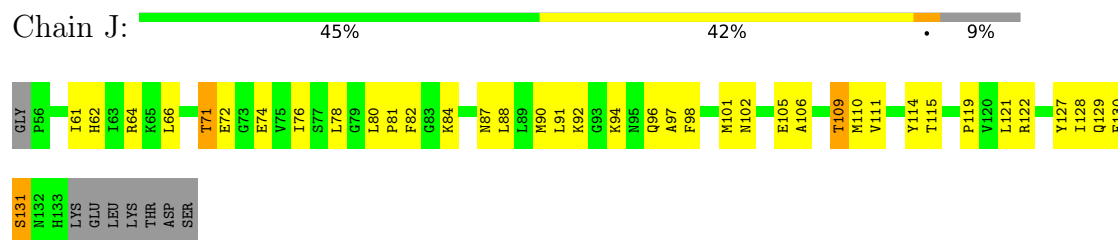


- Molecule 1: Polypyrimidine tract-binding protein 1

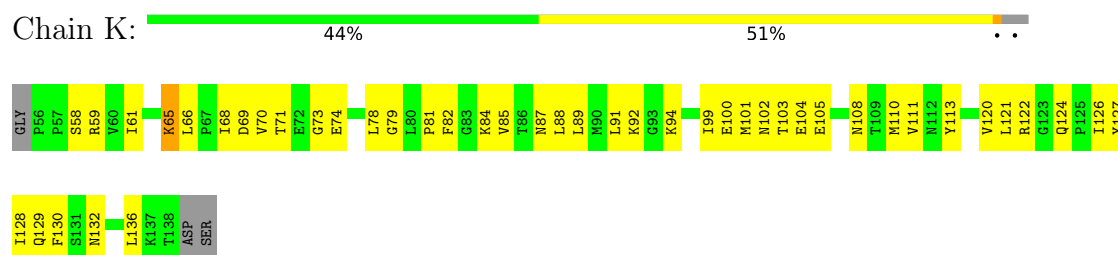
Chain I: 



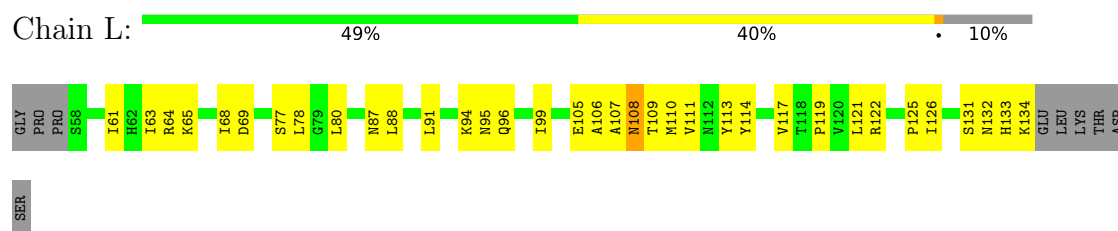
- Molecule 1: Polypyrimidine tract-binding protein 1



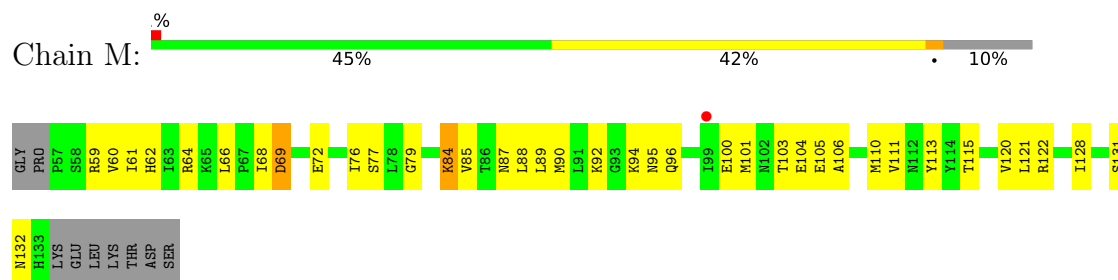
- Molecule 1: Polypyrimidine tract-binding protein 1



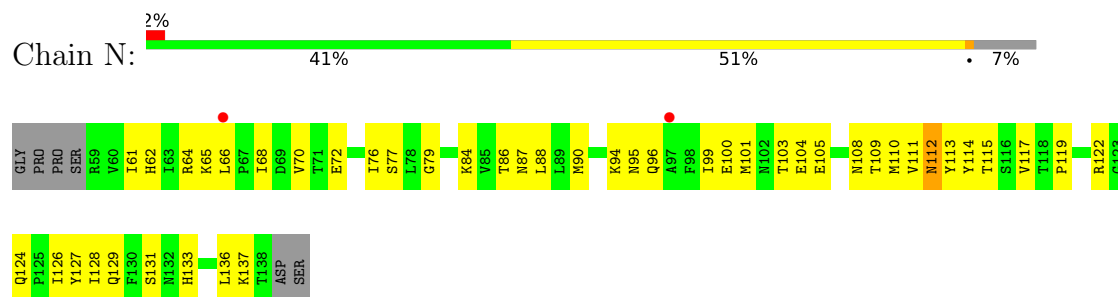
- Molecule 1: Polypyrimidine tract-binding protein 1



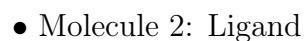
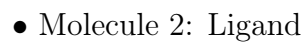
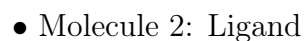
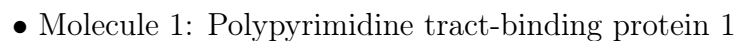
- Molecule 1: Polypyrimidine tract-binding protein 1

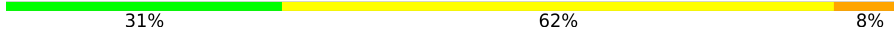


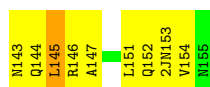
- Molecule 1: Polypyrimidine tract-binding protein 1



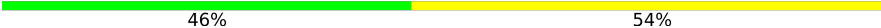
- Molecule 1: Polypyrimidine tract-binding protein 1



Chain e:  31% 62% 8%



• Molecule 2: Ligand

Chain f:  46% 54%



• Molecule 2: Ligand

Chain g:  69% 31%



• Molecule 2: Ligand

Chain h:  77% 23%

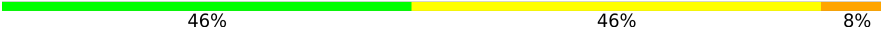


• Molecule 2: Ligand

Chain i:  62% 38%



• Molecule 2: Ligand

Chain j:  46% 46% 8%

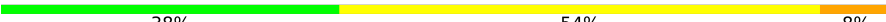


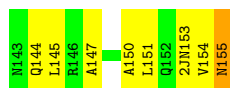
• Molecule 2: Ligand

Chain k:  62% 31% 8%



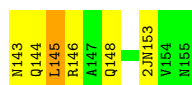
● Molecule 2: Ligand

Chain l:  38% 54% 8%



● Molecule 2: Ligand

Chain m:  54% 38% 8%

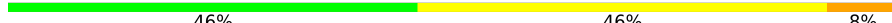


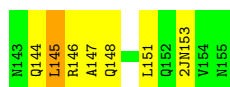
● Molecule 2: Ligand

Chain n:  38% 54% 8%



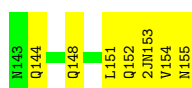
● Molecule 2: Ligand

Chain o:  46% 46% 8%



● Molecule 2: Ligand

Chain p:  46% 54%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	244.20Å 76.63Å 94.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.21 – 2.90 46.21 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.21-2.90) 99.4 (46.21-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.243 , 0.340 0.243 , 0.341	Depositor DCC
R_{free} test set	1992 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	97.1	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 75.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11682	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: GOL, 2JN, NH2, S9X, SO4, MK8

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	0.53	0/627	0.68	0/851
1	B	0.56	0/616	0.76	0/836
1	C	0.49	0/631	0.66	0/857
1	D	0.45	0/620	0.66	0/839
1	E	0.50	0/600	0.67	0/813
1	F	0.70	1/631 (0.2%)	0.91	2/857 (0.2%)
1	G	0.47	0/645	0.72	0/874
1	H	0.63	1/619 (0.2%)	0.76	1/839 (0.1%)
1	I	0.46	0/620	0.66	0/841
1	J	0.44	0/623	0.66	0/844
1	K	0.56	0/669	0.80	0/906
1	L	0.51	0/620	0.74	0/839
1	M	0.49	0/615	0.75	0/833
1	N	0.49	0/647	0.70	0/875
1	O	0.49	0/628	0.69	0/850
1	P	0.46	0/586	0.73	0/794
2	a	0.61	0/75	0.78	0/95
2	b	0.68	0/75	0.75	0/95
2	c	0.52	0/75	0.71	0/95
2	d	0.52	0/75	0.63	0/95
2	e	0.45	0/75	0.86	0/95
2	f	0.67	0/75	0.73	0/95
2	g	0.68	0/75	0.69	0/95
2	h	0.57	0/75	0.85	0/95
2	i	0.47	0/75	0.57	0/95
2	j	0.53	0/75	0.66	0/95
2	k	0.53	0/75	0.65	0/95
2	l	0.61	0/75	0.82	0/95
2	m	0.64	0/75	0.66	0/95
2	n	0.61	0/75	0.76	0/95
2	o	0.65	0/75	0.77	0/95
2	p	0.51	0/75	0.73	0/95

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.53	2/11197 (0.0%)	0.73	3/15068 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	119	PRO	N-CD	-5.59	1.40	1.47
1	F	119	PRO	CB-CG	-5.23	1.23	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	119	PRO	N-CD-CG	-10.51	87.44	103.20
1	H	119	PRO	N-CD-CG	-7.61	91.78	103.20
1	F	119	PRO	CA-N-CD	-5.56	104.22	112.00

There are no chirality outliers.

There are no planarity outliers.

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	614	0	631	31	0
1	B	604	0	624	31	0
1	C	618	0	633	30	0
1	D	609	0	629	30	0
1	E	590	0	609	40	0
1	F	618	0	633	40	0
1	G	632	0	650	47	1
1	H	607	0	624	26	0
1	I	608	0	626	36	0
1	J	611	0	624	37	0
1	K	656	0	681	45	0
1	L	609	0	629	31	0
1	M	604	0	617	32	0
1	N	636	0	661	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	616	0	637	42	0
1	P	576	0	598	50	0
2	a	109	0	94	8	0
2	b	109	0	93	7	0
2	c	109	0	93	14	0
2	d	109	0	92	6	0
2	e	109	0	94	12	0
2	f	109	0	95	5	0
2	g	109	0	94	5	0
2	h	109	0	94	1	0
2	i	109	0	93	3	0
2	j	109	0	93	4	0
2	k	109	0	93	4	0
2	l	109	0	94	6	0
2	m	109	0	93	5	0
2	n	109	0	95	6	0
2	o	109	0	94	7	0
2	p	109	0	93	7	0
3	A	25	0	0	0	1
3	C	5	0	0	1	0
3	D	10	0	0	0	0
3	F	10	0	0	0	0
3	G	10	0	0	1	0
3	H	5	0	0	0	0
3	K	10	0	0	2	0
3	L	5	0	0	0	0
3	O	5	0	0	0	0
3	g	5	0	0	0	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
4	e	1	0	0	0	0
4	f	1	0	0	1	0
4	g	1	0	0	0	0
4	h	1	0	0	1	0
4	i	1	0	0	0	0
4	j	1	0	0	0	0
4	k	1	0	0	0	0
4	l	1	0	0	0	0
4	m	1	0	0	0	0
4	n	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	o	1	0	0	0	0
4	p	1	0	0	0	0
5	C	6	0	8	0	0
5	F	6	0	8	0	0
5	I	6	0	8	0	0
5	i	6	0	8	0	0
All	All	11682	0	11635	612	1

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 26.

