



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:25 PM UTC

PDB ID : 8SW9 / pdb_00008sw9
Title : Plasmodium falciparum M17 (A460S) mutant
Authors : McGowan, S.; Suraweera, C.; Drinkwater, N.
Deposited on : 2023-05-17
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

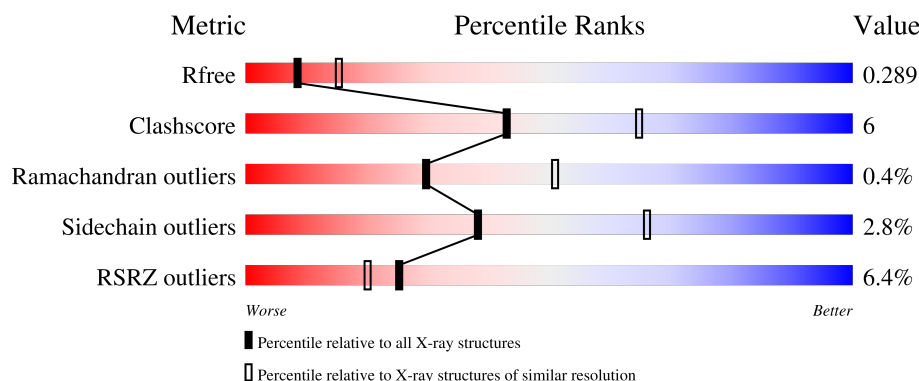
1 Overall quality at a glance

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	528	4% 83% 15% .
1	B	528	9% 79% 17% ..
1	C	528	4% 84% 13% ..
1	D	528	3% 82% 15% ..
1	E	528	2% 82% 14% .

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Mol	Chain	Length	Quality of chain
1	F	528	
1	G	528	
1	H	528	
1	I	528	
1	J	528	
1	K	528	
1	L	528	

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	CO3	H	703	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 93534 atoms, of which 45524 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 Leucine aminopeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	517	Total	C	H	N	O	S	0	1	0
			7782	2533	3841	632	757	19			
1	B	511	Total	C	H	N	O	S	0	0	0
			7528	2470	3698	618	723	19			
1	C	518	Total	C	H	N	O	S	0	0	0
			7820	2540	3871	637	753	19			
1	D	513	Total	C	H	N	O	S	0	0	0
			7748	2520	3832	631	745	20			
1	E	509	Total	C	H	N	O	S	0	0	0
			7674	2499	3789	623	744	19			
1	F	510	Total	C	H	N	O	S	0	0	0
			7365	2428	3589	609	720	19			
1	G	514	Total	C	H	N	O	S	0	0	0
			7798	2530	3862	633	754	19			
1	H	511	Total	C	H	N	O	S	0	0	0
			7605	2485	3742	622	737	19			
1	I	515	Total	C	H	N	O	S	0	0	0
			7736	2518	3827	631	741	19			
1	J	514	Total	C	H	N	O	S	0	0	0
			7753	2521	3840	632	741	19			
1	K	509	Total	C	H	N	O	S	3	0	0
			7624	2489	3757	620	739	19			
1	L	508	Total	C	H	N	O	S	1	0	0
			7424	2442	3623	611	729	19			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP Q8IL11
A	460	SER	ALA	engineered mutation	UNP Q8IL11
A	515	GLN	ASN	engineered mutation	UNP Q8IL11
A	546	GLN	ASN	engineered mutation	UNP Q8IL11
A	606	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
A	607	HIS	-	expression tag	UNP Q8IL11
A	608	HIS	-	expression tag	UNP Q8IL11
A	609	HIS	-	expression tag	UNP Q8IL11
A	610	HIS	-	expression tag	UNP Q8IL11
A	611	HIS	-	expression tag	UNP Q8IL11
B	152	GLN	ASN	engineered mutation	UNP Q8IL11
B	460	SER	ALA	engineered mutation	UNP Q8IL11
B	515	GLN	ASN	engineered mutation	UNP Q8IL11
B	546	GLN	ASN	engineered mutation	UNP Q8IL11
B	606	HIS	-	expression tag	UNP Q8IL11
B	607	HIS	-	expression tag	UNP Q8IL11
B	608	HIS	-	expression tag	UNP Q8IL11
B	609	HIS	-	expression tag	UNP Q8IL11
B	610	HIS	-	expression tag	UNP Q8IL11
B	611	HIS	-	expression tag	UNP Q8IL11
C	152	GLN	ASN	engineered mutation	UNP Q8IL11
C	460	SER	ALA	engineered mutation	UNP Q8IL11
C	515	GLN	ASN	engineered mutation	UNP Q8IL11
C	546	GLN	ASN	engineered mutation	UNP Q8IL11
C	606	HIS	-	expression tag	UNP Q8IL11
C	607	HIS	-	expression tag	UNP Q8IL11
C	608	HIS	-	expression tag	UNP Q8IL11
C	609	HIS	-	expression tag	UNP Q8IL11
C	610	HIS	-	expression tag	UNP Q8IL11
C	611	HIS	-	expression tag	UNP Q8IL11
D	152	GLN	ASN	engineered mutation	UNP Q8IL11
D	460	SER	ALA	engineered mutation	UNP Q8IL11
D	515	GLN	ASN	engineered mutation	UNP Q8IL11
D	546	GLN	ASN	engineered mutation	UNP Q8IL11
D	606	HIS	-	expression tag	UNP Q8IL11
D	607	HIS	-	expression tag	UNP Q8IL11
D	608	HIS	-	expression tag	UNP Q8IL11
D	609	HIS	-	expression tag	UNP Q8IL11
D	610	HIS	-	expression tag	UNP Q8IL11
D	611	HIS	-	expression tag	UNP Q8IL11
E	152	GLN	ASN	engineered mutation	UNP Q8IL11
E	460	SER	ALA	engineered mutation	UNP Q8IL11
E	515	GLN	ASN	engineered mutation	UNP Q8IL11
E	546	GLN	ASN	engineered mutation	UNP Q8IL11
E	606	HIS	-	expression tag	UNP Q8IL11
E	607	HIS	-	expression tag	UNP Q8IL11
E	608	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
E	609	HIS	-	expression tag	UNP Q8IL11
E	610	HIS	-	expression tag	UNP Q8IL11
E	611	HIS	-	expression tag	UNP Q8IL11
F	152	GLN	ASN	engineered mutation	UNP Q8IL11
F	460	SER	ALA	engineered mutation	UNP Q8IL11
F	515	GLN	ASN	engineered mutation	UNP Q8IL11
F	546	GLN	ASN	engineered mutation	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression tag	UNP Q8IL11
G	152	GLN	ASN	engineered mutation	UNP Q8IL11
G	460	SER	ALA	engineered mutation	UNP Q8IL11
G	515	GLN	ASN	engineered mutation	UNP Q8IL11
G	546	GLN	ASN	engineered mutation	UNP Q8IL11
G	606	HIS	-	expression tag	UNP Q8IL11
G	607	HIS	-	expression tag	UNP Q8IL11
G	608	HIS	-	expression tag	UNP Q8IL11
G	609	HIS	-	expression tag	UNP Q8IL11
G	610	HIS	-	expression tag	UNP Q8IL11
G	611	HIS	-	expression tag	UNP Q8IL11
H	152	GLN	ASN	engineered mutation	UNP Q8IL11
H	460	SER	ALA	engineered mutation	UNP Q8IL11
H	515	GLN	ASN	engineered mutation	UNP Q8IL11
H	546	GLN	ASN	engineered mutation	UNP Q8IL11
H	606	HIS	-	expression tag	UNP Q8IL11
H	607	HIS	-	expression tag	UNP Q8IL11
H	608	HIS	-	expression tag	UNP Q8IL11
H	609	HIS	-	expression tag	UNP Q8IL11
H	610	HIS	-	expression tag	UNP Q8IL11
H	611	HIS	-	expression tag	UNP Q8IL11
I	152	GLN	ASN	engineered mutation	UNP Q8IL11
I	460	SER	ALA	engineered mutation	UNP Q8IL11
I	515	GLN	ASN	engineered mutation	UNP Q8IL11
I	546	GLN	ASN	engineered mutation	UNP Q8IL11
I	606	HIS	-	expression tag	UNP Q8IL11
I	607	HIS	-	expression tag	UNP Q8IL11
I	608	HIS	-	expression tag	UNP Q8IL11
I	609	HIS	-	expression tag	UNP Q8IL11
I	610	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
I	611	HIS	-	expression tag	UNP Q8IL11
J	152	GLN	ASN	engineered mutation	UNP Q8IL11
J	460	SER	ALA	engineered mutation	UNP Q8IL11
J	515	GLN	ASN	engineered mutation	UNP Q8IL11
J	546	GLN	ASN	engineered mutation	UNP Q8IL11
J	606	HIS	-	expression tag	UNP Q8IL11
J	607	HIS	-	expression tag	UNP Q8IL11
J	608	HIS	-	expression tag	UNP Q8IL11
J	609	HIS	-	expression tag	UNP Q8IL11
J	610	HIS	-	expression tag	UNP Q8IL11
J	611	HIS	-	expression tag	UNP Q8IL11
K	152	GLN	ASN	engineered mutation	UNP Q8IL11
K	460	SER	ALA	engineered mutation	UNP Q8IL11
K	515	GLN	ASN	engineered mutation	UNP Q8IL11
K	546	GLN	ASN	engineered mutation	UNP Q8IL11
K	606	HIS	-	expression tag	UNP Q8IL11
K	607	HIS	-	expression tag	UNP Q8IL11
K	608	HIS	-	expression tag	UNP Q8IL11
K	609	HIS	-	expression tag	UNP Q8IL11
K	610	HIS	-	expression tag	UNP Q8IL11
K	611	HIS	-	expression tag	UNP Q8IL11
L	152	GLN	ASN	engineered mutation	UNP Q8IL11
L	460	SER	ALA	engineered mutation	UNP Q8IL11
L	515	GLN	ASN	engineered mutation	UNP Q8IL11
L	546	GLN	ASN	engineered mutation	UNP Q8IL11
L	606	HIS	-	expression tag	UNP Q8IL11
L	607	HIS	-	expression tag	UNP Q8IL11
L	608	HIS	-	expression tag	UNP Q8IL11
L	609	HIS	-	expression tag	UNP Q8IL11
L	610	HIS	-	expression tag	UNP Q8IL11
L	611	HIS	-	expression tag	UNP Q8IL11

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

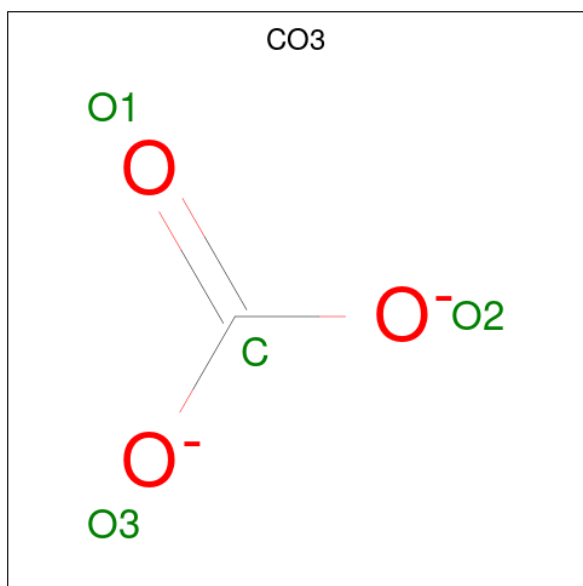
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		
2	G	2	Total	Zn	0	0
			2	2		
2	H	2	Total	Zn	0	0
			2	2		
2	I	2	Total	Zn	0	0
			2	2		
2	J	2	Total	Zn	0	0
			2	2		
2	K	2	Total	Zn	0	0
			2	2		
2	L	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



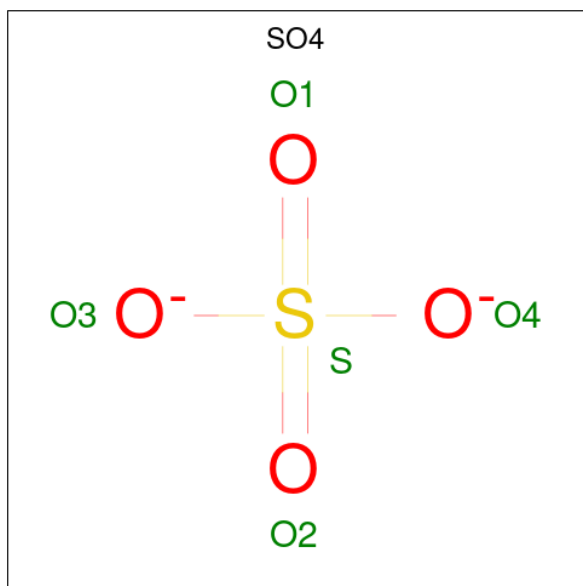
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	B	1	Total	C	O	0	0
			4	1	3		
3	C	1	Total	C	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 4 1 3	0	0
3	E	1	Total C O 4 1 3	0	0
3	F	1	Total C O 4 1 3	0	0
3	G	1	Total C O 4 1 3	0	0
3	H	1	Total C O 4 1 3	0	0
3	I	1	Total C O 4 1 3	0	0
3	J	1	Total C O 4 1 3	0	0
3	K	1	Total C O 4 1 3	0	0
3	L	1	Total C O 4 1 3	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



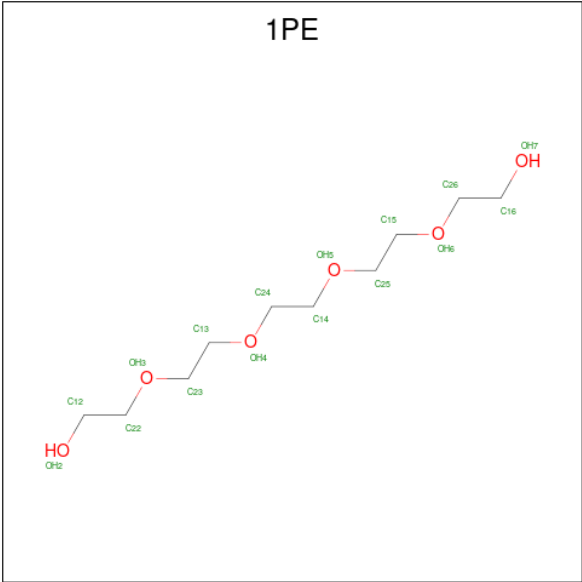
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			19	6	10	3		
5	A	1	Total	C	H	O	0	0
			23	6	13	4		
5	B	1	Total	C	H	O	0	0
			13	5	6	2		
5	C	1	Total	C	H	O	0	0
			27	9	14	4		
5	C	1	Total	C	H	O	0	0
			19	6	10	3		
5	C	1	Total	C	H	O	0	0
			23	6	13	4		
5	D	1	Total	C	H	O	0	0
			20	7	10	3		
5	D	1	Total	C	H	O	0	0
			20	7	10	3		
5	D	1	Total	C	H	O	0	0
			20	6	11	3		
5	E	1	Total	C	H	O	0	0
			26	8	14	4		
5	E	1	Total	C	H	O	0	0
			20	6	11	3		
5	F	1	Total	C	H	O	0	0
			23	6	13	4		
5	G	1	Total	C	H	O	0	0
			19	6	10	3		
5	G	1	Total	C	H	O	0	0
			23	6	13	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	H	O	0	0
			30	8	17	5		
5	H	1	Total	C	H	O	0	0
			20	7	10	3		
5	J	1	Total	C	H	O	0	0
			23	6	13	4		
5	K	1	Total	C	H	O	0	0
			20	6	11	3		
5	K	1	Total	C	H	O	0	0
			38	10	22	6		
5	L	1	Total	C	H	O	0	0
			38	10	22	6		