All (612) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:PRO:HD3	1:E:124:GLN:HG2	1.43	0.99
1:H:74:GLU:HG2	1:H:121:LEU:HD11	1.48	0.94
1:F:76:ILE:HD11	1:F:88:LEU:HD12	1.49	0.93
1:K:71:THR:HB	1:K:74:GLU:HG3	1.51	0.92
1:A:61:ILE:HD12	1:A:110:MET:HE3	1.49	0.91
1:M:62:HIS:HD2	1:M:132:ASN:HB2	1.36	0.90
1:O:120:VAL:HG13	1:P:81:PRO:HB3	1.55	0.87
1:O:63:ILE:HD11	1:O:126:ILE:HD13	1.58	0.85
1:I:69:ASP:OD1	1:I:122:ARG:NH1	2.12	0.83
2:c:146:ARG:HE	2:e:152:GLN:HG2	1.42	0.82
1:M:61:ILE:HG12	1:M:110:MET:HE3	1.64	0.79
1:O:63:ILE:HG23	1:O:66:LEU:HD21	1.64	0.79
1:H:66:LEU:O	1:H:95:ASN:ND2	2.16	0.77
1:K:79:GLY:HA2	1:K:110:MET:CE	2.13	0.77
1:K:66:LEU:HG	1:K:70:VAL:HG11	1.67	0.77
1:E:69:ASP:O	1:E:122:ARG:NH1	2.19	0.76
1:J:71:THR:HG23	1:J:74:GLU:H	1.50	0.76
1:K:85:VAL:HG22	1:K:101:MET:HE1	1.67	0.76
1:P:104:GLU:OE2	1:P:107:ALA:HB3	1.85	0.76
1:I:79:GLY:HA2	1:I:110:MET:HE1	1.68	0.75
1:N:94:LYS:HD3	1:N:96:GLN:NE2	2.01	0.75
1:P:64:ARG:HG2	1:P:96:GLN:HG3	1.67	0.75
1:E:79:GLY:HA2	1:E:110:MET:HE1	1.67	0.75
1:E:88:LEU:H	2:e:151:LEU:HD11	1.52	0.75
1:C:85:VAL:O	2:c:155:ASN:ND2	2.19	0.75
1:G:92:LYS:HD2	1:G:93:GLY:N	2.02	0.74
1:M:105:GLU:OE2	1:M:105:GLU:N	2.14	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:PHE:HD1	1:G:131:SER:H	1.34	0.73
1:L:119:PRO:HB2	1:L:126:ILE:HG13	1.71	0.73
1:P:75:VAL:HG21	1:P:90:MET:HE1	1.71	0.73
1:E:85:VAL:HG22	1:E:101:MET:HE1	1.70	0.73
1:B:59:ARG:HG3	1:B:104:GLU:HG2	1.69	0.72
1:A:66:LEU:HD23	1:A:126:ILE:HG21	1.70	0.72
1:D:82:PHE:CD1	1:D:110:MET:HG3	2.24	0.72
1:E:72:GLU:O	1:E:76:ILE:HD12	1.90	0.71
1:L:91:LEU:HD22	1:L:96:GLN:HG3	1.71	0.71
1:A:114:TYR:HB3	1:A:119:PRO:HG3	1.70	0.71
1:G:72:GLU:HA	1:G:90:MET:HE2	1.72	0.71
1:K:88:LEU:HD13	1:K:99:ILE:HG22	1.73	0.71
1:D:59:ARG:HH21	1:D:102:ASN:HA	1.55	0.71
1:P:70:VAL:HG11	1:P:121:LEU:HD13	1.71	0.71
1:B:105:GLU:O	1:B:109:THR:HG23	1.91	0.71
1:F:77:SER:HA	1:F:80:LEU:HD12	1.73	0.70
1:M:111:VAL:HG12	1:M:128:ILE:HG22	1.72	0.70
1:D:112:ASN:HD21	1:G:112:ASN:HD21	1.39	0.70
1:G:104:GLU:O	1:G:107:ALA:N	2.25	0.70
1:E:66:LEU:O	1:E:95:ASN:ND2	2.25	0.69
1:M:84:LYS:HZ3	1:M:85:VAL:H	1.38	0.69
2:m:144:GLN:HG2	2:m:148:GLN:HE21	1.56	0.69
1:I:111:VAL:O	1:I:115:THR:HG23	1.92	0.69
1:C:114:TYR:HB3	1:C:119:PRO:HG3	1.73	0.69
1:H:111:VAL:HG11	1:H:130:PHE:CZ	2.27	0.69
1:P:61:ILE:HB	1:P:99:ILE:HG23	1.75	0.69
1:K:61:ILE:HD11	1:K:99:ILE:HG12	1.75	0.69
1:P:114:TYR:HA	1:P:117:VAL:HG12	1.74	0.69
1:B:105:GLU:OE1	1:G:65:LYS:HD2	1.93	0.69
1:L:61:ILE:HD12	1:L:110:MET:HE3	1.75	0.69
1:D:60:VAL:HB	1:D:131:SER:HB2	1.74	0.69
1:K:59:ARG:NH1	1:K:100:GLU:OE2	2.26	0.68
1:O:72:GLU:OE2	2:o:146:ARG:NH1	2.26	0.68
1:N:64:ARG:HG2	1:N:96:GLN:HG2	1.75	0.68
1:L:114:TYR:HB3	1:L:119:PRO:HG3	1.75	0.67
1:N:61:ILE:HG13	1:N:129:GLN:O	1.93	0.67
1:C:80:LEU:HD21	2:c:154:VAL:HG21	1.75	0.67
1:G:114:TYR:CD1	1:G:119:PRO:HG3	2.30	0.67
1:A:62:HIS:HD2	1:A:63:ILE:H	1.41	0.67
1:K:79:GLY:HA2	1:K:110:MET:HE1	1.76	0.66
1:I:114:TYR:HB2	1:I:128:ILE:HG12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ARG:NH1	3:C:201:SO4:O3	2.28	0.66
1:H:86:THR:OG1	1:H:100:GLU:OE1	2.12	0.66
1:J:84:LYS:H	1:J:101:MET:HE1	1.61	0.66
1:N:136:LEU:C	1:N:137:LYS:HD3	2.21	0.66
1:G:78:LEU:HD21	1:G:126:ILE:HD12	1.76	0.66
1:J:64:ARG:HH12	1:J:94:LYS:HE2	1.60	0.66
1:O:103:THR:HG23	1:O:106:ALA:H	1.60	0.66
2:g:154:VAL:HA	1:H:73:GLY:HA3	1.79	0.65
1:J:88:LEU:HD21	1:J:90:MET:HG3	1.77	0.65
1:P:79:GLY:HA2	1:P:82:PHE:HD1	1.61	0.65
1:B:66:LEU:HD22	1:B:70:VAL:HG21	1.79	0.65
1:G:121:LEU:HG	1:G:126:ILE:HD13	1.79	0.65
1:B:132:ASN:OD1	1:B:132:ASN:N	2.29	0.65
1:G:94:LYS:HB3	1:G:96:GLN:HE21	1.63	0.64
1:E:79:GLY:HA2	1:E:110:MET:CE	2.26	0.64
1:A:105:GLU:N	1:A:105:GLU:OE1	2.29	0.64
2:a:152:GLN:HE22	4:n:201:NH2:N	1.96	0.64
1:K:100:GLU:HB2	1:K:136:LEU:HD23	1.77	0.64
2:o:144:GLN:CD	2:o:144:GLN:H	2.04	0.64
1:N:94:LYS:HD3	1:N:96:GLN:HE21	1.60	0.64
1:I:58:SER:H	1:I:130:PHE:HZ	1.44	0.64
1:A:61:ILE:HD12	1:A:110:MET:CE	2.25	0.64
1:F:72:GLU:HG3	1:F:90:MET:HE2	1.78	0.64
1:M:69:ASP:OD1	1:M:69:ASP:N	2.18	0.64
1:P:88:LEU:HB3	2:p:151:LEU:HD11	1.78	0.64
1:K:108:ASN:HA	1:K:130:PHE:HZ	1.63	0.64
1:N:112:ASN:HD21	1:P:124:GLN:HG3	1.63	0.64
1:F:119:PRO:HB3	1:F:128:ILE:HD13	1.80	0.64
1:G:71:THR:OG1	1:G:74:GLU:HG3	1.98	0.64
1:L:77:SER:HA	1:L:80:LEU:HG	1.79	0.64
1:P:64:ARG:HB2	1:P:127:TYR:HB2	1.79	0.64
1:B:63:ILE:HD13	1:B:128:ILE:HG22	1.80	0.63
1:I:66:LEU:HB3	1:I:70:VAL:HG11	1.79	0.63
1:O:111:VAL:HA	1:O:128:ILE:HD13	1.78	0.63
1:O:115:THR:O	1:O:127:TYR:OH	2.15	0.63
2:o:147:ALA:O	2:o:151:LEU:HD12	1.99	0.63
1:N:111:VAL:O	1:N:115:THR:HG23	1.99	0.63
1:M:69:ASP:O	1:M:122:ARG:NH2	2.31	0.63
1:A:80:LEU:HD21	2:a:154:VAL:HG11	1.81	0.63
1:N:104:GLU:O	1:N:108:ASN:ND2	2.32	0.63
1:G:119:PRO:HB2	1:G:126:ILE:HD11	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:101:MET:HE3	1:J:102:ASN:H	1.62	0.62
1:K:94:LYS:HD3	1:K:94:LYS:N	2.14	0.62
2:c:146:ARG:HG3	2:c:146:ARG:HH11	1.64	0.62
1:B:105:GLU:HB3	1:G:127:TYR:CD1	2.34	0.62
1:M:60:VAL:HG21	1:M:101:MET:HG3	1.81	0.62
1:J:114:TYR:HB3	1:J:119:PRO:HG3	1.81	0.62
1:M:103:THR:HG22	1:M:106:ALA:H	1.64	0.62
1:I:114:TYR:HB3	1:I:119:PRO:HG3	1.80	0.61
1:N:62:HIS:HB3	1:N:129:GLN:HG3	1.82	0.61
1:K:78:LEU:HD21	1:K:121:LEU:HD11	1.82	0.61
1:M:60:VAL:HG22	1:M:100:GLU:HA	1.82	0.61
2:f:143:ASN:HB3	2:f:146:ARG:CZ	2.30	0.61
1:G:84:LYS:H	1:G:84:LYS:HD2	1.65	0.61
1:K:71:THR:HG22	1:K:73:GLY:N	2.15	0.61
1:O:69:ASP:OD1	1:O:122:ARG:NH1	2.29	0.61
1:P:82:PHE:HD2	1:P:109:THR:HG23	1.66	0.61
1:G:129:GLN:HG2	1:G:130:PHE:N	2.16	0.60
1:K:121:LEU:HD12	1:K:126:ILE:HD13	1.83	0.60
1:N:84:LYS:NZ	2:n:155:ASN:OD1	2.25	0.60
1:E:79:GLY:CA	1:E:110:MET:HE1	2.31	0.60
1:K:92:LYS:HD2	3:K:201:SO4:O3	2.01	0.60
1:N:61:ILE:HD11	1:N:128:ILE:HG23	1.82	0.60
1:P:66:LEU:N	1:P:95:ASN:HB3	2.16	0.60
1:N:66:LEU:HD12	1:N:70:VAL:HG21	1.82	0.60
1:G:119:PRO:O	1:G:126:ILE:HG12	2.02	0.60
1:P:61:ILE:HD11	1:P:107:ALA:HB1	1.82	0.60
1:A:85:VAL:HG12	2:a:151:LEU:HD21	1.84	0.59
1:A:112:ASN:O	1:A:115:THR:OG1	2.20	0.59
1:E:68:ILE:HD12	1:E:95:ASN:ND2	2.17	0.59
1:M:68:ILE:HD13	1:M:95:ASN:ND2	2.17	0.59
1:F:72:GLU:HG3	1:F:90:MET:CE	2.32	0.59
1:K:102:ASN:ND2	1:K:103:THR:HG23	2.18	0.59
1:P:93:GLY:C	1:P:95:ASN:H	2.10	0.59
2:m:144:GLN:HG2	2:m:148:GLN:NE2	2.16	0.59
1:N:72:GLU:HG3	1:N:90:MET:HE2	1.85	0.59
1:O:79:GLY:HA2	1:O:110:MET:HE3	1.85	0.59
1:A:59:ARG:HH22	1:M:92:LYS:HE3	1.67	0.59
1:D:88:LEU:HD21	1:D:90:MET:HG3	1.84	0.59
1:D:64:ARG:HB2	1:D:127:TYR:HB2	1.85	0.59
2:c:146:ARG:NE	2:e:152:GLN:HG2	2.16	0.59
1:J:101:MET:HE2	1:J:106:ALA:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:60:VAL:HG12	1:M:104:GLU:OE2	2.02	0.58
1:D:86:THR:OG1	1:D:100:GLU:HG2	2.02	0.58
1:E:68:ILE:HD12	1:E:95:ASN:HD22	1.68	0.58
1:B:60:VAL:HG13	1:B:131:SER:CB	2.33	0.58
1:G:111:VAL:O	1:G:115:THR:HG23	2.03	0.58
1:A:60:VAL:O	1:A:131:SER:OG	2.21	0.58
1:B:74:GLU:O	1:B:77:SER:OG	2.20	0.58
1:E:109:THR:HG22	1:L:68:ILE:HG12	1.86	0.58
1:F:83:GLY:C	1:F:84:LYS:HD3	2.27	0.58
1:H:69:ASP:HB3	1:H:122:ARG:HH12	1.66	0.58
1:I:129:GLN:HG3	1:I:131:SER:H	1.68	0.58
1:K:128:ILE:HD12	1:K:128:ILE:O	2.03	0.58
1:D:59:ARG:NE	1:D:102:ASN:O	2.37	0.58
1:D:59:ARG:HE	1:D:102:ASN:C	2.12	0.58
1:J:101:MET:HE3	1:J:102:ASN:N	2.19	0.58
1:E:115:THR:HB	1:L:65:LYS:HZ1	1.69	0.58
1:J:105:GLU:O	1:J:109:THR:OG1	2.18	0.58
1:M:76:ILE:HD12	1:M:85:VAL:HG21	1.87	0.57
1:O:119:PRO:HD2	1:O:126:ILE:O	2.05	0.57
1:O:129:GLN:NE2	1:O:130:PHE:O	2.38	0.57
2:a:148:GLN:HB3	2:m:145:MK8:HDA	1.87	0.57
1:G:93:GLY:O	1:G:96:GLN:HG3	2.04	0.57
1:C:88:LEU:N	2:c:151:LEU:HD11	2.20	0.57
1:N:64:ARG:HB3	1:N:65:LYS:HD3	1.87	0.57
1:C:119:PRO:HB2	1:C:126:ILE:HG13	1.87	0.56
1:D:87:ASN:OD1	1:D:88:LEU:N	2.39	0.56
1:K:71:THR:HG22	1:K:73:GLY:H	1.69	0.56
2:l:151:LEU:O	2:l:155:ASN:HB2	2.05	0.56
1:E:66:LEU:C	1:E:95:ASN:HD21	2.13	0.56
1:F:72:GLU:O	1:F:76:ILE:HG12	2.06	0.56
1:H:107:ALA:O	1:H:111:VAL:HG12	2.06	0.56
1:I:79:GLY:HA2	1:I:110:MET:CE	2.34	0.56
1:C:94:LYS:O	1:C:96:GLN:HG3	2.05	0.56
1:F:83:GLY:HA2	1:F:84:LYS:HD3	1.87	0.56
1:G:129:GLN:HG2	1:G:130:PHE:H	1.71	0.55
1:O:62:HIS:HB3	1:O:129:GLN:HG3	1.88	0.55
1:N:136:LEU:O	1:N:137:LYS:HD3	2.06	0.55
1:H:69:ASP:O	1:H:122:ARG:NH2	2.34	0.55
1:J:84:LYS:N	1:J:101:MET:HE1	2.21	0.55
1:N:131:SER:HB2	1:N:133:HIS:O	2.07	0.55
1:H:63:ILE:HB	1:H:128:ILE:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:143:ASN:N	2:e:146:ARG:HB2	2.21	0.55
1:P:61:ILE:HD11	1:P:107:ALA:CB	2.37	0.55
2:g:145:MK8:HGA	2:k:148:GLN:HB3	1.89	0.55
1:K:127:TYR:OH	1:K:129:GLN:OE1	2.23	0.55
1:F:61:ILE:HG22	1:F:63:ILE:CD1	2.36	0.55
2:b:145:MK8:HDA	2:b:145:MK8:C	2.37	0.54
2:f:143:ASN:HB3	2:f:146:ARG:NH2	2.22	0.54
1:A:113:TYR:OH	1:D:117:VAL:HG11	2.07	0.54
1:N:62:HIS:HB2	1:N:131:SER:HA	1.90	0.54
1:N:94:LYS:O	1:N:94:LYS:HG2	2.06	0.54
2:d:145:MK8:HD	2:d:145:MK8:HB1B	1.88	0.54
1:O:111:VAL:HA	1:O:128:ILE:CD1	2.37	0.54
1:D:84:LYS:HD2	1:D:84:LYS:N	2.22	0.54
2:c:150:ALA:O	2:c:154:VAL:HG12	2.08	0.54
1:E:108:ASN:HB3	1:L:68:ILE:HG21	1.90	0.54
1:H:76:ILE:HD13	2:h:151:LEU:HD13	1.90	0.54
1:N:105:GLU:O	1:N:109:THR:OG1	2.26	0.54
1:F:58:SER:OG	1:F:133:HIS:NE2	2.39	0.53
1:L:133:HIS:HB3	1:L:134:LYS:HE3	1.89	0.53
1:M:88:LEU:HD12	1:M:89:LEU:N	2.22	0.53
1:M:94:LYS:HG3	1:M:96:GLN:NE2	2.23	0.53
1:O:112:ASN:O	1:O:115:THR:HG23	2.08	0.53
1:J:62:HIS:HB2	1:J:131:SER:HB2	1.90	0.53
1:C:88:LEU:HD12	1:C:89:LEU:H	1.73	0.53
1:F:62:HIS:CD2	1:F:98:PHE:HE1	2.27	0.53
1:B:64:ARG:HD2	1:B:129:GLN:HE21	1.74	0.53
1:L:99:ILE:HD11	1:L:110:MET:HE1	1.91	0.53
1:C:57:PRO:HG3	1:F:104:GLU:OE1	2.09	0.53
1:O:63:ILE:HG22	1:O:97:ALA:O	2.09	0.53
1:J:72:GLU:HG2	2:j:147:ALA:HA	1.90	0.53
1:B:76:ILE:O	1:B:80:LEU:HD13	2.09	0.52
1:J:62:HIS:N	1:J:129:GLN:O	2.42	0.52
2:j:144:GLN:O	2:j:147:ALA:HB3	2.09	0.52
1:D:65:LYS:HD3	1:D:127:TYR:CE2	2.43	0.52
1:O:60:VAL:HG13	1:O:131:SER:HB2	1.92	0.52
1:O:71:THR:O	1:O:75:VAL:HG23	2.08	0.52
1:E:115:THR:HB	1:L:65:LYS:NZ	2.24	0.52
1:F:119:PRO:O	1:F:126:ILE:HG12	2.08	0.52
1:I:62:HIS:HB3	1:I:129:GLN:HB3	1.91	0.52
1:P:111:VAL:HG13	1:P:128:ILE:HG23	1.91	0.52
1:B:60:VAL:HG13	1:B:131:SER:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:VAL:O	1:C:99:ILE:HD11	2.09	0.52
1:D:80:LEU:HD11	2:d:154:VAL:HB	1.92	0.52
1:I:101:MET:HE2	1:I:110:MET:CE	2.40	0.52
1:I:103:THR:OG1	1:I:105:GLU:HG3	2.10	0.52
2:b:145:MK8:HB1A	2:b:148:GLN:HB2	1.90	0.52
1:F:82:PHE:CD2	1:F:110:MET:HA	2.45	0.52
2:f:144:GLN:N	2:f:144:GLN:OE1	2.41	0.52
2:o:145:MK8:HB1A	2:o:148:GLN:HB2	1.92	0.52
1:P:117:VAL:HG22	1:P:118:THR:H	1.75	0.52
1:C:113:TYR:CE2	1:C:117:VAL:HG21	2.45	0.51
1:G:62:HIS:CG	1:G:98:PHE:HE2	2.28	0.51
1:I:102:ASN:ND2	1:P:69:ASP:OD1	2.43	0.51
1:E:76:ILE:HG23	1:E:85:VAL:HG21	1.92	0.51
1:H:72:GLU:O	1:H:76:ILE:HG13	2.10	0.51
1:I:56:PRO:O	1:I:130:PHE:HE2	1.93	0.51
1:A:102:ASN:OD1	1:A:102:ASN:N	2.43	0.51
2:b:153:2JN:H9	2:c:149:S9X:CD1	2.40	0.51
2:e:154:VAL:HA	1:J:71:THR:HG21	1.92	0.51
1:G:67:PRO:HG3	1:G:121:LEU:O	2.11	0.51
1:E:84:LYS:O	1:E:102:ASN:ND2	2.43	0.51
1:G:86:THR:HG22	1:G:100:GLU:OE1	2.10	0.51
1:O:65:LYS:HB2	1:O:126:ILE:HA	1.91	0.51
1:B:73:GLY:HA3	2:c:154:VAL:HA	1.93	0.51
1:C:71:THR:HG23	1:C:74:GLU:H	1.76	0.51
1:F:119:PRO:HB2	1:F:126:ILE:HG13	1.92	0.51
1:L:63:ILE:HD11	1:L:99:ILE:HG12	1.92	0.51
1:A:89:LEU:HD23	1:A:98:PHE:CD1	2.44	0.51
1:F:64:ARG:HH21	1:F:65:LYS:NZ	2.09	0.51
1:K:81:PRO:HB2	1:K:82:PHE:CE1	2.46	0.51
1:B:80:LEU:HD21	2:b:154:VAL:HG13	1.93	0.51
1:A:62:HIS:CD2	1:A:63:ILE:H	2.26	0.51
1:C:88:LEU:HD12	1:C:89:LEU:N	2.26	0.51
1:I:57:PRO:HA	1:I:130:PHE:HZ	1.76	0.51
1:I:101:MET:HE2	1:I:110:MET:HE3	1.93	0.51
2:n:143:ASN:HB3	2:n:144:GLN:OE1	2.11	0.51
1:P:113:TYR:O	1:P:117:VAL:N	2.44	0.51
1:A:59:ARG:HG3	1:A:104:GLU:HG2	1.94	0.50
1:B:64:ARG:HB3	1:B:65:LYS:HE2	1.93	0.50
1:H:119:PRO:HB2	1:H:126:ILE:HG12	1.93	0.50
1:I:128:ILE:O	1:I:128:ILE:HD12	2.11	0.50
1:K:92:LYS:HE3	3:K:201:SO4:O4	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:82:PHE:CD2	1:P:109:THR:HG23	2.45	0.50
1:L:80:LEU:HD11	2:l:154:VAL:HG22	1.93	0.50
1:P:85:VAL:HG13	1:P:99:ILE:HG13	1.94	0.50
2:p:144:GLN:O	2:p:148:GLN:HG2	2.11	0.50
1:B:60:VAL:HG13	1:B:131:SER:HB3	1.93	0.50
1:K:104:GLU:O	1:K:104:GLU:HG2	2.11	0.50
1:E:105:GLU:O	1:E:109:THR:HG23	2.11	0.50
4:f:201:NH2:N	2:i:146:ARG:HH21	2.09	0.50
1:K:105:GLU:H	1:K:105:GLU:CD	2.19	0.50
1:O:122:ARG:HG2	1:P:83:GLY:O	2.11	0.50
1:A:76:ILE:O	1:A:80:LEU:HD13	2.11	0.50
1:C:128:ILE:HD12	1:C:128:ILE:O	2.11	0.50
1:M:62:HIS:CD2	1:M:132:ASN:HB2	2.29	0.50
1:F:120:VAL:HG22	1:I:81:PRO:O	2.12	0.50
1:P:119:PRO:O	1:P:125:PRO:HA	2.12	0.50
1:O:106:ALA:HA	1:O:109:THR:HG22	1.92	0.50
1:F:82:PHE:HD2	1:F:110:MET:CG	2.24	0.49
1:B:64:ARG:HG2	1:B:96:GLN:HG2	1.94	0.49
1:O:76:ILE:HD11	2:o:151:LEU:HG	1.94	0.49
1:O:128:ILE:HD12	1:O:128:ILE:O	2.12	0.49
1:E:66:LEU:HD21	1:E:121:LEU:HD23	1.94	0.49
1:K:66:LEU:HD23	1:K:70:VAL:HG21	1.95	0.49
1:K:81:PRO:HB2	1:K:82:PHE:CD1	2.47	0.49
2:k:145:MK8:HB1A	2:k:148:GLN:HB2	1.93	0.49
1:D:66:LEU:HD23	1:D:96:GLN:HA	1.93	0.49
1:H:114:TYR:HB3	1:H:119:PRO:HG3	1.94	0.49
1:K:87:ASN:HB3	1:K:136:LEU:HD23	1.92	0.49
1:M:120:VAL:HG13	1:M:120:VAL:O	2.12	0.49
1:O:114:TYR:CD2	1:O:119:PRO:HG3	2.48	0.49
1:G:88:LEU:HD12	1:G:89:LEU:N	2.26	0.49
1:M:59:ARG:NH2	1:M:87:ASN:HD22	2.11	0.49
1:N:76:ILE:HD11	1:N:88:LEU:HD22	1.94	0.49
1:N:86:THR:HB	1:N:100:GLU:HG2	1.94	0.49
2:c:144:GLN:O	2:c:148:GLN:HG2	2.12	0.49
1:A:107:ALA:O	1:A:110:MET:HB2	2.13	0.49
1:E:85:VAL:HG22	1:E:101:MET:CE	2.41	0.49
1:F:83:GLY:CA	1:F:84:LYS:HD3	2.42	0.49
1:F:119:PRO:HB2	1:F:126:ILE:CG1	2.43	0.49
1:D:84:LYS:HD3	1:D:102:ASN:ND2	2.28	0.49
1:F:76:ILE:CD1	1:F:88:LEU:HD12	2.33	0.49
1:H:60:VAL:HA	1:H:99:ILE:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:66:LEU:HD12	1:I:95:ASN:O	2.12	0.49
1:B:67:PRO:HG2	1:B:121:LEU:CD2	2.43	0.49
1:L:87:ASN:HA	2:l:151:LEU:HD11	1.95	0.49
1:M:113:TYR:HH	1:N:113:TYR:HH	1.60	0.49
1:G:91:LEU:HB2	1:G:96:GLN:O	2.12	0.48
1:M:79:GLY:HA2	1:M:110:MET:SD	2.53	0.48
1:N:79:GLY:HA2	1:N:110:MET:HE1	1.95	0.48
2:p:152:GLN:HA	2:p:155:ASN:HB2	1.94	0.48
1:J:111:VAL:O	1:J:115:THR:OG1	2.30	0.48
1:K:91:LEU:HD23	1:K:91:LEU:HA	1.63	0.48
1:L:61:ILE:HD12	1:L:110:MET:CE	2.41	0.48
1:L:107:ALA:O	1:L:111:VAL:HG23	2.13	0.48
1:B:74:GLU:HG2	1:C:80:LEU:HD12	1.94	0.48
1:J:111:VAL:HG23	1:J:128:ILE:HD11	1.95	0.48
1:N:66:LEU:O	1:N:95:ASN:HB3	2.14	0.48
1:G:64:ARG:NH2	3:G:202:SO4:S	2.87	0.48
1:H:71:THR:OG1	1:H:74:GLU:HB2	2.13	0.48
2:l:144:GLN:O	2:l:145:MK8:C	2.61	0.48
1:K:61:ILE:HG22	1:K:130:PHE:HA	1.95	0.48
1:M:111:VAL:O	1:M:115:THR:HG23	2.13	0.48
1:P:72:GLU:HG3	1:P:90:MET:HG3	1.95	0.48
1:F:127:TYR:C	1:F:128:ILE:HD12	2.39	0.48
1:D:75:VAL:O	1:D:78:LEU:HB2	2.14	0.48
1:O:76:ILE:HG13	1:O:88:LEU:HD12	1.95	0.48
1:E:114:TYR:CD2	1:E:128:ILE:HD13	2.49	0.47
1:F:62:HIS:HB3	1:F:129:GLN:HG2	1.96	0.47
1:P:67:PRO:HA	1:P:124:GLN:HE21	1.78	0.47
1:P:72:GLU:HA	1:P:90:MET:HE2	1.96	0.47
1:A:115:THR:HG22	1:B:125:PRO:HG3	1.95	0.47
2:a:149:S9X:CD1	2:d:153:2JN:H12	2.45	0.47
2:c:146:ARG:HG3	2:c:146:ARG:NH1	2.25	0.47
1:L:113:TYR:CE2	1:L:117:VAL:HG21	2.50	0.47
1:C:66:LEU:HD23	1:C:126:ILE:HG21	1.96	0.47
1:C:69:ASP:OD1	1:C:69:ASP:N	2.46	0.47
1:P:103:THR:OG1	1:P:105:GLU:HG2	2.13	0.47
1:E:115:THR:CG2	1:L:65:LYS:HZ1	2.28	0.47
1:K:69:ASP:O	1:K:69:ASP:OD2	2.31	0.47
1:N:87:ASN:HA	2:n:151:LEU:HD11	1.95	0.47
1:A:76:ILE:HG13	1:A:88:LEU:HD22	1.96	0.47
2:d:144:GLN:CD	2:d:144:GLN:H	2.21	0.47
1:F:64:ARG:HE	1:F:65:LYS:HZ3	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:68:ILE:HD12	1:G:68:ILE:H	1.78	0.47
1:I:61:ILE:HD12	1:I:110:MET:SD	2.55	0.47
1:J:64:ARG:HB2	1:J:127:TYR:HD2	1.79	0.47
1:C:62:HIS:CG	1:C:98:PHE:HE1	2.33	0.47
2:d:150:ALA:O	2:d:154:VAL:HG13	2.14	0.47
1:C:72:GLU:O	1:C:75:VAL:HG22	2.13	0.47
1:G:63:ILE:HG12	1:G:128:ILE:HG23	1.96	0.47
1:M:79:GLY:O	1:M:101:MET:HE1	2.14	0.47
2:m:143:ASN:OD1	2:m:144:GLN:N	2.35	0.47
1:I:89:LEU:HD22	1:I:90:MET:N	2.30	0.47
1:K:61:ILE:O	1:K:61:ILE:HD12	2.15	0.47
1:K:65:LYS:HA	1:K:65:LYS:HD3	1.62	0.47
1:L:64:ARG:HA	1:L:96:GLN:HB3	1.97	0.47
1:B:80:LEU:HD21	2:b:154:VAL:CG1	2.45	0.47
2:c:145:MK8:HDA	2:c:145:MK8:C	2.45	0.47
1:D:61:ILE:HG13	1:D:110:MET:CE	2.45	0.47
1:D:64:ARG:HB3	1:D:96:GLN:NE2	2.30	0.47
1:E:121:LEU:HB2	1:E:126:ILE:CD1	2.45	0.47
1:K:108:ASN:HA	1:K:130:PHE:CZ	2.46	0.47
1:L:94:LYS:HB3	1:L:96:GLN:HG2	1.97	0.47
1:O:60:VAL:HG13	1:O:131:SER:CB	2.45	0.47
1:E:121:LEU:HB2	1:E:126:ILE:HD11	1.95	0.47
2:e:144:GLN:CD	2:e:144:GLN:N	2.73	0.47
1:J:71:THR:HG22	1:J:74:GLU:OE1	2.15	0.47
1:G:92:LYS:HD2	1:G:92:LYS:C	2.39	0.46
1:K:124:GLN:O	1:K:126:ILE:HD12	2.16	0.46
1:D:60:VAL:HB	1:D:131:SER:CB	2.45	0.46
1:F:93:GLY:O	1:F:95:ASN:N	2.47	0.46
1:G:77:SER:OG	1:H:81:PRO:HD3	2.16	0.46
1:G:119:PRO:HG2	1:G:128:ILE:HD11	1.97	0.46
1:I:86:THR:OG1	1:I:100:GLU:HG2	2.15	0.46
1:B:82:PHE:CD1	1:B:110:MET:HG2	2.50	0.46
1:E:94:LYS:O	1:E:95:ASN:HB3	2.16	0.46
1:F:60:VAL:HG13	1:F:131:SER:HB3	1.96	0.46
1:G:80:LEU:HD21	2:g:154:VAL:HG21	1.96	0.46
1:I:72:GLU:HG3	1:I:90:MET:HG3	1.98	0.46
1:N:94:LYS:O	1:N:96:GLN:HG3	2.15	0.46
2:b:144:GLN:H	2:b:144:GLN:CD	2.22	0.46
1:D:82:PHE:CE1	1:D:110:MET:HG3	2.50	0.46
1:H:114:TYR:HB2	1:H:128:ILE:HD11	1.96	0.46
1:P:74:GLU:O	1:P:77:SER:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:ILE:HG21	2:f:154:VAL:HG21	1.96	0.46
1:O:122:ARG:HD3	1:P:84:LYS:HG3	1.96	0.46
1:B:119:PRO:HB2	1:B:126:ILE:HG13	1.98	0.46
1:G:114:TYR:CE1	1:G:119:PRO:HG3	2.51	0.46
1:J:82:PHE:CD2	1:J:110:MET:HG3	2.51	0.46
1:O:91:LEU:HD12	1:O:96:GLN:HG3	1.97	0.46
2:c:154:VAL:HG13	2:c:155:ASN:H	1.81	0.46
1:G:93:GLY:O	1:G:95:ASN:N	2.49	0.46
1:C:121:LEU:HD12	1:C:121:LEU:HA	1.73	0.46
1:G:80:LEU:HD21	2:g:154:VAL:CG2	2.46	0.46
1:H:79:GLY:O	1:H:101:MET:HE1	2.15	0.46
1:J:111:VAL:HG23	1:J:128:ILE:CD1	2.46	0.46