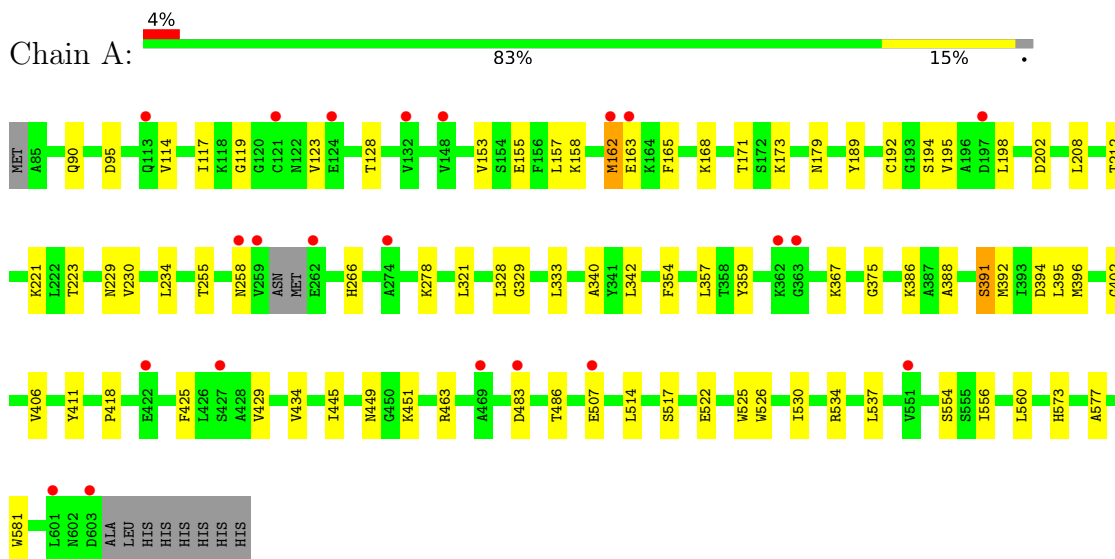
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	97	Total	O	0	0
			97	97		
6	B	78	Total	O	0	0
			78	78		
6	C	79	Total	O	0	0
			79	79		
6	D	87	Total	O	0	0
			87	87		
6	E	119	Total	O	0	0
			119	119		
6	F	94	Total	O	0	0
			94	94		
6	G	85	Total	O	0	0
			85	85		
6	H	79	Total	O	0	0
			79	79		
6	I	98	Total	O	0	0
			98	98		
6	J	86	Total	O	0	0
			86	86		
6	K	88	Total	O	0	0
			88	88		
6	L	66	Total	O	0	0
			66	66		

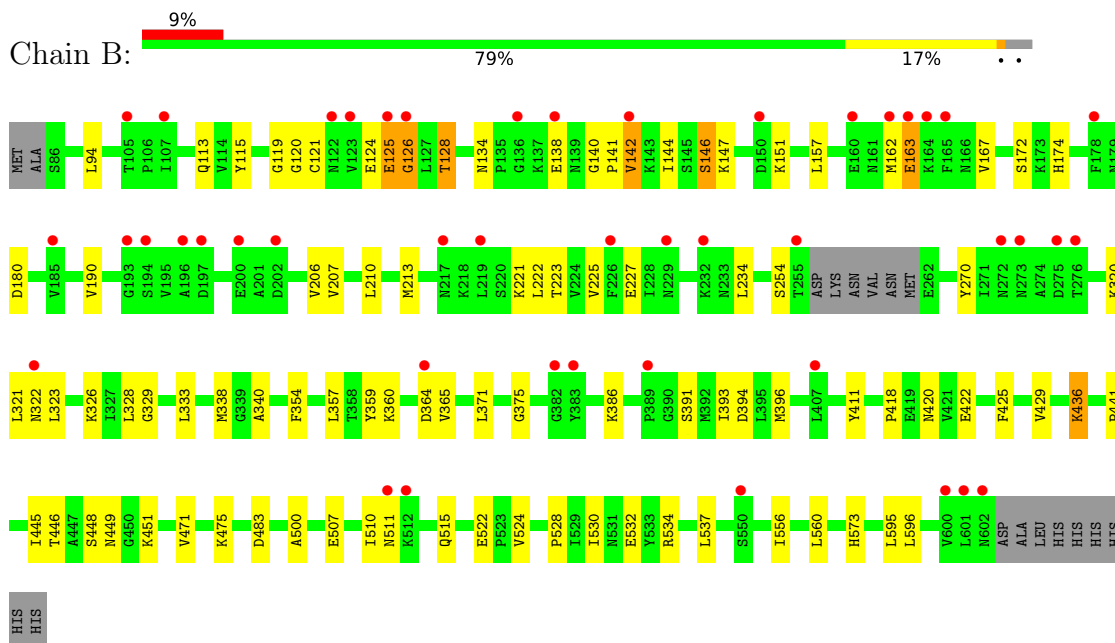
3 Residue-property plots [i](#)

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

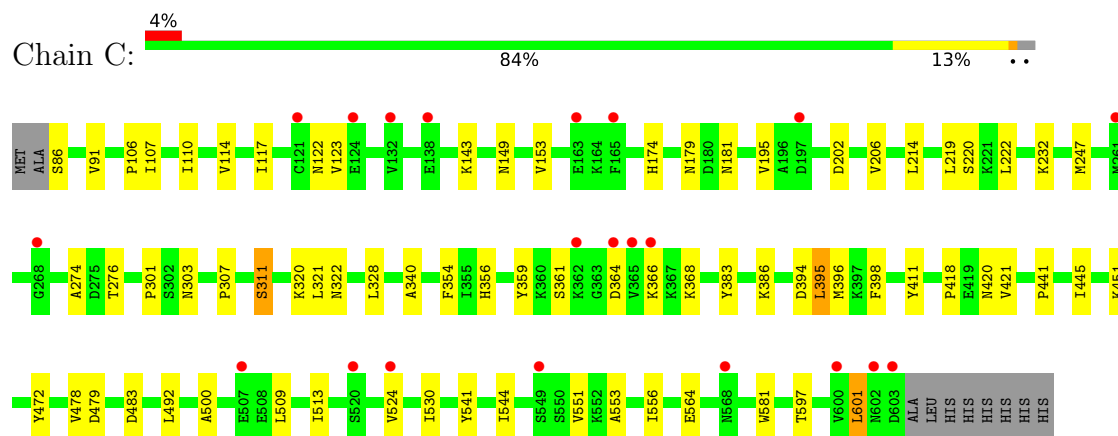
- Molecule 1: Leucine aminopeptidase



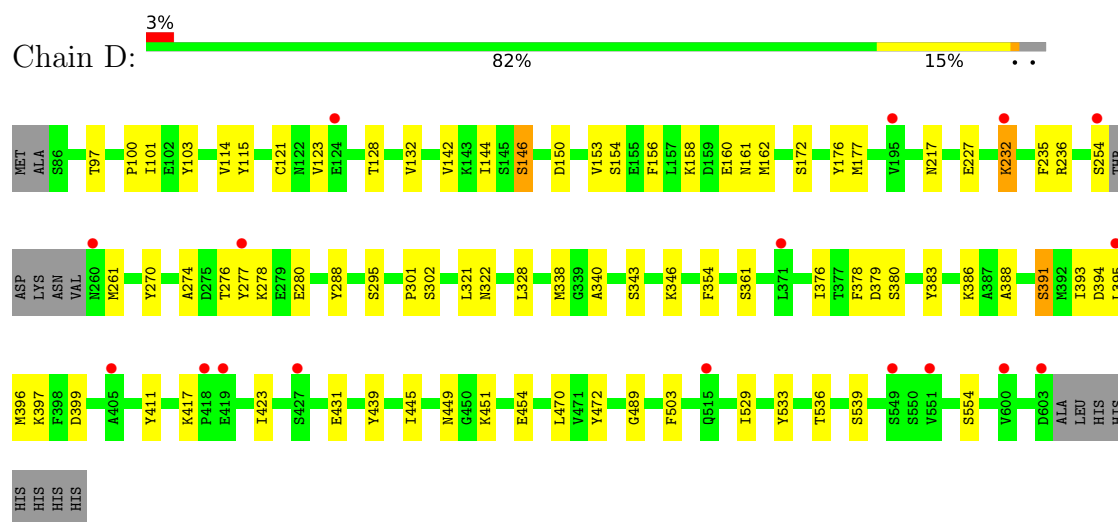
- Molecule 1: Leucine aminopeptidase



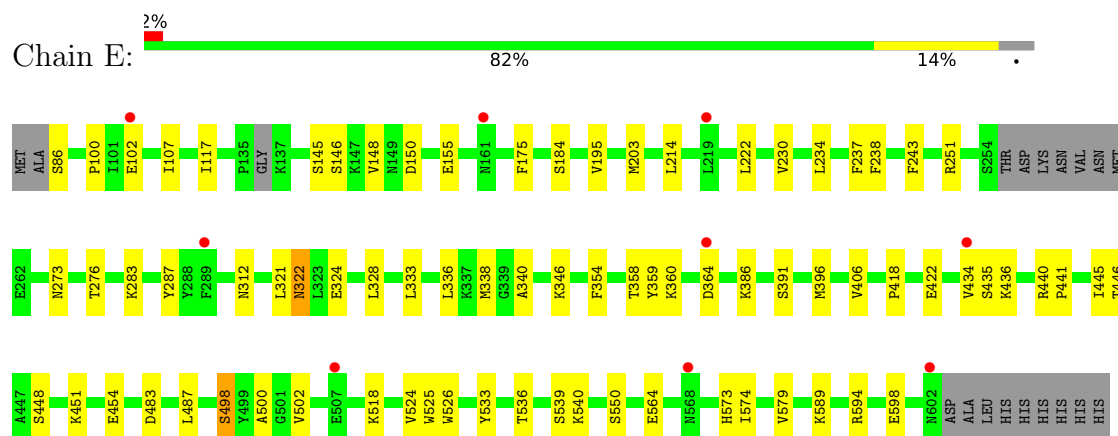
- Molecule 1: Leucine aminopeptidase



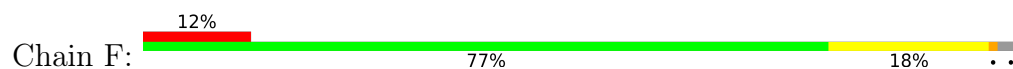
- Molecule 1: Leucine aminopeptidase

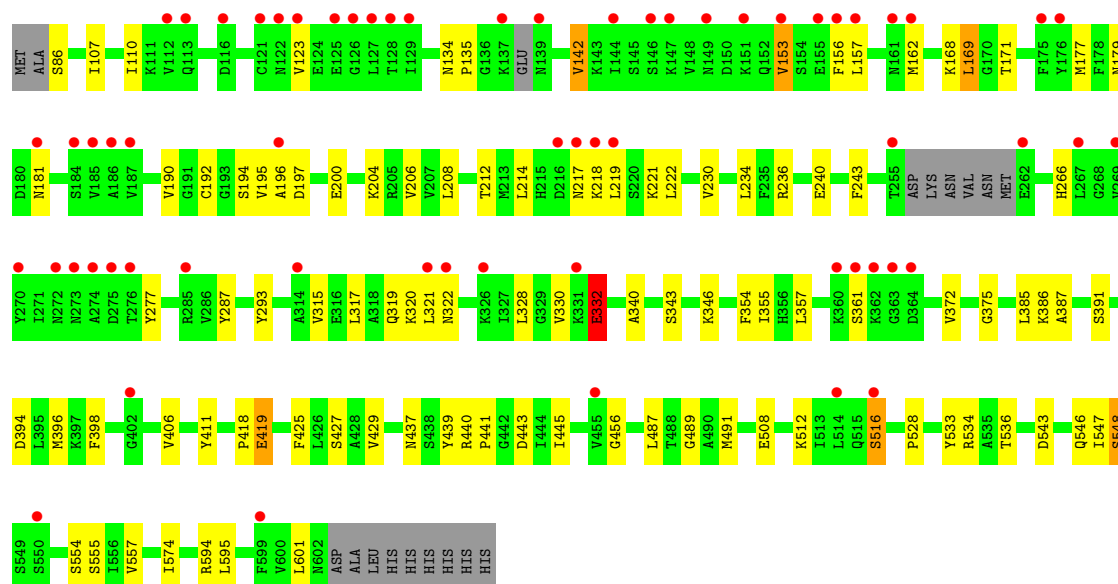


- Molecule 1: Leucine aminopeptidase

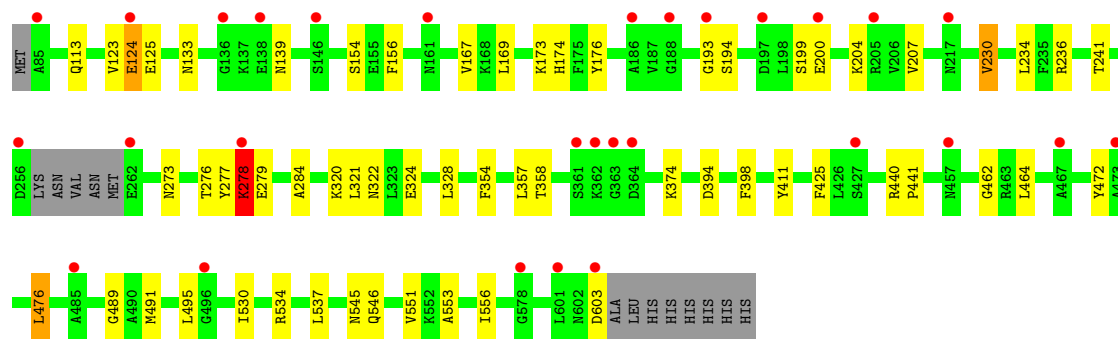
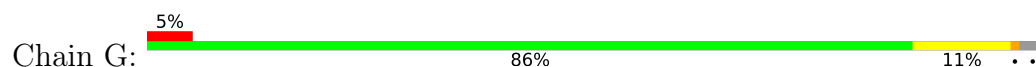


- Molecule 1: Leucine aminopeptidase

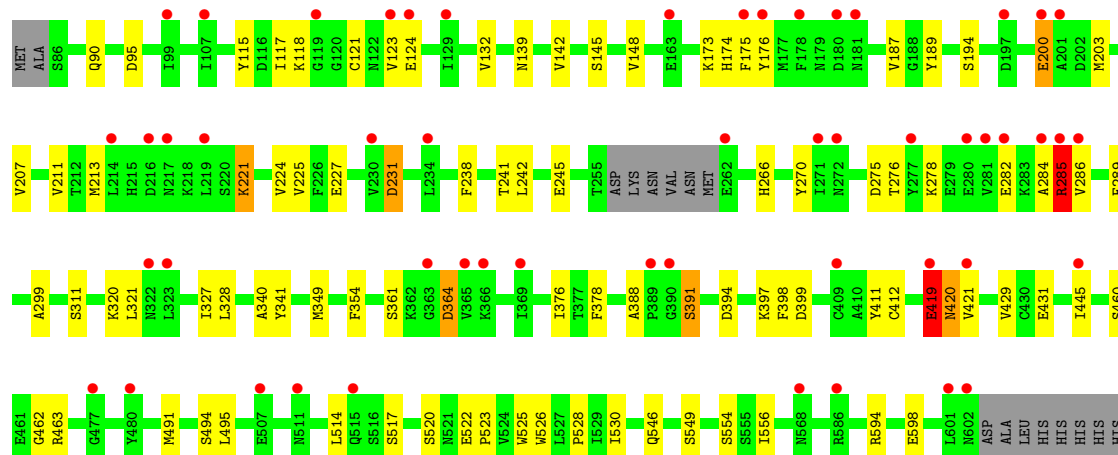
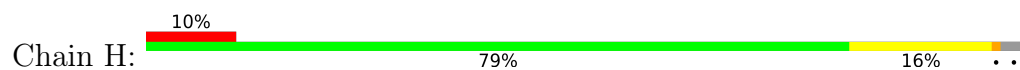




• Molecule 1: Leucine aminopeptidase



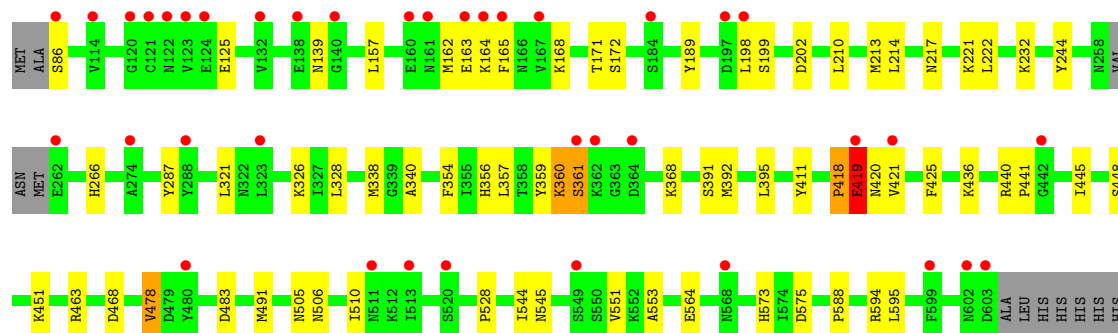
• Molecule 1: Leucine aminopeptidase



HIS

- Molecule 1: Leucine aminopeptidase

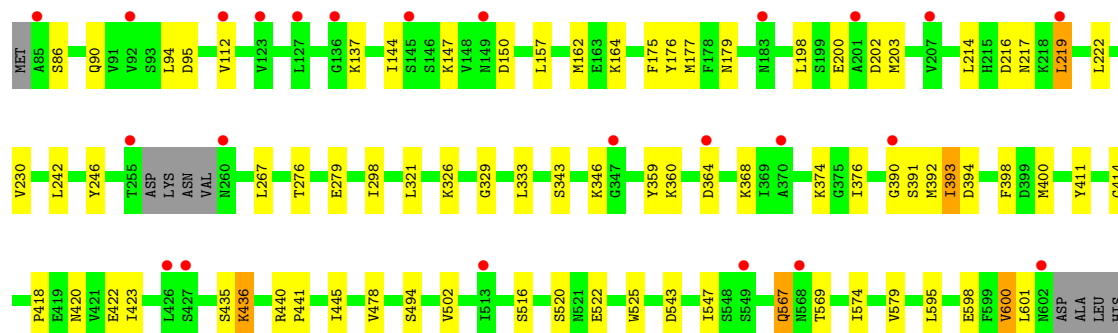
Chain I: 7% 84% 12% ..



HIS

- Molecule 1: Leucine aminopeptidase

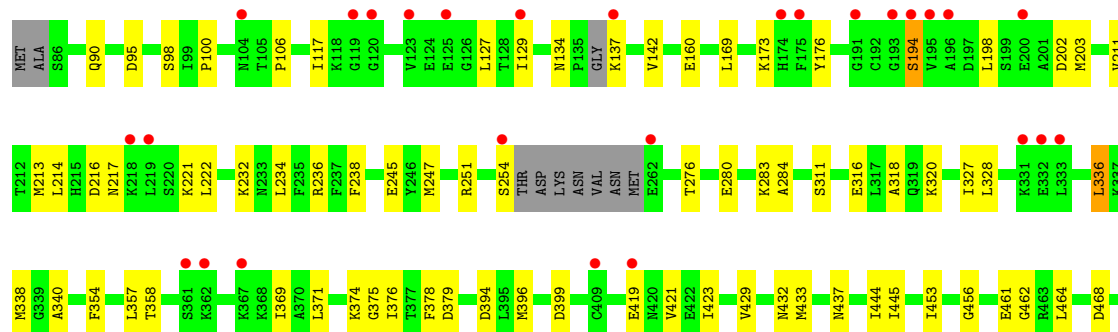
Chain J: 5% 82% 14% ..



HIS

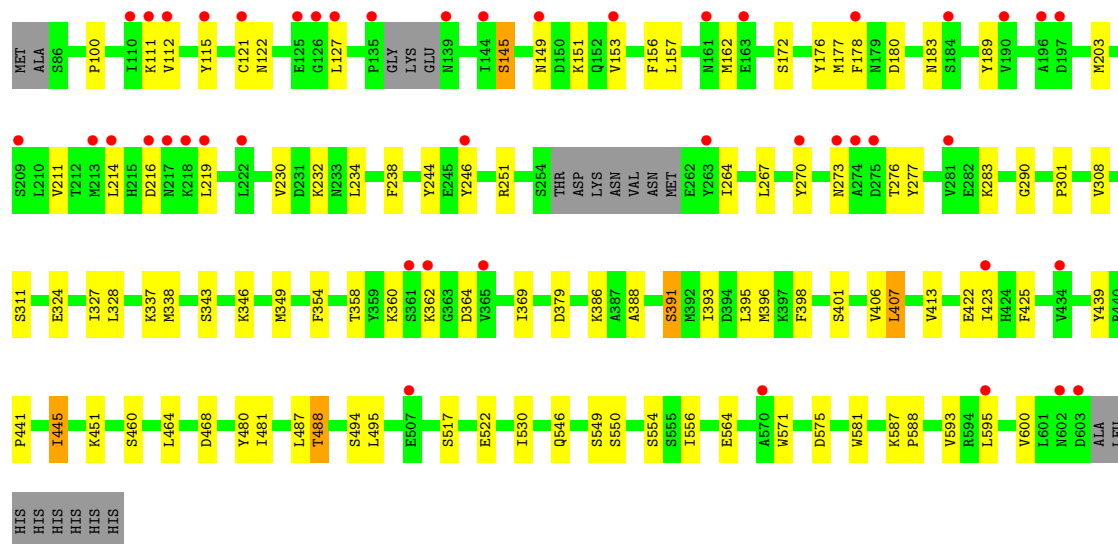
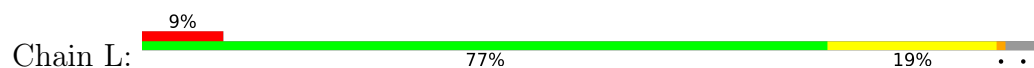
- Molecule 1: Leucine aminopeptidase

Chain K: 6% 79% 17% .





● Molecule 1: Leucine aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	174.34Å 176.72Å 225.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 2.60 49.57 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.57-2.60) 100.0 (49.57-2.60)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.235 , 0.281 (Not available) , 0.289	Depositor DCC
R_{free} test set	10861 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.882	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	93534	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1391e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 1PE, SO4, ZN, CO3

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	0.16	1/4021 (0.0%)	0.32	0/5459
1	B	0.16	0/3907	0.54	3/5312 (0.1%)
1	C	0.10	0/4027	0.29	0/5465
1	D	0.18	0/3993	0.30	0/5417
1	E	0.09	0/3961	0.27	0/5375
1	F	0.10	0/3850	0.27	0/5241
1	G	0.09	0/4012	0.28	0/5442
1	H	0.11	0/3940	0.32	0/5354
1	I	0.15	1/3986 (0.0%)	0.30	0/5410
1	J	0.09	0/3990	0.28	0/5414
1	K	0.13	0/3943	0.28	0/5354
1	L	0.09	0/3876	0.28	0/5277
All	All	0.13	2/47506 (0.0%)	0.32	3/64520 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	F	0	1
1	G	0	1
1	H	0	2
1	I	0	4
1	K	0	1
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	ASN	CG-OD1	5.40	1.33	1.23
1	I	545	ASN	CG-OD1	5.02	1.33	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	GLU	CG-CD-OE2	-18.07	76.84	118.40
1	B	125	GLU	OE1-CD-OE2	-17.93	79.88	122.90
1	B	125	GLU	CG-CD-OE1	16.57	156.51	118.40

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	MET	Peptide
1	D	232	LYS	Peptide
1	F	332	GLU	Peptide
1	G	277	TYR	Peptide
1	H	284	ALA	Peptide
1	H	419	GLU	Peptide
1	I	360	LYS	Peptide
1	I	361	SER	Peptide
1	I	418	PRO	Peptide
1	I	419	GLU	Peptide
1	K	194	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3941	3841	3841	47	1
1	B	3830	3698	3698	52	0
1	C	3949	3871	3871	39	0
1	D	3916	3832	3832	51	0
1	E	3885	3789	3789	47	0
1	F	3776	3589	3588	61	0
1	G	3936	3862	3862	37	1
1	H	3863	3742	3742	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	3909	3827	3827	41	0
1	J	3913	3840	3836	49	0
1	K	3867	3757	3757	60	0
1	L	3801	3623	3623	61	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	4	0	0	1	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	2	0
3	I	4	0	0	1	0
3	J	4	0	0	0	0
3	K	4	0	0	0	0
3	L	4	0	0	0	0
4	A	10	0	0	1	0
4	B	5	0	0	1	0
4	C	10	0	0	1	0
4	D	5	0	0	1	0
4	E	5	0	0	1	0
4	F	5	0	0	0	0
4	G	10	0	0	0	0
4	H	5	0	0	0	0
4	I	10	0	0	1	0
4	J	5	0	0	1	0
4	K	5	0	0	0	0
4	L	10	0	0	0	0
5	A	19	23	23	3	0
5	B	7	6	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	37	37	1	0
5	D	29	31	31	2	0
5	E	21	25	25	1	0
5	F	10	13	13	4	0
5	G	32	40	40	4	0
5	H	10	10	10	1	0
5	J	10	13	13	0	0
5	K	25	33	33	2	0
5	L	16	22	22	2	0
6	A	97	0	0	1	0
6	B	78	0	0	1	0
6	C	79	0	0	0	0
6	D	87	0	0	2	0
6	E	119	0	0	4	0
6	F	94	0	0	7	0
6	G	85	0	0	4	0
6	H	79	0	0	1	0
6	I	98	0	0	2	0
6	J	86	0	0	5	0
6	K	88	0	0	3	0
6	L	66	0	0	0	0
All	All	48010	45524	45519	573	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 6.