2:l:150:ALA:O	2:l:154:VAL:HG12	2.16	0.46
1:D:70:VAL:HA	1:D:74:GLU:OE1	2.16	0.46
1:E:119:PRO:HG2	1:E:128:ILE:HD12	1.98	0.45
1:F:64:ARG:HH21	1:F:65:LYS:HZ3	1.64	0.45
1:G:104:GLU:OE1	1:G:108:ASN:HB2	2.16	0.45
2:j:145:MK8:HG	2:j:146:ARG:N	2.28	0.45
1:A:111:VAL:O	1:A:115:THR:HG23	2.17	0.45
1:D:61:ILE:HG13	1:D:110:MET:HE1	1.97	0.45
1:G:76:ILE:HG13	1:G:88:LEU:HD22	1.97	0.45
1:G:61:ILE:HB	1:G:99:ILE:HG23	1.99	0.45
1:L:108:ASN:O	1:L:110:MET:N	2.50	0.45
2:n:151:LEU:HA	2:n:151:LEU:HD23	1.73	0.45
1:P:67:PRO:HG2	1:P:121:LEU:HB3	1.98	0.45
1:K:127:TYR:CE2	1:K:129:GLN:HB2	2.51	0.45
1:P:93:GLY:O	1:P:95:ASN:N	2.49	0.45
1:E:112:ASN:OD1	1:L:95:ASN:ND2	2.49	0.45
1:K:68:ILE:O	1:K:122:ARG:NH1	2.49	0.45
1:G:107:ALA:O	1:G:111:VAL:HG22	2.17	0.45
1:I:107:ALA:O	1:I:111:VAL:HG12	2.16	0.45
1:H:111:VAL:O	1:H:115:THR:HG23	2.16	0.45
1:H:119:PRO:HB2	1:H:126:ILE:CG1	2.47	0.45
2:o:145:MK8:HB1B	2:o:145:MK8:HGA	1.76	0.45
1:P:65:LYS:HA	1:P:65:LYS:HD2	1.81	0.45
1:P:113:TYR:O	1:P:113:TYR:HD1	1.99	0.45
1:E:84:LYS:N	1:E:102:ASN:HD21	2.14	0.45
1:F:93:GLY:C	1:F:95:ASN:H	2.23	0.45
1:G:119:PRO:HD2	1:G:126:ILE:O	2.17	0.45
1:L:69:ASP:OD1	1:L:122:ARG:NH1	2.49	0.45
1:P:93:GLY:C	1:P:95:ASN:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:101:MET:HB3	1:P:101:MET:HE2	1.70	0.45
1:J:64:ARG:HD2	1:J:127:TYR:HE2	1.82	0.45
1:J:80:LEU:HD23	1:J:80:LEU:HA	1.58	0.45
1:O:65:LYS:O	1:O:126:ILE:HG22	2.17	0.45
1:P:82:PHE:CE1	1:P:110:MET:HG3	2.52	0.45
1:C:65:LYS:HE3	1:H:115:THR:OG1	2.17	0.44
1:E:115:THR:CB	1:L:65:LYS:HZ1	2.31	0.44
1:F:82:PHE:HD2	1:F:110:MET:HG3	1.81	0.44
1:I:58:SER:N	1:I:130:PHE:CZ	2.84	0.44
1:O:122:ARG:CD	1:P:84:LYS:HG3	2.47	0.44
1:G:121:LEU:HG	1:G:126:ILE:CD1	2.47	0.44
1:O:74:GLU:HG3	2:p:154:VAL:HG12	1.98	0.44
1:O:88:LEU:HD23	1:O:89:LEU:N	2.33	0.44
1:G:114:TYR:HA	1:G:117:VAL:O	2.17	0.44
1:M:62:HIS:CE1	1:M:64:ARG:HG2	2.53	0.44
1:O:120:VAL:HG13	1:P:81:PRO:CB	2.37	0.44
1:A:62:HIS:HD2	1:A:63:ILE:N	2.11	0.44
1:I:88:LEU:HD23	2:i:151:LEU:HG	2.00	0.44
1:J:72:GLU:CD	1:J:90:MET:HE2	2.41	0.44
1:E:88:LEU:HD12	1:E:98:PHE:O	2.17	0.44
1:F:113:TYR:CE1	1:F:117:VAL:HG21	2.53	0.44
1:J:88:LEU:C	1:J:88:LEU:HD23	2.41	0.44
1:J:97:ALA:C	1:J:98:PHE:HD1	2.25	0.44
1:P:92:LYS:O	1:P:93:GLY:C	2.60	0.44
1:D:101:MET:HE3	1:D:101:MET:HB3	1.81	0.44
1:L:78:LEU:HD21	1:L:121:LEU:HD13	1.99	0.44
1:B:80:LEU:HD23	1:C:73:GLY:C	2.42	0.44
2:d:144:GLN:CD	2:d:144:GLN:N	2.76	0.44
1:I:71:THR:OG1	1:I:74:GLU:HG3	2.17	0.44
2:m:146:ARG:H	2:m:146:ARG:HG3	1.54	0.44
1:A:71:THR:HG22	1:A:74:GLU:CD	2.42	0.43
1:B:64:ARG:HD2	1:B:129:GLN:NE2	2.32	0.43
2:n:148:GLN:HA	2:n:151:LEU:HB2	1.99	0.43
1:C:76:ILE:HG22	1:C:80:LEU:HD23	2.00	0.43
1:E:84:LYS:HG3	1:J:122:ARG:NE	2.33	0.43
1:E:90:MET:HG2	1:E:97:ALA:HB2	1.99	0.43
1:H:113:TYR:HD1	1:H:114:TYR:CD2	2.36	0.43
1:J:111:VAL:HB	1:J:130:PHE:CE1	2.53	0.43
1:K:84:LYS:N	1:K:102:ASN:OD1	2.46	0.43
1:N:68:ILE:HD12	1:N:68:ILE:HA	1.79	0.43
1:O:63:ILE:HG22	1:O:97:ALA:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:MET:C	1:D:91:LEU:HD23	2.44	0.43
1:F:119:PRO:CB	1:F:128:ILE:HD13	2.48	0.43
1:G:104:GLU:O	1:G:105:GLU:C	2.61	0.43
1:K:89:LEU:HD12	2:k:144:GLN:OE1	2.18	0.43
2:a:150:ALA:O	2:a:154:VAL:HG23	2.19	0.43
1:F:65:LYS:O	1:F:126:ILE:HG22	2.19	0.43
1:F:73:GLY:C	2:i:154:VAL:HG12	2.43	0.43
1:F:120:VAL:HG13	1:I:81:PRO:HB3	2.00	0.43
1:D:63:ILE:HG23	1:D:126:ILE:HD12	2.00	0.43
1:J:71:THR:OG1	1:J:72:GLU:N	2.51	0.43
1:C:79:GLY:HA2	1:C:110:MET:SD	2.58	0.43
1:D:76:ILE:HG13	1:D:88:LEU:CD1	2.49	0.43
1:M:94:LYS:HG3	1:M:96:GLN:HE22	1.84	0.43
2:o:144:GLN:CD	2:o:144:GLN:N	2.74	0.43
1:A:61:ILE:CD1	1:A:110:MET:HE3	2.36	0.43
1:A:69:ASP:OD2	1:A:69:ASP:C	2.62	0.43
1:A:90:MET:O	1:A:91:LEU:HD23	2.19	0.43
1:C:128:ILE:HD12	1:C:128:ILE:C	2.44	0.43
1:E:88:LEU:N	2:e:151:LEU:HD11	2.28	0.43
1:E:117:VAL:HG23	1:L:125:PRO:HG2	2.01	0.43
1:I:88:LEU:HD12	1:I:89:LEU:N	2.34	0.43
1:M:61:ILE:HG23	1:M:128:ILE:HG23	2.00	0.43
1:N:122:ARG:O	1:N:124:GLN:NE2	2.50	0.43
1:P:76:ILE:HG22	1:P:88:LEU:HG	2.01	0.43
1:A:62:HIS:CD2	1:A:63:ILE:N	2.86	0.43
1:G:114:TYR:CD2	1:G:128:ILE:HD12	2.54	0.43
1:M:72:GLU:HG3	1:M:90:MET:SD	2.59	0.43
1:N:79:GLY:HA2	1:N:110:MET:CE	2.48	0.43
1:I:89:LEU:HD22	1:I:90:MET:H	1.83	0.42
1:J:84:LYS:NZ	1:J:84:LYS:HB3	2.34	0.42
1:K:61:ILE:CD1	1:K:99:ILE:HG12	2.45	0.42
1:L:114:TYR:HD1	1:L:117:VAL:HG23	1.83	0.42
1:G:104:GLU:O	1:G:106:ALA:N	2.53	0.42
1:J:128:ILE:HD12	1:J:128:ILE:C	2.44	0.42
1:A:105:GLU:H	1:A:105:GLU:CD	2.26	0.42
1:K:111:VAL:HG21	1:K:130:PHE:CD1	2.55	0.42
1:M:61:ILE:HG12	1:M:110:MET:CE	2.41	0.42
1:C:99:ILE:HD13	1:C:99:ILE:HG21	1.83	0.42
4:h:201:NH2:N	2:k:152:GLN:HE22	2.17	0.42
1:K:78:LEU:HD21	1:K:121:LEU:HD21	2.01	0.42
1:P:110:MET:O	1:P:114:TYR:HD1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLU:OE2	2:a:146:ARG:HD3	2.19	0.42
2:e:154:VAL:O	1:J:71:THR:HG21	2.20	0.42
1:C:125:PRO:HB2	1:H:116:SER:HB2	2.01	0.42
2:e:143:ASN:HB3	2:e:144:GLN:NE2	2.35	0.42
1:I:65:LYS:O	1:I:126:ILE:HG22	2.20	0.42
1:I:105:GLU:O	1:I:109:THR:OG1	2.37	0.42
2:c:145:MK8:HG	2:e:145:MK8:HB1B	2.02	0.42
1:E:121:LEU:HD12	1:E:121:LEU:HA	1.86	0.42
1:F:107:ALA:HB1	1:F:130:PHE:HE1	1.84	0.42
2:g:150:ALA:O	2:g:154:VAL:HG12	2.20	0.42
1:O:75:VAL:HG11	1:O:97:ALA:HB3	2.01	0.42
1:P:66:LEU:HG	1:P:95:ASN:C	2.45	0.42
1:A:82:PHE:CD1	1:A:110:MET:SD	3.13	0.42
1:D:89:LEU:O	1:D:98:PHE:N	2.43	0.42
1:D:60:VAL:C	1:D:61:ILE:HG12	2.45	0.42
1:F:65:LYS:HA	1:F:65:LYS:HD3	1.87	0.42
1:H:118:THR:HA	1:H:119:PRO:HD3	1.70	0.42
1:M:77:SER:HB2	1:N:77:SER:O	2.20	0.42
2:n:145:MK8:HB1A	2:n:148:GLN:HG2	2.01	0.42
1:B:87:ASN:HA	2:b:151:LEU:HD11	2.02	0.41
2:f:144:GLN:O	2:f:148:GLN:HG2	2.20	0.41
1:G:75:VAL:O	1:G:78:LEU:HB2	2.20	0.41
1:I:92:LYS:HZ2	1:I:92:LYS:HG2	1.70	0.41
1:K:69:ASP:HB3	1:K:122:ARG:NH1	2.34	0.41
1:O:60:VAL:HG22	1:O:131:SER:OG	2.20	0.41
1:P:128:ILE:HG23	1:P:128:ILE:O	2.19	0.41
1:F:58:SER:OG	1:F:59:ARG:N	2.53	0.41
1:L:63:ILE:O	1:L:96:GLN:HB2	2.20	0.41
1:L:105:GLU:OE2	1:L:106:ALA:HB2	2.20	0.41
1:N:64:ARG:HB2	1:N:127:TYR:CD2	2.55	0.41
1:O:69:ASP:OD1	1:O:69:ASP:O	2.38	0.41
2:a:148:GLN:H	2:a:148:GLN:HG2	1.63	0.41
1:A:71:THR:HG23	1:A:74:GLU:H	1.84	0.41
1:I:114:TYR:CB	1:I:128:ILE:HG12	2.48	0.41
1:E:118:THR:HA	1:E:119:PRO:HD3	1.79	0.41
1:E:120:VAL:HG13	1:E:123:GLY:HA2	2.03	0.41
1:F:72:GLU:O	1:F:75:VAL:HG22	2.20	0.41
1:J:66:LEU:HD23	1:J:121:LEU:HD23	2.01	0.41
1:K:113:TYR:C	1:K:113:TYR:CD1	2.98	0.41
1:N:88:LEU:HB2	1:N:99:ILE:HG22	2.02	0.41
1:O:69:ASP:CG	1:O:122:ARG:HH12	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:MET:HB2	1:B:107:ALA:HB2	2.01	0.41
1:K:120:VAL:HG13	1:K:124:GLN:H	1.84	0.41
1:N:112:ASN:HD21	1:P:124:GLN:CG	2.31	0.41
1:O:74:GLU:HG3	2:p:154:VAL:CG1	2.51	0.41
1:O:79:GLY:HA2	1:O:110:MET:CE	2.50	0.41
2:e:145:MK8:HDA	2:e:145:MK8:C	2.51	0.41
1:H:90:MET:HB3	1:H:90:MET:HE3	1.65	0.41
1:K:82:PHE:CE2	1:K:110:MET:HA	2.56	0.41
2:p:148:GLN:OE1	2:p:151:LEU:HD22	2.20	0.41
1:F:111:VAL:O	1:F:115:THR:OG1	2.38	0.41
1:J:80:LEU:N	1:J:81:PRO:CD	2.84	0.41
1:O:73:GLY:HA3	2:p:154:VAL:HA	2.02	0.41
1:O:128:ILE:HD12	1:O:128:ILE:C	2.45	0.41
1:P:91:LEU:O	1:P:93:GLY:N	2.53	0.41
1:B:90:MET:HE3	1:B:97:ALA:HB2	2.02	0.41
1:C:66:LEU:HB2	1:C:95:ASN:O	2.20	0.41
1:K:105:GLU:CD	1:K:105:GLU:N	2.79	0.41
1:N:119:PRO:O	1:N:126:ILE:HG12	2.21	0.41
1:P:80:LEU:N	1:P:81:PRO:HD2	2.36	0.41
1:G:101:MET:HE2	1:G:101:MET:HB3	1.99	0.41
1:I:57:PRO:HA	1:I:130:PHE:CZ	2.56	0.41
1:M:66:LEU:H	1:M:66:LEU:HD12	1.86	0.41
1:P:66:LEU:O	1:P:95:ASN:ND2	2.54	0.41
1:C:62:HIS:ND1	1:C:98:PHE:HE1	2.18	0.40
1:C:104:GLU:O	1:C:108:ASN:HB2	2.20	0.40
1:G:134:LYS:C	1:G:134:LYS:HD3	2.46	0.40
1:H:114:TYR:HD1	1:H:128:ILE:HD11	1.86	0.40
1:J:76:ILE:C	1:J:78:LEU:N	2.77	0.40
1:M:60:VAL:HG23	1:M:61:ILE:H	1.86	0.40
1:M:88:LEU:HD12	1:M:89:LEU:H	1.86	0.40
1:N:64:ARG:HB2	1:N:127:TYR:HD2	1.85	0.40
1:O:120:VAL:HA	1:O:125:PRO:HA	2.02	0.40
1:P:106:ALA:O	1:P:110:MET:HB2	2.22	0.40
1:B:66:LEU:HB2	1:B:95:ASN:O	2.22	0.40
1:B:90:MET:HE2	1:B:90:MET:HB3	1.98	0.40
1:C:76:ILE:HG13	1:C:88:LEU:HD22	2.03	0.40
1:E:76:ILE:HG23	1:E:85:VAL:CG2	2.52	0.40
2:l:144:GLN:O	2:l:147:ALA:N	2.54	0.40
1:N:113:TYR:O	1:N:117:VAL:HG23	2.22	0.40
1:N:122:ARG:HB3	1:N:124:GLN:OE1	2.21	0.40
1:E:84:LYS:H	1:E:102:ASN:HD21	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:110:MET:HE3	1:I:110:MET:HB2	1.80	0.40
1:J:94:LYS:HB3	1:J:96:GLN:HG2	2.04	0.40
1:L:88:LEU:HD23	1:L:99:ILE:HG22	2.04	0.40
1:N:79:GLY:O	1:N:101:MET:HE1	2.22	0.40
1:D:94:LYS:HE3	1:D:94:LYS:HA	2.03	0.40
2:e:147:ALA:O	2:e:151:LEU:HG	2.21	0.40
1:J:91:LEU:HD13	1:J:92:LYS:N	2.37	0.40
1:N:72:GLU:OE1	1:N:72:GLU:N	2.47	0.40
1:J:87:ASN:HA	2:j:151:LEU:HD11	2.03	0.40
1:L:65:LYS:O	1:L:126:ILE:HG22	2.21	0.40
1:P:102:ASN:ND2	1:P:103:THR:HG23	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:LYS:NZ	3:A:202:SO4:O3[3_455]	2.11	0.09

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	76/86 (88%)	67 (88%)	9 (12%)	0	100	100
1	B	75/86 (87%)	71 (95%)	4 (5%)	0	100	100
1	C	77/86 (90%)	72 (94%)	5 (6%)	0	100	100
1	D	75/86 (87%)	71 (95%)	4 (5%)	0	100	100
1	E	73/86 (85%)	69 (94%)	4 (6%)	0	100	100
1	F	77/86 (90%)	69 (90%)	6 (8%)	2 (3%)	4	17
1	G	78/86 (91%)	71 (91%)	6 (8%)	1 (1%)	9	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	75/86 (87%)	72 (96%)	3 (4%)	0	100	100
1	I	76/86 (88%)	70 (92%)	6 (8%)	0	100	100
1	J	76/86 (88%)	71 (93%)	5 (7%)	0	100	100
1	K	81/86 (94%)	77 (95%)	4 (5%)	0	100	100
1	L	75/86 (87%)	68 (91%)	5 (7%)	2 (3%)	4	16
1	M	75/86 (87%)	63 (84%)	12 (16%)	0	100	100
1	N	78/86 (91%)	71 (91%)	7 (9%)	0	100	100
1	O	76/86 (88%)	68 (90%)	7 (9%)	1 (1%)	9	32
1	P	71/86 (83%)	56 (79%)	11 (16%)	4 (6%)	1	4
2	a	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	b	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	c	8/13 (62%)	8 (100%)	0	0	100	100
2	d	8/13 (62%)	8 (100%)	0	0	100	100
2	e	8/13 (62%)	8 (100%)	0	0	100	100
2	f	8/13 (62%)	8 (100%)	0	0	100	100
2	g	8/13 (62%)	8 (100%)	0	0	100	100
2	h	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	i	8/13 (62%)	8 (100%)	0	0	100	100
2	j	8/13 (62%)	8 (100%)	0	0	100	100
2	k	8/13 (62%)	8 (100%)	0	0	100	100
2	l	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	m	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	n	8/13 (62%)	8 (100%)	0	0	100	100
2	o	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
2	p	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
All	All	1342/1584 (85%)	1227 (91%)	105 (8%)	10 (1%)	18	48