All (573) 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:J:400:MET:HE2	6:J:805:HOH:O	1.44	1.17
1:J:400:MET:CE	6:J:805:HOH:O	2.04	1.00
1:J:298:ILE:HA	1:J:400:MET:HE1	1.45	0.96
1:H:286:VAL:HG11	1:H:412:CYS:HA	1.60	0.81
1:E:273:ASN:OD1	1:E:276:THR:OG1	1.99	0.81
1:L:386:LYS:HB2	1:L:393:ILE:HD12	1.63	0.79
1:J:390:GLY:O	1:J:392:MET:N	2.17	0.77
1:I:419:GLU:HB2	1:I:421:VAL:H	1.50	0.75
1:B:142:VAL:HG12	1:B:167:VAL:HG12	1.70	0.74
1:B:532:GLU:OE1	1:E:498:SER:OG	2.04	0.74
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.69	0.74
1:L:338:MET:HE3	1:L:468:ASP:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:157:LEU:HD23	1:J:162:MET:HE3	1.70	0.73
1:L:451:LYS:HZ2	5:L:706:1PE:H232	1.54	0.72
1:F:221:LYS:HG3	1:F:266:HIS:HB2	1.71	0.71
1:H:231:ASP:OD1	1:H:231:ASP:N	2.22	0.71
1:D:232:LYS:HA	1:D:235:PHE:H	1.54	0.71
1:I:172:SER:HB2	1:I:213:MET:HE2	1.72	0.70
1:B:134:ASN:ND2	1:B:141:PRO:O	2.24	0.70
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.73	0.69
1:F:321:LEU:HD11	1:F:411:TYR:HA	1.72	0.69
1:H:462:GLY:N	3:H:703:CO3:O2	2.24	0.69
1:F:214:LEU:HD21	1:F:222:LEU:HD13	1.72	0.69
1:I:419:GLU:HG3	1:I:420:ASN:H	1.58	0.69
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.73	0.69
1:D:503:PHE:HB3	1:D:529:ILE:HD11	1.75	0.68
1:K:378:PHE:HD2	1:K:433:MET:HE1	1.59	0.68
1:E:518:LYS:NZ	6:E:801:HOH:O	2.26	0.68
1:K:374:LYS:HE3	1:K:462:GLY:HA3	1.76	0.68
1:F:195:VAL:O	1:F:197:ASP:N	2.26	0.67
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.76	0.67
1:B:326:LYS:HE2	1:B:328:LEU:HD21	1.75	0.67
1:G:489:GLY:HA3	5:G:706:1PE:H241	1.75	0.66
1:B:320:LYS:NZ	6:B:1101:HOH:O	2.29	0.66
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.76	0.66
1:A:123:VAL:HG21	1:A:153:VAL:HG11	1.76	0.66
1:L:423:ILE:HD11	1:L:600:VAL:HG11	1.78	0.65
1:F:157:LEU:HA	1:F:162:MET:HE2	1.79	0.65
1:G:230:VAL:HG12	1:G:234:LEU:HD23	1.77	0.65
1:H:388:ALA:O	1:H:391:SER:OG	2.15	0.65
1:I:163:GLU:HG3	1:I:164:LYS:N	2.11	0.65
1:K:374:LYS:HE2	1:K:376:ILE:HG13	1.79	0.65
1:K:129:ILE:HD11	1:K:213:MET:HE1	1.79	0.64
1:H:463:ARG:NE	3:H:703:CO3:O1	2.27	0.64
1:F:361:SER:HB3	1:F:419:GLU:HA	1.78	0.64
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.79	0.64
1:G:534:ARG:O	1:G:534:ARG:NH1	2.27	0.64
1:H:419:GLU:O	1:H:421:VAL:N	2.30	0.64
1:A:157:LEU:HA	1:A:162:MET:HE3	1.78	0.63
1:J:436:LYS:NZ	1:K:437:ASN:OD1	2.31	0.63
1:F:489:GLY:HA3	5:F:705:1PE:H222	1.80	0.63
1:H:285:ARG:HG2	1:H:286:VAL:HG23	1.79	0.63
1:I:359:TYR:OH	1:I:418:PRO:O	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:144:ILE:HG21	1:J:157:LEU:HD22	1.79	0.63
1:D:380:SER:HA	1:D:393:ILE:HD11	1.79	0.62
1:A:114:VAL:HG11	1:A:278:LYS:HB3	1.80	0.62
1:H:364:ASP:O	1:H:420:ASN:ND2	2.18	0.62
1:D:388:ALA:O	1:D:391:SER:OG	2.15	0.62
1:E:451:LYS:NZ	1:E:564:GLU:O	2.32	0.62
1:F:534:ARG:O	1:F:534:ARG:NH1	2.33	0.62
1:B:134:ASN:HB2	1:B:167:VAL:HG11	1.80	0.62
1:D:343:SER:HA	1:D:346:LYS:HD3	1.81	0.62
1:B:151:LYS:N	1:B:180:ASP:OD2	2.33	0.62
1:D:161:ASN:ND2	6:D:807:HOH:O	2.32	0.61
1:D:232:LYS:HB3	1:D:235:PHE:HB3	1.81	0.61
1:K:483:ASP:OD1	1:K:573:HIS:ND1	2.27	0.61
1:F:340:ALA:HA	1:F:445:ILE:HD12	1.82	0.61
1:G:394:ASP:HA	1:I:441:PRO:HB2	1.81	0.61
1:F:123:VAL:HG21	1:F:153:VAL:HG21	1.82	0.60
1:H:491:MET:HE2	1:H:491:MET:HA	1.84	0.60
1:F:168:LYS:O	1:F:171:THR:HG22	2.00	0.60
1:A:173:LYS:NZ	6:A:803:HOH:O	2.34	0.60
1:D:533:TYR:O	1:D:536:THR:HG22	2.02	0.60
1:D:146:SER:OG	1:D:227:GLU:OE2	2.20	0.60
1:J:198:LEU:HD22	1:J:202:ASP:HB3	1.83	0.60
1:F:107:ILE:HA	1:F:110:ILE:HD12	1.84	0.60
1:H:123:VAL:HG23	1:H:124:GLU:H	1.67	0.59
1:B:507:GLU:HA	1:B:510:ILE:HD12	1.85	0.59
1:L:324:GLU:HB3	1:L:358:THR:HB	1.84	0.59
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.83	0.59
1:L:244:TYR:OH	1:L:588:PRO:O	2.18	0.59
1:K:316:GLU:HG3	5:K:705:1PE:H121	1.85	0.59
1:L:388:ALA:O	1:L:391:SER:OG	2.19	0.59
1:G:357:LEU:HB2	1:G:425:PHE:HB2	1.84	0.59
1:I:214:LEU:HD21	1:I:222:LEU:HD22	1.85	0.59
1:K:160:GLU:OE2	1:K:160:GLU:N	2.25	0.59
1:K:203:MET:HE2	1:K:234:LEU:HG	1.83	0.59
1:E:540:LYS:NZ	6:E:806:HOH:O	2.36	0.59
1:B:500:ALA:HB3	1:B:524:VAL:HG22	1.85	0.58
1:A:198:LEU:HD22	1:A:202:ASP:HB3	1.86	0.58
1:C:551:VAL:HG12	1:C:553:ALA:H	1.68	0.58
1:L:115:TYR:HB2	1:L:270:TYR:CE2	2.38	0.58
4:A:704:SO4:O4	1:C:541:TYR:OH	2.17	0.58
1:I:451:LYS:NZ	1:I:564:GLU:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:137:LYS:N	6:K:809:HOH:O	2.36	0.58
1:D:346:LYS:NZ	6:D:809:HOH:O	2.34	0.58
1:B:386:LYS:HB3	1:B:391:SER:HB3	1.85	0.58
1:L:172:SER:OG	1:L:189:TYR:O	2.19	0.58
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.84	0.58
1:D:132:VAL:HG21	1:D:142:VAL:HG13	1.85	0.57
1:J:214:LEU:HD21	1:J:222:LEU:HD22	1.86	0.57
1:A:340:ALA:HA	1:A:445:ILE:HD12	1.86	0.57
1:L:219:LEU:HB2	1:L:264:ILE:HG22	1.87	0.57
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.86	0.57
1:I:440:ARG:NH1	6:I:802:HOH:O	2.37	0.57
1:H:494:SER:OG	1:H:495:LEU:N	2.38	0.57
1:H:286:VAL:CG1	1:H:412:CYS:HA	2.31	0.56
1:F:320:LYS:NZ	6:F:807:HOH:O	2.35	0.56
1:H:419:GLU:O	1:H:421:VAL:HG22	2.05	0.56
1:B:338:MET:HG2	1:B:448:SER:HB3	1.87	0.56
1:H:460:SER:O	1:H:546:GLN:NE2	2.35	0.56
1:L:530:ILE:HD12	1:L:556:ILE:HD13	1.87	0.56
1:B:125:GLU:HG2	1:B:126:GLY:N	2.20	0.56
1:G:156:PHE:CZ	1:G:156:PHE:CD2	2.92	0.56
1:I:217:ASN:HB2	1:K:173:LYS:HZ1	1.70	0.56
1:K:221:LYS:NZ	6:K:806:HOH:O	2.33	0.56
1:D:301:PRO:HA	1:D:397:LYS:HD2	1.87	0.56
1:E:203:MET:HE2	1:E:238:PHE:HD1	1.71	0.56
1:F:156:PHE:CD2	1:F:177:MET:HE1	2.41	0.56
1:F:386:LYS:HB3	1:F:391:SER:HB2	1.87	0.56
1:A:388:ALA:O	1:A:391:SER:OG	2.23	0.56
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.88	0.56
1:H:174:HIS:CE1	1:H:213:MET:HG2	2.42	0.55
1:A:530:ILE:HD12	1:A:556:ILE:HD13	1.89	0.55
1:A:192:CYS:HB3	1:A:198:LEU:HD11	1.88	0.55
1:F:134:ASN:O	1:F:194:SER:OG	2.25	0.55
1:I:221:LYS:HG3	1:I:266:HIS:HB2	1.88	0.55
1:C:361:SER:OG	1:C:421:VAL:O	2.13	0.55
1:E:386:LYS:HB3	1:E:391:SER:HB2	1.88	0.54
1:J:321:LEU:HD11	1:J:411:TYR:HA	1.89	0.54
1:L:364:ASP:OD2	1:L:364:ASP:N	2.39	0.54
1:L:145:SER:O	1:L:145:SER:OG	2.25	0.54
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.88	0.54
1:L:156:PHE:CG	1:L:177:MET:HE1	2.42	0.54
1:D:321:LEU:HD11	1:D:411:TYR:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:543:ASP:OD2	1:K:254:SER:OG	2.26	0.54
1:C:214:LEU:HD21	1:C:222:LEU:HD22	1.90	0.54
1:E:483:ASP:OD1	1:E:573:HIS:ND1	2.41	0.54
1:F:533:TYR:O	1:F:536:THR:OG1	2.24	0.54
1:E:454:GLU:OE1	1:E:539:SER:OG	2.26	0.54
1:E:346:LYS:NZ	6:E:807:HOH:O	2.39	0.53
1:I:326:LYS:HB3	1:I:356:HIS:HB3	1.90	0.53
1:B:113:GLN:HG2	1:B:115:TYR:CZ	2.43	0.53
1:F:386:LYS:NZ	5:F:705:1PE:OH5	2.40	0.53
1:J:374:LYS:HE3	1:J:376:ILE:HG13	1.91	0.53
1:C:500:ALA:HB3	1:C:524:VAL:HG22	1.91	0.53
1:L:311:SER:HB2	1:L:327:ILE:HD12	1.89	0.53
1:A:90:GLN:HB3	1:A:95:ASP:HB2	1.90	0.53
1:B:441:PRO:HB2	1:C:394:ASP:HA	1.90	0.53
1:H:289:PHE:HD2	1:H:411:TYR:CE2	2.27	0.53
1:K:236:ARG:HD2	1:K:283:LYS:HG2	1.91	0.53
1:K:445:ILE:HD11	1:K:464:LEU:HD22	1.89	0.53
1:D:338:MET:HE1	1:D:472:TYR:HB2	1.90	0.53
1:E:203:MET:HB3	1:E:237:PHE:HE2	1.73	0.53
1:F:427:SER:O	6:F:801:HOH:O	2.18	0.53
1:H:225:VAL:HG22	1:H:270:TYR:HB2	1.90	0.53
1:D:431:GLU:OE2	1:F:440:ARG:NH1	2.42	0.53
1:B:128:THR:HG23	1:B:223:THR:HB	1.91	0.53
1:J:90:GLN:NE2	1:J:95:ASP:O	2.42	0.53
1:K:419:GLU:O	1:K:421:VAL:HG13	2.09	0.53
1:D:254:SER:OG	1:F:543:ASP:OD2	2.22	0.52
1:E:230:VAL:HG12	1:E:234:LEU:HD23	1.90	0.52
1:K:444:ILE:HG13	1:L:301:PRO:HG3	1.90	0.52
1:K:453:ILE:HD13	1:K:561:PHE:HZ	1.74	0.52
1:A:514:LEU:HD11	1:A:526:TRP:HB2	1.92	0.52
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.92	0.52
1:B:386:LYS:HE3	1:B:396:MET:HE2	1.91	0.52
1:K:90:GLN:NE2	1:K:95:ASP:O	2.36	0.52
1:L:230:VAL:O	1:L:277:TYR:OH	2.23	0.52
1:F:322:ASN:HB3	1:K:160:GLU:OE1	2.10	0.52
1:A:359:TYR:OH	1:A:418:PRO:O	2.24	0.52
1:H:282:GLU:O	1:H:285:ARG:NE	2.36	0.52
1:C:366:LYS:HG2	1:C:420:ASN:HB3	1.91	0.52
1:D:454:GLU:OE1	1:D:539:SER:OG	2.26	0.52
1:J:440:ARG:NH1	6:J:809:HOH:O	2.42	0.52
1:I:436:LYS:NZ	4:I:704:SO4:O1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:ASP:OD1	1:B:573:HIS:ND1	2.41	0.51
1:H:594:ARG:NH2	6:H:808:HOH:O	2.43	0.51
1:J:216:ASP:OD1	6:J:801:HOH:O	2.19	0.51
1:K:311:SER:HB2	1:K:327:ILE:HD12	1.92	0.51
1:C:320:LYS:NZ	5:C:705:1PE:OH3	2.42	0.51
1:E:359:TYR:OH	1:E:418:PRO:O	2.26	0.51
1:L:115:TYR:HB2	1:L:270:TYR:HE2	1.75	0.51
1:E:324:GLU:HB2	1:E:358:THR:HB	1.93	0.51
1:I:164:LYS:NZ	1:K:176:TYR:OH	2.23	0.51
1:D:232:LYS:HE3	1:D:277:TYR:HA	1.91	0.51
1:H:282:GLU:HB3	1:H:285:ARG:NE	2.25	0.51
1:I:357:LEU:HB2	1:I:425:PHE:HB2	1.92	0.51
1:C:107:ILE:HG12	1:C:247:MET:HG2	1.92	0.51
1:E:502:VAL:HG12	1:E:526:TRP:HA	1.92	0.51
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.92	0.51
1:D:394:ASP:HA	1:F:441:PRO:HB2	1.91	0.51
1:G:193:GLY:N	6:G:802:HOH:O	2.44	0.51
1:J:321:LEU:HD13	1:J:414:GLY:HA3	1.91	0.51
1:J:343:SER:HA	1:J:346:LYS:HG3	1.92	0.51
1:D:123:VAL:HG12	1:D:128:THR:HG21	1.93	0.51
1:F:142:VAL:HG22	1:F:162:MET:HB3	1.93	0.51
1:B:144:ILE:HG13	1:B:157:LEU:HD22	1.93	0.51
1:D:103:TYR:HB3	5:D:705:1PE:H242	1.93	0.51
1:F:230:VAL:HG12	1:F:234:LEU:HD23	1.93	0.51
1:F:512:LYS:O	1:F:516:SER:OG	2.26	0.51
1:F:548:SER:HB3	1:F:557:VAL:HG11	1.92	0.51
1:F:440:ARG:NH2	6:F:802:HOH:O	2.43	0.50
1:A:255:THR:HG21	1:C:451:LYS:HG2	1.93	0.50
1:H:118:LYS:HD2	1:H:118:LYS:N	2.27	0.50
1:L:413:VAL:HG11	1:L:423:ILE:HD12	1.93	0.50
1:G:440:ARG:NE	1:H:431:GLU:OE2	2.43	0.50
1:K:379:ASP:O	1:K:396:MET:HG3	2.10	0.50
1:A:434:VAL:HG23	1:C:383:TYR:HE1	1.76	0.50
1:H:376:ILE:HB	1:H:399:ASP:HB3	1.92	0.50
1:C:122:ASN:OD1	1:C:149:ASN:ND2	2.41	0.50
1:J:520:SER:HB3	1:J:598:GLU:HG3	1.93	0.50
1:E:184:SER:OG	4:E:704:SO4:O4	2.29	0.50
1:E:502:VAL:HG23	1:E:574:ILE:HG12	1.94	0.50
1:G:324:GLU:HB2	1:G:358:THR:HB	1.94	0.50
1:B:360:LYS:HG3	1:B:422:GLU:HG3	1.92	0.50
1:G:176:TYR:HB3	1:J:177:MET:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:134:ASN:H	1:K:194:SER:HB3	1.76	0.50
1:B:140:GLY:O	1:B:167:VAL:HG13	2.12	0.50
1:C:220:SER:OG	4:C:704:SO4:O3	2.30	0.50
1:J:217:ASN:HD21	1:J:219:LEU:HB2	1.76	0.50
1:L:121:CYS:HA	1:L:270:TYR:CE1	2.47	0.50
1:E:364:ASP:OD1	1:E:364:ASP:N	2.44	0.50
1:I:321:LEU:HD11	1:I:411:TYR:HA	1.94	0.50
1:H:525:TRP:CZ3	1:K:528:PRO:HB3	2.47	0.49
1:I:244:TYR:OH	1:I:588:PRO:O	2.29	0.49
1:J:94:LEU:HD21	1:L:337:LYS:HA	1.94	0.49
1:J:435:SER:OG	4:J:705:SO4:O2	2.25	0.49
1:B:471:VAL:HG12	1:B:475:LYS:HE3	1.95	0.49
1:H:517:SER:OG	1:H:522:GLU:O	2.24	0.49
1:A:165:PHE:HB3	1:A:189:TYR:OH	2.13	0.49
1:F:287:TYR:CD2	1:F:594:ARG:HG2	2.47	0.49
1:A:411:TYR:CE1	5:A:706:1PE:H242	2.48	0.49
1:F:236:ARG:NE	1:F:240:GLU:OE2	2.42	0.49
1:K:456:GLY:N	1:K:546:GLN:OE1	2.42	0.49
1:E:287:TYR:CD2	1:E:594:ARG:HG2	2.48	0.49
1:H:221:LYS:HD3	1:H:266:HIS:HB2	1.95	0.49
1:K:100:PRO:O	1:K:251:ARG:NH1	2.39	0.49
1:L:451:LYS:HE2	1:L:564:GLU:HB3	1.93	0.49
1:D:376:ILE:HB	1:D:399:ASP:HB3	1.95	0.49
1:I:491:MET:HE2	1:I:575:ASP:HB3	1.93	0.49
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.93	0.49
1:D:489:GLY:HA3	5:D:707:1PE:H132	1.94	0.49
1:G:273:ASN:O	1:G:276:THR:OG1	2.28	0.49
1:H:275:ASP:HA	1:H:278:LYS:HG2	1.95	0.49
1:A:168:LYS:O	1:A:171:THR:HG22	2.12	0.49
1:B:190:VAL:HG11	1:B:206:VAL:HG13	1.94	0.49
1:F:443:ASP:OD2	6:F:802:HOH:O	2.20	0.49
1:B:225:VAL:HG22	1:B:270:TYR:HB2	1.93	0.48
1:J:359:TYR:OH	1:J:418:PRO:O	2.29	0.48
1:L:153:VAL:O	1:L:157:LEU:HG	2.12	0.48
1:B:125:GLU:HG3	1:B:221:LYS:HB3	1.95	0.48
1:H:115:TYR:HD1	1:H:270:TYR:CZ	2.31	0.48
1:I:506:ASN:O	1:I:510:ILE:HG13	2.12	0.48
1:K:320:LYS:NZ	5:K:705:1PE:OH3	2.44	0.48
1:J:441:PRO:HB2	1:K:394:ASP:HA	1.93	0.48
1:D:232:LYS:HD2	1:D:280:GLU:HG3	1.96	0.48
1:I:165:PHE:HB3	1:I:189:TYR:OH	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:THR:HG23	1:A:223:THR:HB	1.93	0.48
1:A:230:VAL:HG12	1:A:234:LEU:HD23	1.95	0.48
1:C:597:THR:HG22	1:C:601:LEU:HD22	1.95	0.48
1:E:500:ALA:HB3	1:E:524:VAL:HG22	1.95	0.48
1:G:321:LEU:HD11	1:G:411:TYR:HA	1.94	0.48
1:K:232:LYS:NZ	1:K:276:THR:O	2.38	0.48
1:K:338:MET:HE2	1:K:468:ASP:HB3	1.95	0.48
1:K:371:LEU:HD13	1:K:596:LEU:HD22	1.95	0.48
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.94	0.48
1:L:203:MET:HE3	1:L:238:PHE:HB2	1.95	0.48
1:I:287:TYR:CD2	1:I:594:ARG:HG2	2.49	0.48
1:H:514:LEU:HD11	1:H:526:TRP:HB2	1.96	0.48
1:J:360:LYS:HG3	1:J:422:GLU:HG3	1.95	0.48
1:A:449:ASN:HD21	1:A:451:LYS:HD2	1.76	0.48
1:L:111:LYS:O	1:L:267:LEU:N	2.39	0.48
1:F:418:PRO:HB3	1:F:601:LEU:HD23	1.94	0.48
1:I:164:LYS:NZ	1:K:217:ASN:HB3	2.29	0.48
1:J:203:MET:HE2	1:J:230:VAL:HG11	1.96	0.48
1:H:341:TYR:OH	1:H:429:VAL:O	2.29	0.47
1:G:124:GLU:O	6:G:801:HOH:O	2.20	0.47
1:H:282:GLU:OE1	1:H:285:ARG:HD3	2.14	0.47
1:K:214:LEU:HD11	1:K:222:LEU:HD22	1.96	0.47
1:K:461:GLU:HA	1:K:464:LEU:HD12	1.96	0.47
1:D:386:LYS:HB3	1:D:391:SER:HB2	1.96	0.47
1:I:326:LYS:HE2	1:I:328:LEU:HD21	1.96	0.47
1:J:368:LYS:HB3	1:J:478:VAL:HA	1.96	0.47