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	94	LYS
1	L	109	THR
1	P	92	LYS

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Mol	Chain	Res	Type
1	P	93	GLY
1	G	94	LYS
1	L	108	ASN
1	F	102	ASN
1	P	67	PRO
1	P	94	LYS
1	O	117	VAL

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	70/77 (91%)	66 (94%)	4 (6%)	18	49
1	B	69/77 (90%)	66 (96%)	3 (4%)	26	60
1	C	70/77 (91%)	65 (93%)	5 (7%)	13	40
1	D	69/77 (90%)	63 (91%)	6 (9%)	9	30
1	E	67/77 (87%)	62 (92%)	5 (8%)	12	37
1	F	70/77 (91%)	68 (97%)	2 (3%)	37	71
1	G	72/77 (94%)	66 (92%)	6 (8%)	10	32
1	H	69/77 (90%)	63 (91%)	6 (9%)	9	30
1	I	69/77 (90%)	66 (96%)	3 (4%)	26	60
1	J	69/77 (90%)	65 (94%)	4 (6%)	18	49
1	K	75/77 (97%)	72 (96%)	3 (4%)	28	62
1	L	69/77 (90%)	67 (97%)	2 (3%)	37	71
1	M	68/77 (88%)	64 (94%)	4 (6%)	18	48
1	N	72/77 (94%)	69 (96%)	3 (4%)	26	60
1	O	70/77 (91%)	68 (97%)	2 (3%)	37	71
1	P	65/77 (84%)	57 (88%)	8 (12%)	4	15
2	a	8/8 (100%)	7 (88%)	1 (12%)	4	15
2	b	8/8 (100%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	c	8/8 (100%)	7 (88%)	1 (12%)	4	15
2	d	8/8 (100%)	7 (88%)	1 (12%)	4	15
2	e	8/8 (100%)	8 (100%)	0	100	100
2	f	8/8 (100%)	8 (100%)	0	100	100
2	g	8/8 (100%)	8 (100%)	0	100	100
2	h	8/8 (100%)	8 (100%)	0	100	100
2	i	8/8 (100%)	8 (100%)	0	100	100
2	j	8/8 (100%)	7 (88%)	1 (12%)	4	15
2	k	8/8 (100%)	8 (100%)	0	100	100
2	l	8/8 (100%)	7 (88%)	1 (12%)	4	15
2	m	8/8 (100%)	8 (100%)	0	100	100
2	n	8/8 (100%)	7 (88%)	1 (12%)	4	15
2	o	8/8 (100%)	8 (100%)	0	100	100
2	p	8/8 (100%)	8 (100%)	0	100	100
All	All	1241/1360 (91%)	1169 (94%)	72 (6%)	18	49

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	105	GLU
1	A	131	SER
1	A	132	ASN
2	a	146	ARG
1	B	61	ILE
1	B	131	SER
1	B	132	ASN
1	C	65	LYS
1	C	69	ASP
1	C	94	LYS
1	C	115	THR
1	C	133	HIS
2	c	144	GLN
1	D	58	SER
1	D	96	GLN
1	D	104	GLU
1	D	109	THR

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Mol	Chain	Res	Type
1	D	133	HIS
1	D	134	LYS
2	d	146	ARG
1	E	58	SER
1	E	92	LYS
1	E	103	THR
1	E	124	GLN
1	E	131	SER
1	F	115	THR
1	F	129	GLN
1	G	69	ASP
1	G	75	VAL
1	G	88	LEU
1	G	103	THR
1	G	130	PHE
1	G	134	LYS
1	H	64	ARG
1	H	69	ASP
1	H	74	GLU
1	H	86	THR
1	H	109	THR
1	H	131	SER
1	I	63	ILE
1	I	89	LEU
1	I	105	GLU
1	J	61	ILE
1	J	71	THR
1	J	109	THR
1	J	131	SER
2	j	155	ASN
1	K	58	SER
1	K	65	LYS
1	K	132	ASN
1	L	131	SER
1	L	132	ASN
2	l	155	ASN
1	M	69	ASP
1	M	84	LYS
1	M	121	LEU
1	M	131	SER
1	N	103	THR
1	N	112	ASN

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Mol	Chain	Res	Type
1	N	114	TYR
2	n	146	ARG
1	O	118	THR
1	O	134	LYS
1	P	72	GLU
1	P	76	ILE
1	P	80	LEU
1	P	88	LEU
1	P	91	LEU
1	P	99	ILE
1	P	101	MET
1	P	131	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	133	HIS
1	C	124	GLN
2	c	143	ASN
2	c	144	GLN
1	D	96	GLN
1	D	112	ASN
1	D	124	GLN
1	E	102	ASN
1	E	129	GLN
2	e	144	GLN
1	F	62	HIS
1	F	96	GLN
1	F	124	GLN
2	f	155	ASN
1	H	132	ASN
2	h	155	ASN
1	I	96	GLN
2	i	155	ASN
1	J	95	ASN
2	j	148	GLN
2	j	155	ASN
1	K	96	GLN
1	K	124	GLN
1	K	132	ASN
2	k	155	ASN

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Mol	Chain	Res	Type
1	L	95	ASN
1	L	96	GLN
1	M	62	HIS
1	M	87	ASN
1	M	96	GLN
2	m	148	GLN
1	N	95	ASN
1	N	112	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