1:C:232:LYS:HE2	1:C:276:THR:O	2.15	0.47
1:C:395:LEU:HD21	1:C:581:TRP:CG	2.50	0.47
1:H:132:VAL:HG11	1:H:142:VAL:HG13	1.96	0.47
1:A:208:LEU:O	1:A:212:THR:HG23	2.15	0.47
1:B:371:LEU:HD22	1:B:596:LEU:HD22	1.97	0.47
1:E:436:LYS:NZ	6:F:803:HOH:O	2.27	0.47
1:F:361:SER:CB	1:F:419:GLU:HA	2.45	0.47
1:G:207:VAL:HG11	1:G:241:THR:HG22	1.97	0.47
1:K:236:ARG:HG2	1:K:284:ALA:HB2	1.96	0.47
1:D:115:TYR:HB2	1:D:270:TYR:CD2	2.49	0.47
1:D:274:ALA:HA	1:D:277:TYR:HB2	1.96	0.47
1:D:386:LYS:HB2	1:D:393:ILE:HD13	1.97	0.47
1:I:368:LYS:C	1:I:478:VAL:HG22	2.40	0.47
1:E:321:LEU:O	1:E:322:ASN:HB2	2.14	0.47
1:F:330:VAL:C	1:F:332:GLU:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:177:MET:HE2	1:J:177:MET:HB3	1.71	0.47
1:L:178:PHE:HA	1:L:183:ASN:O	2.15	0.47
1:H:285:ARG:CG	1:H:286:VAL:HG23	2.44	0.47
1:L:460:SER:O	1:L:546:GLN:NE2	2.48	0.47
1:D:176:TYR:HB3	4:D:704:SO4:O1	2.15	0.47
1:D:383:TYR:HE1	1:E:434:VAL:HG23	1.80	0.47
1:G:537:LEU:HA	1:G:545:ASN:HB2	1.96	0.47
1:F:546:GLN:HG2	1:F:547:ILE:HG23	1.97	0.46
1:H:311:SER:HB2	1:H:327:ILE:HD12	1.97	0.46
1:C:107:ILE:HA	1:C:110:ILE:HD12	1.96	0.46
1:G:441:PRO:HB2	1:H:394:ASP:HA	1.95	0.46
1:B:329:GLY:O	1:B:333:LEU:HG	2.15	0.46
1:D:232:LYS:CB	1:D:235:PHE:HB3	2.45	0.46
1:F:396:MET:HE1	5:F:705:1PE:H131	1.97	0.46
1:G:374:LYS:HE3	1:G:462:GLY:HA3	1.97	0.46
1:H:282:GLU:HB3	1:H:285:ARG:CZ	2.45	0.46
1:H:299:ALA:HA	1:H:397:LYS:HE3	1.96	0.46
1:J:522:GLU:OE2	1:J:595:LEU:N	2.49	0.46
1:J:600:VAL:HG12	1:J:601:LEU:HD23	1.97	0.46
1:K:211:VAL:HG21	1:K:245:GLU:HB2	1.97	0.46
1:C:143:LYS:HB3	1:C:143:LYS:HE2	1.69	0.46
1:I:544:ILE:HD12	1:I:544:ILE:HA	1.82	0.46
1:A:517:SER:OG	1:A:522:GLU:O	2.34	0.46
1:E:396:MET:HA	1:E:396:MET:HE3	1.98	0.46
1:J:400:MET:HE1	6:J:805:HOH:O	1.93	0.46
1:A:367:LYS:HA	1:A:367:LYS:HD3	1.77	0.46
1:C:114:VAL:HG12	1:C:274:ALA:HB1	1.98	0.46
1:D:232:LYS:CE	1:D:277:TYR:HA	2.46	0.46
1:K:375:GLY:O	1:K:429:VAL:HA	2.16	0.46
1:K:530:ILE:HD12	1:K:556:ILE:HD13	1.98	0.46
1:B:120:GLY:HA2	1:B:147:LYS:O	2.16	0.46
1:B:321:LEU:HD11	1:B:411:TYR:HA	1.98	0.46
1:F:346:LYS:HB3	1:F:437:ASN:O	2.16	0.46
1:I:172:SER:HB2	1:I:213:MET:CE	2.43	0.46
1:A:342:LEU:HD12	1:B:94:LEU:HD12	1.98	0.46
1:E:287:TYR:OH	1:E:598:GLU:OE2	2.29	0.46
1:F:574:ILE:HD13	1:F:595:LEU:HD21	1.97	0.46
1:L:100:PRO:O	1:L:251:ARG:NH1	2.33	0.46
1:L:488:THR:OG1	1:L:575:ASP:OD2	2.32	0.46
1:F:204:LYS:O	1:F:208:LEU:HD12	2.16	0.46
1:H:364:ASP:OD1	1:H:364:ASP:N	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:112:VAL:HG22	1:J:267:LEU:HB3	1.98	0.46
1:L:360:LYS:HG2	1:L:422:GLU:HG3	1.98	0.46
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.98	0.45
1:D:236:ARG:HD3	1:D:280:GLU:OE1	2.15	0.45
1:F:293:TYR:CZ	1:F:317:LEU:HD13	2.50	0.45
1:K:106:PRO:HD2	1:K:247:MET:HE1	1.96	0.45
1:H:207:VAL:HG13	1:H:242:LEU:HD12	1.98	0.45
1:I:198:LEU:HD22	1:I:202:ASP:HB3	1.97	0.45
1:F:217:ASN:OD1	1:F:219:LEU:N	2.41	0.45
1:G:321:LEU:O	1:G:322:ASN:HB2	2.15	0.45
1:H:145:SER:H	1:H:227:GLU:CD	2.25	0.45
1:I:528:PRO:HB3	1:J:525:TRP:CZ3	2.51	0.45
1:A:221:LYS:HG3	1:A:266:HIS:HB2	1.96	0.45
1:L:445:ILE:HD11	1:L:464:LEU:HD22	1.98	0.45
1:B:364:ASP:O	1:B:420:ASN:HA	2.17	0.45
1:D:232:LYS:HA	1:D:235:PHE:HB3	1.98	0.45
1:E:440:ARG:NH1	6:E:810:HOH:O	2.42	0.45
1:F:217:ASN:OD1	1:F:218:LYS:N	2.49	0.45
1:I:157:LEU:HA	1:I:162:MET:HE2	1.99	0.45
1:B:522:GLU:OE1	1:B:595:LEU:N	2.49	0.45
1:E:533:TYR:O	1:E:536:THR:OG1	2.34	0.45
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.97	0.45
1:A:530:ILE:O	1:A:560:LEU:HD11	2.16	0.45
1:F:375:GLY:O	1:F:429:VAL:HA	2.16	0.45
1:G:464:LEU:HD21	1:G:546:GLN:HG3	1.98	0.45
1:A:157:LEU:HD23	1:A:162:MET:HE3	1.98	0.45
1:B:210:LEU:HD21	1:B:222:LEU:HD21	1.98	0.45
1:L:122:ASN:OD1	1:L:149:ASN:ND2	2.44	0.45
1:L:487:LEU:HA	1:L:487:LEU:HD12	1.79	0.45
1:B:375:GLY:O	1:B:429:VAL:HA	2.17	0.45
1:E:441:PRO:HB2	1:F:394:ASP:HA	1.98	0.45
1:E:336:LEU:HD13	1:E:338:MET:HE3	1.98	0.44
1:G:167:VAL:HB	6:G:802:HOH:O	2.17	0.44
1:B:357:LEU:HB2	1:B:425:PHE:HB2	2.00	0.44
1:H:207:VAL:HG11	1:H:241:THR:HG22	1.99	0.44
1:C:368:LYS:HB3	1:C:478:VAL:HG12	2.00	0.44
1:D:144:ILE:HD11	1:D:162:MET:HE2	1.98	0.44
1:E:579:VAL:O	1:E:589:LYS:NZ	2.50	0.44
1:F:230:VAL:O	1:F:277:TYR:OH	2.31	0.44
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.53	0.44
1:J:147:LYS:HD2	1:J:147:LYS:HA	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:GLY:O	1:A:429:VAL:HA	2.17	0.44
1:H:175:PHE:HD1	1:L:176:TYR:HB2	1.83	0.44
1:J:359:TYR:HD2	1:J:423:ILE:HD12	1.81	0.44
1:L:157:LEU:HA	1:L:162:MET:HE2	2.00	0.44
1:L:386:LYS:HB3	1:L:391:SER:HB3	2.00	0.44
1:A:155:GLU:O	1:A:158:LYS:HG2	2.18	0.44
1:H:320:LYS:HB3	5:H:704:1PE:H141	2.00	0.44
1:L:230:VAL:HB	1:L:234:LEU:HB3	1.99	0.44
1:H:528:PRO:HB3	1:K:525:TRP:CZ3	2.52	0.44
1:J:364:ASP:O	1:J:420:ASN:HA	2.17	0.44
1:A:525:TRP:CZ3	1:F:528:PRO:HB3	2.52	0.44
1:F:315:VAL:O	1:F:319:GLN:HG3	2.18	0.44
1:H:121:CYS:HA	1:H:270:TYR:CE2	2.53	0.43
1:H:200:GLU:OE2	1:H:523:PRO:HD3	2.17	0.43
1:I:483:ASP:OD1	1:I:573:HIS:ND1	2.41	0.43
1:C:356:HIS:ND1	1:C:472:TYR:OH	2.49	0.43
1:D:121:CYS:HA	1:D:270:TYR:CZ	2.54	0.43
1:H:361:SER:OG	1:H:419:GLU:O	2.29	0.43
1:B:162:MET:O	1:B:163:GLU:C	2.60	0.43
1:B:449:ASN:ND2	1:B:451:LYS:HG3	2.33	0.43
1:H:176:TYR:HB3	1:L:177:MET:HE2	2.00	0.43
1:K:160:GLU:H	1:K:160:GLU:CD	2.17	0.43
1:K:493:TYR:O	6:K:801:HOH:O	2.21	0.43
1:A:114:VAL:HG11	1:A:278:LYS:CB	2.48	0.43
1:D:340:ALA:HA	1:D:445:ILE:HD12	1.99	0.43
1:H:530:ILE:HD12	1:H:556:ILE:HD13	2.00	0.43
1:J:150:ASP:OD1	1:J:179:ASN:HB2	2.19	0.43
1:J:164:LYS:HB2	1:J:164:LYS:HE3	1.84	0.43
1:K:378:PHE:CD2	1:K:433:MET:HE1	2.47	0.43
1:L:369:ILE:HG23	1:L:480:TYR:HB2	2.01	0.43
1:F:190:VAL:HG11	1:F:206:VAL:HG13	2.00	0.43
1:I:505:ASN:ND2	6:I:805:HOH:O	2.47	0.43
1:L:290:GLY:C	1:L:593:VAL:HG11	2.44	0.43
1:C:321:LEU:HD11	1:C:411:TYR:HA	2.00	0.43
1:J:329:GLY:O	1:J:333:LEU:HG	2.19	0.43
1:J:393:ILE:HG12	1:L:441:PRO:HG2	2.00	0.43
1:L:273:ASN:HB3	1:L:276:THR:OG1	2.17	0.43
1:C:123:VAL:HG21	1:C:153:VAL:HG21	2.00	0.43
1:E:333:LEU:HD21	1:E:354:PHE:HB2	2.01	0.43
1:H:419:GLU:HG2	1:H:420:ASN:HB2	2.01	0.43
1:I:419:GLU:HA	1:I:421:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:516:SER:O	1:J:520:SER:OG	2.32	0.43
1:D:379:ASP:O	1:D:396:MET:HG3	2.19	0.43
1:F:214:LEU:HA	1:F:214:LEU:HD23	1.75	0.43
1:G:411:TYR:HE1	5:G:707:1PE:H141	1.84	0.43
1:H:211:VAL:HG21	1:H:245:GLU:HB2	2.00	0.43
1:A:411:TYR:HE1	5:A:706:1PE:H242	1.83	0.43
1:B:528:PRO:HB3	1:E:525:TRP:CZ3	2.53	0.43
1:C:544:ILE:HD12	1:C:564:GLU:HG3	2.01	0.43
1:E:107:ILE:HG21	1:E:243:PHE:HB3	2.01	0.43
1:F:355:ILE:N	6:F:801:HOH:O	2.48	0.43
1:K:509:LEU:O	1:K:513:ILE:HG12	2.19	0.43
1:B:365:VAL:HG11	1:B:422:GLU:HB2	2.01	0.43
1:E:86:SER:O	1:E:312:ASN:ND2	2.43	0.43
1:E:100:PRO:O	1:E:251:ARG:NH1	2.47	0.43
1:E:214:LEU:HD21	1:E:222:LEU:HD22	2.01	0.43
1:A:117:ILE:C	1:A:119:GLY:H	2.26	0.42
1:A:402:GLY:O	1:A:406:VAL:HG23	2.18	0.42
1:B:146:SER:OG	1:B:227:GLU:OE2	2.36	0.42
1:C:509:LEU:O	1:C:513:ILE:HG12	2.18	0.42
1:D:394:ASP:OD2	1:D:395:LEU:HD22	2.19	0.42
1:E:148:VAL:HG12	1:E:150:ASP:H	1.84	0.42
1:F:491:MET:HE3	1:F:491:MET:HB3	1.89	0.42
1:G:173:LYS:NZ	1:J:176:TYR:OH	2.52	0.42
1:G:320:LYS:HG2	5:G:705:1PE:H222	2.01	0.42
1:I:463:ARG:N	3:I:703:CO3:O2	2.39	0.42
1:L:494:SER:OG	1:L:495:LEU:N	2.52	0.42
1:E:487:LEU:HA	1:E:487:LEU:HD12	1.83	0.42
1:F:487:LEU:HD12	1:F:487:LEU:HA	1.81	0.42
1:G:236:ARG:HG2	1:G:284:ALA:HB2	2.01	0.42
1:G:551:VAL:HG12	1:G:553:ALA:H	1.84	0.42
1:H:173:LYS:HB2	1:H:189:TYR:CE2	2.54	0.42
1:I:551:VAL:HG12	1:I:553:ALA:H	1.84	0.42
1:K:198:LEU:HG	1:K:202:ASP:HB3	2.00	0.42
1:K:236:ARG:HG3	1:K:280:GLU:HB3	2.01	0.42
1:K:328:LEU:HD23	1:K:328:LEU:HA	1.81	0.42
1:H:118:LYS:HD2	1:H:118:LYS:H	1.82	0.42
1:B:323:LEU:HD23	1:B:359:TYR:HB2	2.01	0.42
1:C:301:PRO:HB2	1:C:303:ASN:OD1	2.19	0.42
1:C:364:ASP:O	1:C:420:ASN:HA	2.19	0.42
1:D:114:VAL:HB	1:D:278:LYS:HD2	2.02	0.42
1:F:456:GLY:N	1:F:546:GLN:OE1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:200:GLU:H	1:J:200:GLU:HG3	1.68	0.42
1:B:436:LYS:HG2	4:B:1004:SO4:O2	2.19	0.42
1:C:492:LEU:HD23	1:C:492:LEU:HA	1.88	0.42
1:D:232:LYS:HE3	1:D:276:THR:O	2.20	0.42
1:I:125:GLU:CG	1:I:221:LYS:HD2	2.50	0.42
1:L:398:PHE:O	1:L:401:SER:OG	2.27	0.42
5:L:706:1PE:H231	5:L:706:1PE:H122	1.72	0.42
1:A:329:GLY:O	1:A:333:LEU:HG	2.19	0.42
1:D:302:SER:OG	1:D:378:PHE:HB2	2.20	0.42
1:G:124:GLU:HB3	1:G:125:GLU:H	1.62	0.42
1:G:199:SER:OG	1:G:200:GLU:N	2.53	0.42
1:L:343:SER:HA	1:L:346:LYS:HG3	2.01	0.42
1:L:379:ASP:O	1:L:396:MET:HG3	2.19	0.42
1:L:407:LEU:HD12	1:L:407:LEU:HA	1.94	0.42
1:A:386:LYS:HB3	1:A:391:SER:HB2	2.02	0.42
1:A:534:ARG:NH1	1:A:537:LEU:HB2	2.35	0.42
1:D:150:ASP:HB3	1:D:153:VAL:HB	2.02	0.42
1:J:567:GLN:N	1:J:567:GLN:CD	2.78	0.42
1:A:396:MET:HE1	5:A:707:1PE:H151	2.01	0.42
1:B:530:ILE:HD12	1:B:556:ILE:HD13	2.02	0.42
1:D:449:ASN:HD21	1:D:451:LYS:HD2	1.85	0.42
1:H:90:GLN:HB3	1:H:95:ASP:HB2	2.01	0.42
1:D:156:PHE:CG	1:D:177:MET:HE1	2.55	0.41
1:G:472:TYR:O	1:G:476:LEU:HD13	2.20	0.41
1:K:318:ALA:HB2	1:K:357:LEU:HD22	2.00	0.41
1:A:357:LEU:HB2	1:A:425:PHE:HB2	2.01	0.41
1:A:394:ASP:HA	1:C:441:PRO:HB2	2.01	0.41
1:B:121:CYS:HA	1:B:270:TYR:CE2	2.55	0.41
1:C:106:PRO:HD2	1:C:247:MET:SD	2.60	0.41
1:E:283:LYS:HE2	1:E:287:TYR:CZ	2.55	0.41
1:K:369:ILE:HB	1:K:423:ILE:HD13	2.02	0.41
1:L:151:LYS:N	1:L:180:ASP:OD2	2.52	0.41
1:L:406:VAL:HG12	1:L:425:PHE:HB3	2.02	0.41
1:B:511:ASN:O	1:B:515:GLN:HB2	2.20	0.41
1:E:396:MET:CE	5:E:706:1PE:H121	2.50	0.41
5:F:705:1PE:H132	5:F:705:1PE:H221	1.73	0.41
1:G:491:MET:HE1	1:G:495:LEU:HD12	2.03	0.41
1:C:174:HIS:HB3	1:E:175:PHE:CD2	2.55	0.41
1:C:179:ASN:OD1	1:C:181:ASN:N	2.44	0.41
1:E:214:LEU:HD11	1:E:222:LEU:HD22	2.01	0.41
1:E:340:ALA:HA	1:E:445:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:127:LEU:HD21	1:K:213:MET:HE2	2.01	0.41
1:L:395:LEU:HD11	1:L:581:TRP:CE2	2.55	0.41
1:L:481:ILE:O	1:L:571:TRP:HA	2.21	0.41
1:A:392:MET:HE2	1:A:392:MET:HB2	1.91	0.41
1:B:394:ASP:OD2	1:B:394:ASP:N	2.35	0.41
1:K:432:ASN:O	1:K:433:MET:HE2	2.21	0.41
1:C:386:LYS:HE3	1:C:396:MET:HG3	2.01	0.41
1:D:232:LYS:HD3	1:D:277:TYR:CG	2.55	0.41
1:G:440:ARG:HD3	1:H:378:PHE:CG	2.56	0.41
1:G:530:ILE:HG13	1:G:556:ILE:HG21	2.02	0.41
1:K:444:ILE:HD13	1:K:542:ALA:HB2	2.03	0.41
1:K:585:ALA:HB1	1:K:587:LYS:HD3	2.02	0.41
1:B:530:ILE:O	1:B:560:LEU:HD11	2.20	0.41
1:D:261:MET:HB3	1:D:261:MET:HE3	1.86	0.41
1:E:360:LYS:HD2	1:E:422:GLU:OE1	2.21	0.41
1:F:169:LEU:HD23	1:F:192:CYS:HA	2.02	0.41
1:H:282:GLU:HA	1:H:285:ARG:HB2	2.02	0.41
1:J:242:LEU:O	1:J:246:TYR:HB2	2.20	0.41
1:L:112:VAL:HG22	1:L:267:LEU:HD23	2.03	0.41
1:L:214:LEU:HB3	1:L:246:TYR:CE1	2.55	0.41
1:L:232:LYS:HE2	1:L:232:LYS:HB3	1.89	0.41
1:B:534:ARG:NH1	1:B:537:LEU:HB2	2.36	0.41
1:C:202:ASP:O	1:C:206:VAL:HG23	2.21	0.41
1:C:530:ILE:HD12	1:C:556:ILE:HD13	2.03	0.41
1:D:100:PRO:O	1:D:101:ILE:HD13	2.20	0.41
1:D:158:LYS:HE3	1:D:160:GLU:HB3	2.03	0.41
1:I:168:LYS:HB3	1:I:171:THR:OG1	2.20	0.41
1:I:338:MET:CE	1:I:468:ASP:HB3	2.51	0.41
1:A:395:LEU:HD11	1:A:581:TRP:CE2	2.55	0.41
1:B:174:HIS:NE2	1:B:213:MET:SD	2.94	0.41
1:C:307:PRO:O	1:C:311:SER:OG	2.39	0.41
1:E:435:SER:OG	1:E:436:LYS:N	2.54	0.41
1:F:357:LEU:HB2	1:F:425:PHE:HB2	2.02	0.41
1:F:385:LEU:HD23	1:F:387:ALA:HB2	2.03	0.41
1:G:133:ASN:HA	6:G:802:HOH:O	2.20	0.41
1:G:194:SER:O	1:G:194:SER:OG	2.28	0.41
1:G:411:TYR:CE1	5:G:707:1PE:H141	2.56	0.41
1:H:117:ILE:HD12	1:H:117:ILE:H	1.86	0.41
1:J:279:GLU:H	1:J:279:GLU:HG2	1.63	0.41
1:K:336:LEU:HD13	1:K:336:LEU:HA	1.85	0.41
1:K:487:LEU:HD12	1:K:487:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:TYR:OH	1:C:418:PRO:O	2.32	0.41
1:F:320:LYS:NZ	6:F:817:HOH:O	2.47	0.41
1:I:392:MET:HB3	1:I:395:LEU:HD12	2.02	0.41
1:K:203:MET:HE3	1:K:238:PHE:HB2	2.03	0.41
1:A:321:LEU:HD11	1:A:411:TYR:HA	2.03	0.40
1:A:483:ASP:OD1	1:A:573:HIS:ND1	2.40	0.40
1:B:359:TYR:OH	1:B:418:PRO:O	2.34	0.40
1:E:102:GLU:HG2	1:E:102:GLU:O	2.21	0.40
1:G:278:LYS:HB3	1:G:279:GLU:H	1.40	0.40
1:K:471:VAL:O	1:K:475:LYS:HG3	2.21	0.40
1:L:216:ASP:N	1:L:216:ASP:OD1	2.54	0.40
1:L:349:MET:HE3	1:L:349:MET:HB2	1.84	0.40
1:L:362:LYS:HD3	1:L:362:LYS:HA	1.79	0.40
1:A:463:ARG:HG2	3:A:703:CO3:O2	2.22	0.40
1:D:470:LEU:HD23	1:D:470:LEU:HA	1.97	0.40
1:F:321:LEU:O	1:F:322:ASN:HB2	2.20	0.40
1:J:502:VAL:HG23	1:J:574:ILE:HG12	2.03	0.40
1:F:107:ILE:HG21	1:F:243:PHE:HB3	2.03	0.40
1:L:481:ILE:HG22	1:L:571:TRP:HD1	1.86	0.40
1:A:486:THR:HG22	1:A:577:ALA:HA	2.03	0.40
1:B:172:SER:HB2	1:B:213:MET:HE2	2.03	0.40
1:F:179:ASN:ND2	1:F:181:ASN:H	2.19	0.40
1:H:139:ASN:OD1	1:H:139:ASN:N	2.54	0.40
1:H:203:MET:HE2	1:H:238:PHE:HD2	1.86	0.40
1:H:349:MET:HE3	1:H:349:MET:HB2	1.90	0.40
1:H:520:SER:HB3	1:H:598:GLU:HG3	2.03	0.40
1:I:210:LEU:HD21	1:I:222:LEU:HD21	2.04	0.40
1:L:517:SER:OG	1:L:522:GLU:O	2.32	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:A:179:ASN:HD21	1:G:113:GLN:HE22[2_564]	1.19	0.41

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	514/528 (97%)	493 (96%)	17 (3%)	4 (1%)	16	34
1	B	507/528 (96%)	483 (95%)	19 (4%)	5 (1%)	12	28
1	C	516/528 (98%)	500 (97%)	16 (3%)	0	100	100
1	D	509/528 (96%)	495 (97%)	14 (3%)	0	100	100
1	E	503/528 (95%)	489 (97%)	13 (3%)	1 (0%)	43	66
1	F	504/528 (96%)	486 (96%)	15 (3%)	3 (1%)	21	42
1	G	510/528 (97%)	494 (97%)	14 (3%)	2 (0%)	30	51
1	H	507/528 (96%)	482 (95%)	21 (4%)	4 (1%)	16	34
1	I	511/528 (97%)	489 (96%)	20 (4%)	2 (0%)	30	51
1	J	510/528 (97%)	496 (97%)	12 (2%)	2 (0%)	30	51
1	K	503/528 (95%)	493 (98%)	10 (2%)	0	100	100
1	L	502/528 (95%)	484 (96%)	18 (4%)	0	100	100
All	All	6096/6336 (96%)	5884 (96%)	189 (3%)	23 (0%)	30	51

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	GLU
1	H	285	ARG
1	H	419	GLU
1	H	420	ASN
1	I	419	GLU
1	J	391	SER
1	A	258	ASN
1	B	124	GLU
1	B	126	GLY
1	B	138	GLU
1	I	139	ASN
1	J	137	LYS

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Mol	Chain	Res	Type
1	A	507	GLU
1	F	196	ALA
1	F	332	GLU
1	G	278	LYS
1	B	163	GLU
1	G	124	GLU
1	H	321	LEU
1	E	322	ASN
1	B	119	GLY
1	A	195	VAL
1	F	135	PRO

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	380/456 (83%)	377 (99%)	3 (1%)	73	88
1	B	394/456 (86%)	384 (98%)	10 (2%)	42	69
1	C	419/456 (92%)	407 (97%)	12 (3%)	37	65
1	D	414/456 (91%)	400 (97%)	14 (3%)	32	60
1	E	412/456 (90%)	402 (98%)	10 (2%)	43	70
1	F	382/456 (84%)	365 (96%)	17 (4%)	24	50
1	G	420/456 (92%)	410 (98%)	10 (2%)	43	70
1	H	404/456 (89%)	390 (96%)	14 (4%)	32	59
1	I	412/456 (90%)	403 (98%)	9 (2%)	45	72
1	J	412/456 (90%)	398 (97%)	14 (3%)	32	60
1	K	407/456 (89%)	398 (98%)	9 (2%)	45	72
1	L	391/456 (86%)	376 (96%)	15 (4%)	29	56
All	All	4847/5472 (89%)	4710 (97%)	137 (3%)	38	66