32 non-standard protein/DNA/RNA residues 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	2JN	e	153	2	5,8,9	0.72	0	6,10,12	1.74	2 (33%)
2	MK8	e	145	2	5,8,9	0.85	0	6,10,12	1.78	2 (33%)
2	MK8	j	145	2	5,8,9	0.75	0	6,10,12	1.66	1 (16%)
2	MK8	c	145	2	5,8,9	0.89	0	6,10,12	1.28	1 (16%)
2	MK8	l	145	2	5,8,9	0.75	0	6,10,12	1.31	0
2	2JN	c	153	2	5,8,9	0.98	1 (20%)	6,10,12	1.97	2 (33%)
2	MK8	g	145	2	5,8,9	0.77	0	6,10,12	1.16	0
2	MK8	b	145	2	5,8,9	0.70	0	6,10,12	2.19	3 (50%)
2	MK8	p	145	2	5,8,9	0.80	0	6,10,12	1.26	0
2	2JN	i	153	2	5,8,9	0.93	1 (20%)	6,10,12	1.19	1 (16%)
2	2JN	a	153	2	5,8,9	0.96	1 (20%)	6,10,12	1.23	1 (16%)
2	MK8	h	145	2	5,8,9	0.85	0	6,10,12	1.53	1 (16%)
2	2JN	h	153	2	5,8,9	0.79	0	6,10,12	1.48	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MK8	d	145	2	5,8,9	0.76	0	6,10,12	1.29	1 (16%)
2	2JN	d	153	2	5,8,9	0.66	0	6,10,12	1.46	2 (33%)
2	MK8	m	145	2	5,8,9	0.90	1 (20%)	6,10,12	1.05	0
2	2JN	m	153	2	5,8,9	0.85	0	6,10,12	1.39	1 (16%)
2	MK8	i	145	2	5,8,9	0.72	0	6,10,12	1.34	1 (16%)
2	MK8	a	145	2	5,8,9	0.60	0	6,10,12	1.04	0
2	2JN	j	153	2	5,8,9	0.69	0	6,10,12	1.42	1 (16%)
2	2JN	k	153	2	5,8,9	0.97	1 (20%)	6,10,12	1.38	1 (16%)
2	MK8	o	145	2	5,8,9	0.84	0	6,10,12	1.11	1 (16%)
2	2JN	g	153	2	5,8,9	0.82	0	6,10,12	1.33	1 (16%)
2	MK8	n	145	2	5,8,9	0.72	0	6,10,12	1.41	1 (16%)
2	2JN	n	153	2	5,8,9	0.77	0	6,10,12	1.56	2 (33%)
2	2JN	o	153	2	5,8,9	0.88	0	6,10,12	1.60	1 (16%)
2	MK8	f	145	2	5,8,9	0.94	0	6,10,12	1.68	2 (33%)
2	2JN	f	153	2	5,8,9	0.84	0	6,10,12	1.38	1 (16%)
2	2JN	p	153	2	5,8,9	1.11	1 (20%)	6,10,12	2.43	3 (50%)
2	2JN	b	153	2	5,8,9	0.68	0	6,10,12	1.51	1 (16%)
2	2JN	l	153	2	5,8,9	0.66	0	6,10,12	1.67	1 (16%)
2	MK8	k	145	2	5,8,9	0.68	0	6,10,12	1.24	1 (16%)

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	2JN	e	153	2	-	0/6/8/11	-
2	MK8	e	145	2	-	1/6/8/11	-
2	MK8	j	145	2	-	5/6/8/11	-
2	MK8	c	145	2	-	1/6/8/11	-
2	MK8	l	145	2	-	4/6/8/11	-
2	2JN	c	153	2	-	4/6/8/11	-
2	MK8	g	145	2	-	4/6/8/11	-
2	MK8	b	145	2	-	4/6/8/11	-
2	MK8	p	145	2	-	4/6/8/11	-
2	2JN	i	153	2	-	0/6/8/11	-
2	2JN	a	153	2	-	1/6/8/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MK8	h	145	2	-	4/6/8/11	-
2	2JN	h	153	2	-	0/6/8/11	-
2	MK8	d	145	2	-	4/6/8/11	-
2	2JN	d	153	2	-	0/6/8/11	-
2	MK8	m	145	2	-	1/6/8/11	-
2	2JN	m	153	2	-	4/6/8/11	-
2	MK8	i	145	2	-	1/6/8/11	-
2	MK8	a	145	2	-	1/6/8/11	-
2	2JN	j	153	2	-	4/6/8/11	-
2	2JN	k	153	2	-	4/6/8/11	-
2	MK8	o	145	2	-	1/6/8/11	-
2	2JN	g	153	2	-	4/6/8/11	-
2	MK8	n	145	2	-	1/6/8/11	-
2	2JN	n	153	2	-	1/6/8/11	-
2	2JN	o	153	2	-	4/6/8/11	-
2	MK8	f	145	2	-	1/6/8/11	-
2	2JN	f	153	2	-	4/6/8/11	-
2	2JN	p	153	2	-	0/6/8/11	-
2	2JN	b	153	2	-	1/6/8/11	-
2	2JN	l	153	2	-	4/6/8/11	-
2	MK8	k	145	2	-	1/6/8/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	p	153	2JN	O-C	2.42	1.27	1.20
2	c	153	2JN	O-C	2.15	1.26	1.20
2	k	153	2JN	O-C	2.15	1.26	1.20
2	a	153	2JN	O-C	2.12	1.26	1.20
2	i	153	2JN	O-C	2.06	1.26	1.20
2	m	145	MK8	O-C	2.00	1.26	1.20

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	p	153	2JN	CAA-CA-CAO	-3.91	104.53	110.97
2	j	145	MK8	CB1-CA-CB	-3.73	104.83	110.97
2	c	153	2JN	CAA-CA-CAO	-3.65	104.95	110.97
2	l	153	2JN	CAM-CAO-CA	3.48	120.56	115.41
2	p	153	2JN	CAO-CA-C	3.42	117.28	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	153	2JN	CAA-CA-CAO	-3.42	105.34	110.97
2	b	145	MK8	CB1-CA-CB	-3.35	105.45	110.97
2	e	145	MK8	CB1-CA-CB	-3.25	105.61	110.97
2	e	153	2JN	CAA-CA-CAO	-3.22	105.67	110.97
2	f	145	MK8	CB-CA-C	2.90	115.94	108.47
2	k	145	MK8	CB1-CA-CB	-2.83	106.31	110.97
2	n	145	MK8	CB1-CA-CB	-2.78	106.40	110.97
2	o	153	2JN	CAM-CAO-CA	2.75	119.48	115.41
2	c	153	2JN	CAM-CAO-CA	2.74	119.46	115.41
2	p	153	2JN	CAM-CAO-CA	2.68	119.38	115.41
2	b	145	MK8	CG-CB-CA	2.67	119.35	115.41
2	i	153	2JN	CAA-CA-CAO	-2.58	106.71	110.97
2	n	153	2JN	CAO-CA-C	2.56	115.08	108.47
2	k	153	2JN	CAM-CAO-CA	2.56	119.20	115.41
2	d	153	2JN	CAA-CA-CAO	-2.53	106.80	110.97
2	h	145	MK8	CG-CB-CA	2.49	119.10	115.41
2	c	145	MK8	CB1-CA-CB	-2.49	106.87	110.97
2	h	153	2JN	CAO-CA-C	2.45	114.78	108.47
2	g	153	2JN	CAA-CA-CAO	-2.40	107.02	110.97
2	e	145	MK8	CG-CB-CA	2.38	118.93	115.41
2	e	153	2JN	CAO-CA-C	2.33	114.47	108.47
2	f	153	2JN	CAM-CAO-CA	2.32	118.84	115.41
2	a	153	2JN	CAM-CAO-CA	2.28	118.79	115.41
2	h	153	2JN	CAA-CA-CAO	-2.28	107.21	110.97
2	b	145	MK8	CB-CG-CD	2.27	120.08	113.11
2	f	145	MK8	CG-CB-CA	2.25	118.75	115.41
2	i	145	MK8	CB1-CA-CB	-2.22	107.32	110.97
2	d	153	2JN	CAO-CA-C	2.18	114.08	108.47
2	n	153	2JN	CAA-CA-CAO	-2.17	107.40	110.97
2	o	145	MK8	CB1-CA-CB	-2.14	107.44	110.97
2	d	145	MK8	CB1-CA-CB	-2.12	107.47	110.97
2	j	153	2JN	CAA-CA-CAO	-2.07	107.55	110.97
2	m	153	2JN	CAM-CAO-CA	2.07	118.47	115.41

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	b	145	MK8	C-CA-CB-CG
2	b	145	MK8	N-CA-CB-CG
2	b	145	MK8	CB1-CA-CB-CG
2	g	145	MK8	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	g	145	MK8	N-CA-CB-CG
2	g	145	MK8	CB1-CA-CB-CG
2	h	145	MK8	C-CA-CB-CG
2	h	145	MK8	N-CA-CB-CG
2	h	145	MK8	CB1-CA-CB-CG
2	j	145	MK8	N-CA-CB-CG
2	j	145	MK8	CB1-CA-CB-CG
2	l	145	MK8	N-CA-CB-CG
2	l	145	MK8	CB1-CA-CB-CG
2	p	145	MK8	N-CA-CB-CG
2	p	145	MK8	CB1-CA-CB-CG
2	c	153	2JN	C-CA-CAO-CAM
2	c	153	2JN	CAA-CA-CAO-CAM
2	c	153	2JN	N-CA-CAO-CAM
2	f	153	2JN	C-CA-CAO-CAM
2	f	153	2JN	CAA-CA-CAO-CAM
2	f	153	2JN	N-CA-CAO-CAM
2	g	153	2JN	C-CA-CAO-CAM
2	g	153	2JN	CAA-CA-CAO-CAM
2	g	153	2JN	N-CA-CAO-CAM
2	j	153	2JN	C-CA-CAO-CAM
2	j	153	2JN	CAA-CA-CAO-CAM
2	j	153	2JN	N-CA-CAO-CAM
2	k	153	2JN	C-CA-CAO-CAM
2	k	153	2JN	CAA-CA-CAO-CAM
2	k	153	2JN	N-CA-CAO-CAM
2	l	153	2JN	C-CA-CAO-CAM
2	l	153	2JN	CAA-CA-CAO-CAM
2	l	153	2JN	N-CA-CAO-CAM
2	m	153	2JN	C-CA-CAO-CAM
2	m	153	2JN	CAA-CA-CAO-CAM
2	m	153	2JN	N-CA-CAO-CAM
2	o	153	2JN	C-CA-CAO-CAM
2	o	153	2JN	CAA-CA-CAO-CAM
2	o	153	2JN	N-CA-CAO-CAM
2	b	145	MK8	CA-CB-CG-CD
2	h	145	MK8	CA-CB-CG-CD
2	l	145	MK8	CA-CB-CG-CD
2	m	145	MK8	CA-CB-CG-CD
2	p	145	MK8	CA-CB-CG-CD
2	c	153	2JN	CAK-CAM-CAO-CA
2	f	153	2JN	CAK-CAM-CAO-CA

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Mol	Chain	Res	Type	Atoms
2	g	153	2JN	CAK-CAM-CAO-CA
2	j	153	2JN	CAK-CAM-CAO-CA
2	k	153	2JN	CAK-CAM-CAO-CA
2	l	153	2JN	CAK-CAM-CAO-CA
2	o	153	2JN	CAK-CAM-CAO-CA
2	a	145	MK8	CA-CB-CG-CD
2	c	145	MK8	CA-CB-CG-CD
2	d	145	MK8	CA-CB-CG-CD
2	e	145	MK8	CA-CB-CG-CD
2	f	145	MK8	CA-CB-CG-CD
2	g	145	MK8	CA-CB-CG-CD
2	i	145	MK8	CA-CB-CG-CD
2	k	145	MK8	CA-CB-CG-CD
2	n	145	MK8	CA-CB-CG-CD
2	a	153	2JN	CAK-CAM-CAO-CA
2	b	153	2JN	CAK-CAM-CAO-CA
2	m	153	2JN	CAK-CAM-CAO-CA
2	l	145	MK8	C-CA-CB-CG
2	j	145	MK8	CA-CB-CG-CD
2	o	145	MK8	CA-CB-CG-CD
2	d	145	MK8	CE-CD-CG-CB
2	j	145	MK8	C-CA-CB-CG
2	p	145	MK8	C-CA-CB-CG
2	n	153	2JN	O-C-CA-CAA
2	j	145	MK8	CE-CD-CG-CB
2	d	145	MK8	N-CA-CB-CG
2	d	145	MK8	CB1-CA-CB-CG

There are no ring outliers.