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	SER
1	A	391	SER
1	A	554	SER
1	B	128	THR
1	B	142	VAL
1	B	146	SER
1	B	207	VAL
1	B	234	LEU
1	B	254	SER
1	B	322	ASN
1	B	393	ILE
1	B	436	LYS
1	B	446	THR
1	C	86	SER
1	C	91	VAL
1	C	117	ILE
1	C	195	VAL
1	C	219	LEU
1	C	311	SER
1	C	322	ASN
1	C	395	LEU
1	C	398	PHE
1	C	479	ASP
1	C	483	ASP
1	C	601	LEU
1	D	97	THR
1	D	146	SER
1	D	154	SER
1	D	172	SER
1	D	217	ASN
1	D	288	TYR
1	D	295	SER
1	D	322	ASN
1	D	361	SER
1	D	391	SER
1	D	417	LYS
1	D	423	ILE
1	D	439	TYR
1	D	554	SER
1	E	117	ILE
1	E	145	SER
1	E	146	SER
1	E	155	GLU

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Mol	Chain	Res	Type
1	E	195	VAL
1	E	406	VAL
1	E	446	THR
1	E	448	SER
1	E	498	SER
1	E	550	SER
1	F	86	SER
1	F	142	VAL
1	F	153	VAL
1	F	169	LEU
1	F	200	GLU
1	F	212	THR
1	F	343	SER
1	F	372	VAL
1	F	398	PHE
1	F	406	VAL
1	F	419	GLU
1	F	439	TYR
1	F	508	GLU
1	F	516	SER
1	F	548	SER
1	F	554	SER
1	F	555	SER
1	G	123	VAL
1	G	139	ASN
1	G	154	SER
1	G	169	LEU
1	G	204	LYS
1	G	230	VAL
1	G	278	LYS
1	G	398	PHE
1	G	476	LEU
1	G	603	ASP
1	H	148	VAL
1	H	187	VAL
1	H	194	SER
1	H	200	GLU
1	H	221	LYS
1	H	224	VAL
1	H	231	ASP
1	H	276	THR
1	H	285	ARG

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Mol	Chain	Res	Type
1	H	364	ASP
1	H	391	SER
1	H	398	PHE
1	H	549	SER
1	H	554	SER
1	I	86	SER
1	I	199	SER
1	I	232	LYS
1	I	360	LYS
1	I	361	SER
1	I	391	SER
1	I	448	SER
1	I	478	VAL
1	I	595	LEU
1	J	86	SER
1	J	219	LEU
1	J	276	THR
1	J	326	LYS
1	J	393	ILE
1	J	398	PHE
1	J	436	LYS
1	J	445	ILE
1	J	494	SER
1	J	547	ILE
1	J	567	GLN
1	J	569	THR
1	J	579	VAL
1	J	600	VAL
1	K	98	SER
1	K	117	ILE
1	K	142	VAL
1	K	169	LEU
1	K	216	ASP
1	K	336	LEU
1	K	358	THR
1	K	399	ASP
1	K	550	SER
1	L	127	LEU
1	L	145	SER
1	L	211	VAL
1	L	283	LYS
1	L	308	VAL

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Mol	Chain	Res	Type
1	L	391	SER
1	L	407	LEU
1	L	439	TYR
1	L	445	ILE
1	L	488	THR
1	L	549	SER
1	L	550	SER
1	L	554	SER
1	L	587	LYS
1	L	595	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	ASN
1	B	122	ASN
1	B	183	ASN
1	C	166	ASN
1	C	420	ASN
1	C	506	ASN
1	C	521	ASN
1	D	139	ASN
1	D	161	ASN
1	D	272	ASN
1	D	515	GLN
1	D	567	GLN
1	D	568	ASN
1	E	90	GLN
1	E	266	HIS
1	E	272	ASN
1	E	602	ASN
1	F	174	HIS
1	F	266	HIS
1	F	322	ASN
1	F	420	ASN
1	F	521	ASN
1	F	582	ASN
1	G	104	ASN
1	G	174	HIS
1	G	437	ASN
1	G	521	ASN
1	G	531	ASN

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Mol	Chain	Res	Type
1	G	602	ASN
1	H	90	GLN
1	H	104	ASN
1	H	531	ASN
1	I	161	ASN
1	I	174	HIS
1	I	568	ASN
1	J	217	ASN
1	J	266	HIS
1	J	531	ASN
1	K	161	ASN
1	K	166	ASN
1	K	511	ASN
1	L	90	GLN
1	L	266	HIS
1	L	420	ASN
1	L	545	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 73 ligands modelled in this entry, 24 are monoatomic - leaving 49 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	CO3	B	1001	-	3,3,3	0.82	0	2,3,3	0.11	0
5	1PE	A	706	-	8,8,15	0.17	0	7,7,14	0.16	0
4	SO4	K	706	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	D	704	-	4,4,4	0.24	0	6,6,6	0.12	0
5	1PE	E	705	-	11,11,15	0.15	0	10,10,14	0.14	0
5	1PE	E	706	-	8,8,15	0.15	0	7,7,14	0.10	0
4	SO4	A	705	-	4,4,4	0.23	0	6,6,6	0.07	0
5	1PE	B	1005	-	6,6,15	0.20	0	5,5,14	0.10	0
4	SO4	A	704	-	4,4,4	0.24	0	6,6,6	0.12	0
3	CO3	J	703	-	3,3,3	0.82	0	2,3,3	0.14	0
4	SO4	G	704	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	G	708	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	E	704	-	4,4,4	0.23	0	6,6,6	0.09	0
5	1PE	G	707	-	12,12,15	0.10	0	11,11,14	0.12	0
3	CO3	K	703	-	3,3,3	0.83	0	2,3,3	0.10	0
3	CO3	F	704	-	3,3,3	0.84	0	2,3,3	0.13	0
5	1PE	K	705	-	15,15,15	0.11	0	14,14,14	0.12	0
4	SO4	L	705	-	4,4,4	0.23	0	6,6,6	0.07	0
3	CO3	A	703	-	3,3,3	0.83	0	2,3,3	0.19	0
3	CO3	C	703	-	3,3,3	0.84	0	2,3,3	0.14	0
4	SO4	I	705	-	4,4,4	0.24	0	6,6,6	0.07	0
5	1PE	J	704	-	9,9,15	0.10	0	8,8,14	0.14	0
5	1PE	A	707	-	9,9,15	0.10	0	8,8,14	0.14	0
3	CO3	L	704	-	3,3,3	0.83	0	2,3,3	0.12	0
4	SO4	C	704	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	F	701	-	4,4,4	0.23	0	6,6,6	0.09	0
5	1PE	F	705	-	9,9,15	0.08	0	8,8,14	0.15	0
5	1PE	L	706	-	15,15,15	0.13	0	14,14,14	0.16	0
5	1PE	H	704	-	9,9,15	0.19	0	8,8,14	0.12	0
4	SO4	C	708	-	4,4,4	0.24	0	6,6,6	0.07	0
3	CO3	G	701	-	3,3,3	0.83	0	2,3,3	0.16	0
5	1PE	D	705	-	9,9,15	0.19	0	8,8,14	0.12	0
5	1PE	D	706	-	9,9,15	0.20	0	8,8,14	0.11	0
3	CO3	E	703	-	3,3,3	0.85	0	2,3,3	0.15	0
3	CO3	H	703	-	3,3,3	0.82	0	2,3,3	0.26	0
5	1PE	C	706	-	8,8,15	0.17	0	7,7,14	0.15	0
4	SO4	J	705	-	4,4,4	0.22	0	6,6,6	0.09	0
3	CO3	I	703	-	3,3,3	0.83	0	2,3,3	0.14	0
4	SO4	B	1004	-	4,4,4	0.23	0	6,6,6	0.13	0
5	1PE	K	704	-	8,8,15	0.16	0	7,7,14	0.09	0
4	SO4	H	705	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	L	701	-	4,4,4	0.23	0	6,6,6	0.07	0
5	1PE	C	705	-	12,12,15	0.18	0	11,11,14	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	1PE	D	707	-	8,8,15	0.16	0	7,7,14	0.09	0
4	SO4	I	704	-	4,4,4	0.23	0	6,6,6	0.09	0
5	1PE	G	706	-	9,9,15	0.11	0	8,8,14	0.13	0
3	CO3	D	703	-	3,3,3	0.82	0	2,3,3	0.12	0
5	1PE	C	707	-	9,9,15	0.11	0	8,8,14	0.13	0
5	1PE	G	705	-	8,8,15	0.17	0	7,7,14	0.14	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	1PE	A	706	-	-	3/6/6/13	-
5	1PE	E	705	-	-	5/9/9/13	-
5	1PE	B	1005	-	-	2/4/4/13	-
5	1PE	C	707	-	-	4/7/7/13	-
5	1PE	G	707	-	-	4/10/10/13	-
5	1PE	K	705	-	-	4/13/13/13	-
5	1PE	J	704	-	-	5/7/7/13	-
5	1PE	A	707	-	-	6/7/7/13	-
5	1PE	F	705	-	-	4/7/7/13	-
5	1PE	L	706	-	-	6/13/13/13	-
5	1PE	H	704	-	-	6/7/7/13	-
5	1PE	D	705	-	-	5/7/7/13	-
5	1PE	D	706	-	-	2/7/7/13	-
5	1PE	C	706	-	-	2/6/6/13	-
5	1PE	K	704	-	-	1/6/6/13	-
5	1PE	C	705	-	-	2/10/10/13	-
5	1PE	D	707	-	-	5/6/6/13	-
5	1PE	G	706	-	-	2/7/7/13	-
5	1PE	E	706	-	-	2/6/6/13	-
5	1PE	G	705	-	-	4/6/6/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	706	1PE	C14-C24-OH4-C13
5	L	706	1PE	C12-C22-OH3-C23
5	D	705	1PE	OH4-C13-C23-OH3
5	G	707	1PE	OH5-C14-C24-OH4
5	A	707	1PE	OH5-C14-C24-OH4
5	D	706	1PE	OH5-C14-C24-OH4
5	A	707	1PE	OH6-C15-C25-OH5
5	E	705	1PE	OH6-C15-C25-OH5
5	J	704	1PE	OH6-C15-C25-OH5
5	C	707	1PE	C13-C23-OH3-C22
5	C	707	1PE	OH5-C14-C24-OH4
5	F	705	1PE	OH5-C14-C24-OH4
5	G	707	1PE	OH4-C13-C23-OH3
5	L	706	1PE	OH2-C12-C22-OH3
5	A	707	1PE	OH7-C16-C26-OH6
5	G	705	1PE	OH4-C13-C23-OH3
5	D	707	1PE	OH4-C13-C23-OH3
5	D	705	1PE	OH5-C14-C24-OH4
5	J	704	1PE	C16-C26-OH6-C15
5	F	705	1PE	C13-C23-OH3-C22
5	C	706	1PE	OH5-C14-C24-OH4
5	K	705	1PE	OH4-C13-C23-OH3
5	L	706	1PE	OH5-C14-C24-OH4
5	E	705	1PE	OH4-C13-C23-OH3
5	C	705	1PE	OH4-C13-C23-OH3
5	G	706	1PE	OH5-C14-C24-OH4
5	J	704	1PE	OH7-C16-C26-OH6
5	E	705	1PE	OH5-C14-C24-OH4
5	E	705	1PE	C12-C22-OH3-C23
5	C	705	1PE	C12-C22-OH3-C23
5	G	705	1PE	C12-C22-OH3-C23
5	D	707	1PE	C14-C24-OH4-C13
5	H	704	1PE	OH4-C13-C23-OH3
5	A	706	1PE	OH5-C14-C24-OH4
5	G	707	1PE	C24-C14-OH5-C25
5	D	707	1PE	C13-C23-OH3-C22
5	E	706	1PE	OH4-C13-C23-OH3
5	G	705	1PE	C13-C23-OH3-C22
5	H	704	1PE	C13-C23-OH3-C22
5	K	705	1PE	C25-C15-OH6-C26
5	A	707	1PE	C25-C15-OH6-C26
5	L	706	1PE	C15-C25-OH5-C14

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Mol	Chain	Res	Type	Atoms
5	A	706	1PE	C23-C13-OH4-C24
5	F	705	1PE	C14-C24-OH4-C13
5	K	705	1PE	C12-C22-OH3-C23
5	H	704	1PE	OH5-C14-C24-OH4
5	A	706	1PE	C12-C22-OH3-C23
5	A	707	1PE	C15-C25-OH5-C14
5	L	706	1PE	OH6-C15-C25-OH5
5	B	1005	1PE	C14-C24-OH4-C13
5	J	704	1PE	C25-C15-OH6-C26
5	H	704	1PE	C12-C22-OH3-C23
5	G	705	1PE	C23-C13-OH4-C24
5	H	704	1PE	C23-C13-OH4-C24
5	B	1005	1PE	C24-C14-OH5-C25
5	G	707	1PE	C25-C15-OH6-C26
5	H	704	1PE	C24-C14-OH5-C25
5	C	706	1PE	C23-C13-OH4-C24
5	D	705	1PE	C12-C22-OH3-C23
5	D	705	1PE	C13-C23-OH3-C22
5	D	705	1PE	C14-C24-OH4-C13
5	D	707	1PE	C23-C13-OH4-C24
5	J	704	1PE	C24-C14-OH5-C25
5	K	704	1PE	C23-C13-OH4-C24
5	E	705	1PE	C14-C24-OH4-C13
5	D	707	1PE	C12-C22-OH3-C23
5	G	706	1PE	C14-C24-OH4-C13
5	E	706	1PE	C23-C13-OH4-C24
5	F	705	1PE	OH4-C13-C23-OH3
5	C	707	1PE	OH4-C13-C23-OH3
5	C	707	1PE	OH2-C12-C22-OH3
5	K	705	1PE	C13-C23-OH3-C22
5	D	706	1PE	C12-C22-OH3-C23
5	A	707	1PE	C16-C26-OH6-C15

There are no ring outliers.