13 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	e	145	MK8	2	0
2	j	145	MK8	1	0
2	c	145	MK8	2	0
2	l	145	MK8	1	0
2	g	145	MK8	1	0
2	b	145	MK8	2	0
2	d	145	MK8	1	0
2	d	153	2JN	1	0
2	m	145	MK8	1	0
2	o	145	MK8	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	n	145	MK8	1	0
2	b	153	2JN	1	0
2	k	145	MK8	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 16 are modelled with single atom - leaving 22 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	SO4	F	201	-	4,4,4	0.23	0	6,6,6	0.35	0
3	SO4	A	202	-	4,4,4	0.27	0	6,6,6	0.24	0
3	SO4	g	202	-	4,4,4	0.28	0	6,6,6	0.20	0
3	SO4	G	201	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	A	203	-	4,4,4	0.29	0	6,6,6	0.33	0
3	SO4	D	202	-	4,4,4	0.23	0	6,6,6	0.24	0
5	GOL	I	201	-	5,5,5	1.52	1 (20%)	5,5,5	1.04	0
3	SO4	F	202	-	4,4,4	0.32	0	6,6,6	0.21	0
3	SO4	K	202	-	4,4,4	0.24	0	6,6,6	0.27	0
3	SO4	C	201	-	4,4,4	0.25	0	6,6,6	0.56	0
5	GOL	i	202	-	5,5,5	1.23	1 (20%)	5,5,5	1.07	0
3	SO4	A	204	-	4,4,4	0.39	0	6,6,6	0.57	0
3	SO4	A	201	-	4,4,4	0.25	0	6,6,6	0.82	0
3	SO4	A	205	-	4,4,4	0.29	0	6,6,6	0.39	0
3	SO4	O	201	-	4,4,4	0.27	0	6,6,6	0.13	0
5	GOL	F	203	-	5,5,5	1.42	1 (20%)	5,5,5	0.84	0
3	SO4	D	201	-	4,4,4	0.28	0	6,6,6	0.17	0
5	GOL	C	202	-	5,5,5	1.33	1 (20%)	5,5,5	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	H	201	-	4,4,4	0.27	0	6,6,6	0.16	0
3	SO4	G	202	-	4,4,4	0.33	0	6,6,6	0.14	0
3	SO4	L	201	-	4,4,4	0.29	0	6,6,6	0.35	0
3	SO4	K	201	-	4,4,4	0.33	0	6,6,6	0.38	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	C	202	-	-	0/4/4/4	-
5	GOL	i	202	-	-	2/4/4/4	-
5	GOL	I	201	-	-	0/4/4/4	-
5	GOL	F	203	-	-	3/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	201	GOL	C3-C2	2.62	1.61	1.51
5	F	203	GOL	C3-C2	2.29	1.60	1.51
5	i	202	GOL	C3-C2	2.25	1.60	1.51
5	C	202	GOL	C1-C2	2.14	1.59	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	203	GOL	O1-C1-C2-C3
5	F	203	GOL	C1-C2-C3-O3
5	i	202	GOL	C1-C2-C3-O3
5	F	203	GOL	O1-C1-C2-O2
5	i	202	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	SO4	0	1

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	201	SO4	1	0
3	G	202	SO4	1	0
3	K	201	SO4	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	78/86 (90%)	-0.20	0 100 100	70, 80, 100, 113	0
1	B	77/86 (89%)	-0.19	0 100 100	69, 83, 105, 112	0
1	C	79/86 (91%)	-0.19	0 100 100	76, 94, 114, 123	0
1	D	77/86 (89%)	0.06	1 (1%) 75 67	84, 106, 125, 134	0
1	E	75/86 (87%)	0.04	0 100 100	84, 106, 125, 135	0
1	F	79/86 (91%)	-0.07	0 100 100	81, 92, 107, 114	0
1	G	80/86 (93%)	0.07	2 (2%) 58 48	82, 104, 131, 138	0
1	H	77/86 (89%)	-0.01	0 100 100	82, 109, 131, 139	0
1	I	77/86 (89%)	0.12	2 (2%) 57 48	59, 113, 135, 160	1 (1%)
1	J	78/86 (90%)	0.19	0 100 100	86, 113, 134, 145	0
1	K	83/86 (96%)	-0.06	0 100 100	79, 98, 114, 125	0
1	L	77/86 (89%)	-0.10	0 100 100	70, 92, 113, 130	0
1	M	77/86 (89%)	0.21	1 (1%) 75 67	89, 113, 129, 138	0
1	N	80/86 (93%)	0.22	2 (2%) 58 48	91, 117, 135, 148	0
1	O	78/86 (90%)	0.19	0 100 100	93, 120, 136, 149	0
1	P	73/86 (84%)	0.36	0 100 100	104, 129, 144, 145	0
2	a	10/13 (76%)	0.05	0 100 100	69, 80, 94, 99	0
2	b	10/13 (76%)	-0.15	0 100 100	73, 79, 100, 103	0
2	c	10/13 (76%)	-0.18	0 100 100	83, 90, 99, 117	0
2	d	10/13 (76%)	-0.01	0 100 100	83, 93, 110, 120	0
2	e	10/13 (76%)	-0.18	0 100 100	89, 91, 112, 121	0
2	f	10/13 (76%)	-0.14	0 100 100	80, 85, 100, 111	0
2	g	10/13 (76%)	-0.21	0 100 100	84, 90, 98, 101	0
2	h	10/13 (76%)	-0.10	0 100 100	88, 95, 111, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
2	i	10/13 (76%)	-0.20	0	100	100	90, 99, 109, 117	0
2	j	10/13 (76%)	-0.23	0	100	100	91, 98, 107, 114	0
2	k	10/13 (76%)	-0.09	0	100	100	75, 81, 92, 110	0
2	l	10/13 (76%)	0.28	0	100	100	77, 86, 99, 106	0
2	m	10/13 (76%)	0.19	0	100	100	82, 88, 106, 119	0
2	n	10/13 (76%)	0.02	0	100	100	93, 98, 108, 113	0
2	o	10/13 (76%)	0.06	0	100	100	86, 89, 104, 108	0
2	p	10/13 (76%)	-0.10	0	100	100	93, 104, 117, 121	0
All	All	1405/1584 (88%)	0.03	8 (0%)	85	81	59, 103, 131, 160	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	97	ALA	2.5
1	N	66	LEU	2.4
1	M	99	ILE	2.3
1	D	89	LEU	2.3
1	N	97	ALA	2.2
1	G	89	LEU	2.2
1	I	57	PRO	2.2
1	I	99	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	2JN	a	153	9/10	0.91	0.16	69,81,83,85	0
2	MK8	h	145	9/10	0.93	0.18	76,83,96,102	0
2	MK8	e	145	9/10	0.93	0.16	92,100,102,103	0
2	MK8	b	145	9/10	0.94	0.15	68,79,84,84	0
2	MK8	o	145	9/10	0.94	0.12	76,81,86,88	0
2	MK8	g	145	9/10	0.94	0.10	71,80,81,84	0
2	MK8	j	145	9/10	0.95	0.13	84,92,97,103	0
2	MK8	c	145	9/10	0.95	0.16	82,90,102,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MK8	i	145	9/10	0.95	0.17	89,98,103,104	0
2	2JN	b	153	9/10	0.95	0.10	72,79,86,89	0
2	2JN	e	153	9/10	0.95	0.10	73,78,91,91	0
2	2JN	f	153	9/10	0.95	0.10	77,89,97,99	0
2	2JN	i	153	9/10	0.95	0.12	75,82,87,89	0
2	2JN	n	153	9/10	0.95	0.11	81,87,94,99	0
2	2JN	p	153	9/10	0.95	0.11	82,93,97,99	0
2	MK8	d	145	9/10	0.96	0.12	87,96,100,100	0
2	2JN	c	153	9/10	0.96	0.08	72,76,81,88	0
2	2JN	d	153	9/10	0.96	0.11	68,79,83,87	0
2	MK8	m	145	9/10	0.96	0.20	81,88,94,94	0
2	MK8	n	145	9/10	0.96	0.10	86,90,94,96	0
2	2JN	g	153	9/10	0.96	0.11	79,87,93,94	0
2	2JN	h	153	9/10	0.96	0.10	83,86,92,95	0
2	MK8	a	145	9/10	0.96	0.17	65,68,73,74	0
2	2JN	j	153	9/10	0.96	0.11	83,92,93,97	0
2	MK8	p	145	9/10	0.96	0.15	95,105,107,111	0
2	2JN	o	153	9/10	0.96	0.12	77,87,89,91	0
2	MK8	f	145	9/10	0.96	0.09	77,85,90,93	0
2	2JN	l	153	9/10	0.97	0.10	70,78,84,85	0
2	2JN	m	153	9/10	0.97	0.10	74,83,89,90	0
2	MK8	k	145	9/10	0.97	0.08	71,76,83,89	0
2	MK8	l	145	9/10	0.97	0.12	76,79,84,85	0
2	2JN	k	153	9/10	0.97	0.11	68,77,85,86	0

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
4	NH2	f	201	1/1	0.27	0.14	100,100,100,100	0
3	SO4	G	201	5/5	0.28	0.09	127,134,138,140	5
3	SO4	D	202	5/5	0.41	0.12	109,113,122,123	5
3	SO4	g	202	5/5	0.43	0.12	109,115,120,124	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	O	201	5/5	0.57	0.08	118,123,132,136	5
3	SO4	G	202	5/5	0.62	0.12	107,109,115,122	5
3	SO4	K	202	5/5	0.66	0.08	115,117,124,126	5
3	SO4	K	201	5/5	0.68	0.08	115,121,131,136	5
3	SO4	H	201	5/5	0.68	0.07	118,125,131,137	5
5	GOL	F	203	6/6	0.68	0.10	92,100,112,121	0
3	SO4	F	202	5/5	0.69	0.10	88,99,107,117	5
4	NH2	p	201	1/1	0.71	0.11	101,101,101,101	0
3	SO4	A	205	5/5	0.71	0.10	93,94,99,113	5
5	GOL	C	202	6/6	0.72	0.08	97,103,111,114	0
3	SO4	A	202	5/5	0.72	0.13	100,103,110,117	5
4	NH2	n	201	1/1	0.75	0.10	80,80,80,80	0
5	GOL	I	201	6/6	0.76	0.08	103,114,125,133	0
3	SO4	A	203	5/5	0.79	0.09	117,119,122,127	5
5	GOL	i	202	6/6	0.79	0.08	101,102,112,113	0
3	SO4	D	201	5/5	0.80	0.07	115,116,120,126	5
3	SO4	L	201	5/5	0.80	0.08	106,106,121,122	5
4	NH2	b	201	1/1	0.81	0.15	92,92,92,92	0
3	SO4	F	201	5/5	0.83	0.19	85,89,98,104	5
4	NH2	g	201	1/1	0.83	0.14	107,107,107,107	0
4	NH2	d	201	1/1	0.84	0.08	90,90,90,90	0
4	NH2	k	201	1/1	0.85	0.14	83,83,83,83	0
4	NH2	o	201	1/1	0.86	0.08	95,95,95,95	0
4	NH2	m	201	1/1	0.86	0.22	87,87,87,87	0
4	NH2	a	201	1/1	0.89	0.15	86,86,86,86	0
4	NH2	l	201	1/1	0.93	0.08	94,94,94,94	0
4	NH2	h	201	1/1	0.93	0.08	93,93,93,93	0
4	NH2	e	201	1/1	0.93	0.09	86,86,86,86	0
4	NH2	i	201	1/1	0.94	0.04	90,90,90,90	0
4	NH2	j	201	1/1	0.94	0.07	105,105,105,105	0
3	SO4	C	201	5/5	0.94	0.06	88,89,97,98	5
3	SO4	A	204	5/5	0.94	0.06	79,86,92,93	5
3	SO4	A	201	5/5	0.95	0.06	78,79,88,88	0
4	NH2	c	201	1/1	0.97	0.05	84,84,84,84	0

6.5 Other polymers ⓘ

There are no such residues in this entry.