23 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	706	1PE	2	0
4	D	704	SO4	1	0
5	E	706	1PE	1	0
4	A	704	SO4	1	0
4	E	704	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	707	1PE	2	0
5	K	705	1PE	2	0
3	A	703	CO3	1	0
5	A	707	1PE	1	0
4	C	704	SO4	1	0
5	F	705	1PE	4	0
5	L	706	1PE	2	0
5	H	704	1PE	1	0
5	D	705	1PE	1	0
3	H	703	CO3	2	0
4	J	705	SO4	1	0
3	I	703	CO3	1	0
4	B	1004	SO4	1	0
5	C	705	1PE	1	0
5	D	707	1PE	1	0
4	I	704	SO4	1	0
5	G	706	1PE	1	0
5	G	705	1PE	1	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	517/528 (97%)	0.72	22 (4%)	40	34	26, 37, 59, 88	1 (0%)
1	B	511/528 (96%)	0.81	45 (8%)	15	12	28, 39, 69, 108	0
1	C	518/528 (98%)	0.66	21 (4%)	41	36	27, 36, 59, 87	0
1	D	513/528 (97%)	0.56	17 (3%)	49	43	23, 31, 52, 81	0
1	E	509/528 (96%)	0.48	9 (1%)	67	63	24, 32, 46, 69	0
1	F	510/528 (96%)	0.96	63 (12%)	8	6	24, 38, 70, 92	0
1	G	514/528 (97%)	0.81	29 (5%)	30	24	32, 40, 57, 79	0
1	H	511/528 (96%)	0.95	52 (10%)	12	9	26, 40, 73, 116	1 (0%)
1	I	515/528 (97%)	0.83	38 (7%)	20	16	28, 37, 60, 105	0
1	J	514/528 (97%)	0.65	24 (4%)	36	30	24, 34, 51, 70	0
1	K	509/528 (96%)	0.66	30 (5%)	28	23	26, 33, 49, 77	3 (0%)
1	L	508/528 (96%)	0.92	45 (8%)	15	12	28, 39, 65, 95	1 (0%)
All	All	6149/6336 (97%)	0.75	395 (6%)	25	20	23, 37, 63, 116	6 (0%)

All (395) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	419	GLU	6.1
1	L	603	ASP	6.0
1	I	603	ASP	5.4
1	H	285	ARG	5.3
1	I	361	SER	5.2
1	D	232	LYS	5.1
1	C	549	SER	5.0
1	L	219	LEU	4.9
1	F	121	CYS	4.9
1	A	259	VAL	4.8
1	H	282	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	163	GLU	4.8
1	A	258	ASN	4.7
1	L	144	ILE	4.7
1	I	364	ASP	4.6
1	A	362	LYS	4.6
1	E	507	GLU	4.4
1	H	602	ASN	4.4
1	F	149	ASN	4.3
1	D	603	ASP	4.2
1	B	125	GLU	4.2
1	B	162	MET	4.1
1	G	200	GLU	4.1
1	F	262	GLU	4.0
1	F	360	LYS	4.0
1	F	274	ALA	4.0
1	D	549	SER	3.9
1	F	123	VAL	3.9
1	L	110	ILE	3.9
1	K	119	GLY	3.9
1	L	270	TYR	3.8
1	K	361	SER	3.8
1	D	277	TYR	3.8
1	B	272	ASN	3.8
1	K	550	SER	3.6
1	B	197	ASP	3.6
1	G	603	ASP	3.6
1	L	217	ASN	3.6
1	H	277	TYR	3.6
1	H	421	VAL	3.6
1	B	273	ASN	3.6
1	F	129	ILE	3.5
1	H	390	GLY	3.5
1	B	185	VAL	3.5
1	A	262	GLU	3.5
1	C	600	VAL	3.5
1	H	281	VAL	3.5
1	F	255	THR	3.5
1	H	119	GLY	3.5
1	G	262	GLU	3.5
1	I	419	GLU	3.5
1	F	361	SER	3.4
1	B	160	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	255	THR	3.4
1	F	116	ASP	3.4
1	G	362	LYS	3.4
1	I	362	LYS	3.4
1	I	160	GLU	3.4
1	L	274	ALA	3.4
1	K	218	LYS	3.4
1	K	120	GLY	3.4
1	L	214	LEU	3.4
1	B	142	VAL	3.4
1	H	365	VAL	3.4
1	J	145	SER	3.3
1	H	507	GLU	3.3
1	L	153	VAL	3.3
1	G	278	LYS	3.3
1	F	137	LYS	3.3
1	H	322	ASN	3.3
1	I	602	ASN	3.3
1	F	147	LYS	3.3
1	I	121	CYS	3.2
1	D	515	GLN	3.2
1	H	272	ASN	3.2
1	F	162	MET	3.2
1	L	111	LYS	3.2
1	F	363	GLY	3.2
1	C	163	GLU	3.1
1	H	586	ARG	3.1
1	L	362	LYS	3.1
1	H	197	ASP	3.1
1	F	267	LEU	3.1
1	J	255	THR	3.1
1	J	112	VAL	3.1
1	C	568	ASN	3.1
1	A	197	ASP	3.1
1	A	132	VAL	3.1
1	C	268	GLY	3.1
1	I	167	VAL	3.0
1	F	402	GLY	3.0
1	F	146	SER	3.0
1	F	272	ASN	3.0
1	L	161	ASN	3.0
1	C	362	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	600	VAL	3.0
1	L	178	PHE	3.0
1	L	125	GLU	3.0
1	H	366	LYS	3.0
1	H	216	ASP	3.0
1	K	194	SER	2.9
1	K	409	CYS	2.9
1	K	568	ASN	2.9
1	I	114	VAL	2.9
1	A	507	GLU	2.9
1	B	164	LYS	2.9
1	D	427	SER	2.9
1	B	126	GLY	2.9
1	J	92	VAL	2.9
1	A	124	GLU	2.9
1	C	138	GLU	2.9
1	L	218	LYS	2.9
1	G	361	SER	2.9
1	C	603	ASP	2.9
1	B	322	ASN	2.9
1	F	153	VAL	2.9
1	J	549	SER	2.8
1	L	275	ASP	2.8
1	H	176	TYR	2.8
1	L	112	VAL	2.8
1	I	520	SER	2.8
1	K	362	LYS	2.8
1	K	193	GLY	2.8
1	A	148	VAL	2.8
1	F	112	VAL	2.8
1	H	445	ILE	2.8
1	K	549	SER	2.8
1	B	219	LEU	2.8
1	F	196	ALA	2.8
1	I	123	VAL	2.8
1	B	389	PRO	2.8
1	C	364	ASP	2.8
1	G	364	ASP	2.8
1	I	262	GLU	2.8
1	B	107	ILE	2.7
1	G	188	GLY	2.7
1	F	156	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	269	VAL	2.7
1	K	254	SER	2.7
1	F	175	PHE	2.7
1	F	185	VAL	2.7
1	F	364	ASP	2.7
1	F	218	LYS	2.7
1	F	157	LEU	2.7
1	B	163	GLU	2.7
1	F	181	ASN	2.7
1	B	165	PHE	2.7
1	B	196	ALA	2.7
1	C	165	PHE	2.7
1	G	186	ALA	2.7
1	F	161	ASN	2.7
1	B	123	VAL	2.7
1	J	390	GLY	2.6
1	C	365	VAL	2.6
1	I	184	SER	2.6
1	F	176	TYR	2.6
1	H	323	LEU	2.6
1	D	124	GLU	2.6
1	D	419	GLU	2.6
1	F	362	LYS	2.6
1	H	363	GLY	2.6
1	D	260	ASN	2.6
1	D	254	SER	2.6
1	I	165	PHE	2.6
1	K	137	LYS	2.6
1	C	507	GLU	2.6
1	H	124	GLU	2.6
1	F	314	ALA	2.6
1	H	217	ASN	2.6
1	F	184	SER	2.6
1	G	146	SER	2.6
1	I	197	ASP	2.6
1	A	162	MET	2.6
1	H	480	TYR	2.6
1	F	155	GLU	2.6
1	K	191	GLY	2.6
1	K	195	VAL	2.6
1	F	599	PHE	2.6
1	I	568	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	513	ILE	2.5
1	L	423	ILE	2.5
1	F	321	LEU	2.5
1	H	262	GLU	2.5
1	A	551	VAL	2.5
1	C	121	CYS	2.5
1	L	196	ALA	2.5
1	E	161	ASN	2.5
1	I	511	ASN	2.5
1	J	149	ASN	2.5
1	F	216	ASP	2.5
1	J	219	LEU	2.5
1	B	136	GLY	2.5
1	J	123	VAL	2.5
1	B	202	ASP	2.5
1	F	144	ILE	2.5
1	A	422	GLU	2.5
1	L	115	TYR	2.5
1	L	263	TYR	2.5
1	H	389	PRO	2.5
1	B	550	SER	2.5
1	F	550	SER	2.5
1	H	234	LEU	2.5
1	F	275	ASP	2.5
1	L	216	ASP	2.5
1	G	124	GLU	2.5
1	G	363	GLY	2.5
1	A	113	GLN	2.5
1	H	284	ALA	2.5
1	F	322	ASN	2.4
1	E	219	LEU	2.4
1	L	121	CYS	2.4
1	K	262	GLU	2.4
1	F	187	VAL	2.4
1	H	286	VAL	2.4
1	A	469	ALA	2.4
1	B	276	THR	2.4
1	I	138	GLU	2.4
1	L	213	MET	2.4
1	A	363	GLY	2.4
1	D	195	VAL	2.4
1	I	288	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	365	VAL	2.4
1	I	274	ALA	2.4
1	H	129	ILE	2.4
1	L	127	LEU	2.4
1	B	511	ASN	2.4
1	B	602	ASN	2.4
1	H	511	ASN	2.4
1	F	125	GLU	2.4
1	H	180	ASP	2.4
1	K	419	GLU	2.4
1	D	600	VAL	2.4
1	G	473	ALA	2.4
1	J	370	ALA	2.4
1	K	129	ILE	2.4
1	G	457	ASN	2.4
1	C	520	SER	2.4
1	H	163	GLU	2.4
1	A	483	ASP	2.4
1	A	603	ASP	2.4
1	I	442	GLY	2.4
1	C	524	VAL	2.4
1	D	551	VAL	2.4
1	G	85	ALA	2.4
1	J	201	ALA	2.4
1	H	601	LEU	2.3
1	F	128	THR	2.3
1	F	122	ASN	2.3
1	K	104	ASN	2.3
1	L	163	GLU	2.3
1	I	164	LYS	2.3
1	K	331	LYS	2.3
1	H	477	GLY	2.3
1	C	132	VAL	2.3
1	E	434	VAL	2.3
1	H	99	ILE	2.3
1	J	513	ILE	2.3
1	F	217	ASN	2.3
1	H	568	ASN	2.3
1	B	232	LYS	2.3
1	G	256	ASP	2.3
1	I	549	SER	2.3
1	B	193	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	190	VAL	2.3
1	F	514	LEU	2.3
1	H	280	GLU	2.3
1	I	163	GLU	2.3
1	K	332	GLU	2.3
1	F	113	GLN	2.3
1	H	123	VAL	2.3
1	H	409	CYS	2.3
1	I	323	LEU	2.3
1	K	196	ALA	2.3
1	B	512	LYS	2.3
1	E	102	GLU	2.3
1	F	273	ASN	2.3
1	B	194	SER	2.3
1	E	364	ASP	2.3
1	J	364	ASP	2.3
1	G	578	GLY	2.3
1	I	140	GLY	2.3
1	J	136	GLY	2.3
1	F	127	LEU	2.3
1	H	219	LEU	2.3
1	G	467	ALA	2.2
1	G	485	ALA	2.2
1	B	105	THR	2.2
1	B	229	ASN	2.2
1	F	139	ASN	2.2
1	B	150	ASP	2.2
1	G	197	ASP	2.2
1	G	427	SER	2.2
1	L	361	SER	2.2
1	G	496	GLY	2.2
1	F	455	VAL	2.2
1	H	214	LEU	2.2
1	K	219	LEU	2.2
1	K	333	LEU	2.2
1	L	434	VAL	2.2
1	B	226	PHE	2.2
1	E	289	PHE	2.2
1	F	331	LYS	2.2
1	H	201	ALA	2.2
1	F	270	TYR	2.2
1	I	161	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	183	ASN	2.2
1	L	149	ASN	2.2
1	L	273	ASN	2.2
1	C	197	ASP	2.2
1	F	516	SER	2.2
1	G	136	GLY	2.2
1	L	184	SER	2.2
1	I	421	VAL	2.2
1	C	124	GLU	2.2
1	L	507	GLU	2.2
1	E	568	ASN	2.2
1	I	122	ASN	2.2
1	L	602	ASN	2.2
1	G	193	GLY	2.2
1	C	602	ASN	2.2
1	H	181	ASN	2.2
1	L	135	PRO	2.2
1	H	271	ILE	2.2
1	I	132	VAL	2.2
1	K	123	VAL	2.2
1	A	274	ALA	2.1
1	J	85	ALA	2.1
1	K	200	GLU	2.1
1	J	568	ASN	2.1
1	D	395	LEU	2.1
1	L	222	LEU	2.1
1	F	126	GLY	2.1
1	L	126	GLY	2.1
1	L	197	ASP	2.1
1	L	209	SER	2.1
1	H	178	PHE	2.1
1	K	125	GLU	2.1
1	F	276	THR	2.1
1	F	326	LYS	2.1
1	B	217	ASN	2.1
1	C	261	MET	2.1
1	G	217	ASN	2.1
1	J	260	ASN	2.1
1	B	275	ASP	2.1
1	H	230	VAL	2.1
1	L	281	VAL	2.1
1	A	427	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	405	ALA	2.1
1	G	138	GLU	2.1
1	H	200	GLU	2.1
1	K	367	LYS	2.1
1	I	198	LEU	2.1
1	E	602	ASN	2.1
1	J	602	ASN	2.1
1	B	383	TYR	2.1
1	I	120	GLY	2.1
1	K	174	HIS	2.1
1	L	246	TYR	2.1
1	H	369	ILE	2.1
1	B	178	PHE	2.1
1	B	364	ASP	2.1
1	K	175	PHE	2.1
1	B	200	GLU	2.1
1	D	418	PRO	2.1
1	B	407	LEU	2.1
1	J	127	LEU	2.1
1	A	121	CYS	2.1
1	J	347	GLY	2.1
1	H	107	ILE	2.1
1	B	138	GLU	2.0
1	G	205	ARG	2.0
1	F	186	ALA	2.0
1	I	86	SER	2.0
1	J	427	SER	2.0
1	L	570	ALA	2.0
1	C	366	LYS	2.0
1	F	151	LYS	2.0
1	D	371	LEU	2.0
1	L	595	LEU	2.0
1	B	122	ASN	2.0
1	B	382	GLY	2.0
1	I	480	TYR	2.0
1	H	175	PHE	2.0
1	I	124	GLU	2.0
1	I	599	PHE	2.0
1	A	601	LEU	2.0
1	B	601	LEU	2.0
1	F	219	LEU	2.0
1	G	601	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	515	GLN	2.0
1	J	426	LEU	2.0
1	G	161	ASN	2.0
1	L	139	ASN	2.0
1	F	285	ARG	2.0
1	J	207	VAL	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(Å ²)	Q<0.9
4	SO4	L	701	5/5	0.27	0.12	123,127,143,154	0
4	SO4	L	705	5/5	0.38	0.14	123,128,135,152	0
4	SO4	E	704	5/5	0.58	0.34	122,123,124,148	0
4	SO4	D	704	5/5	0.62	0.27	112,113,119,125	0
4	SO4	A	705	5/5	0.65	0.20	92,92,106,117	0
5	1PE	B	1005	7/16	0.68	0.23	37,47,51,53	0
3	CO3	J	703	4/4	0.72	0.21	26,26,27,44	0
5	1PE	C	705	13/16	0.72	0.17	37,49,62,64	0
5	1PE	D	706	10/16	0.72	0.17	36,55,59,62	0
5	1PE	K	704	9/16	0.73	0.16	31,34,42,42	0
5	1PE	D	707	9/16	0.75	0.18	28,38,51,51	0
5	1PE	K	705	16/16	0.75	0.16	45,59,72,75	0
4	SO4	G	708	5/5	0.76	0.20	75,77,92,95	0
4	SO4	I	705	5/5	0.77	0.16	64,68,75,77	0
5	1PE	G	707	13/16	0.79	0.16	41,50,64,67	0
4	SO4	A	704	5/5	0.79	0.36	84,85,101,116	0
5	1PE	G	705	9/16	0.79	0.18	40,50,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	1PE	L	706	16/16	0.79	0.17	48,64,75,78	0
5	1PE	A	706	9/16	0.80	0.16	37,37,46,49	0
5	1PE	G	706	10/16	0.80	0.16	35,44,54,56	0
5	1PE	A	707	10/16	0.80	0.18	39,43,52,55	0
4	SO4	H	705	5/5	0.81	0.13	52,55,81,85	0
3	CO3	A	703	4/4	0.82	0.18	35,38,38,43	0
5	1PE	C	707	10/16	0.82	0.17	28,35,50,51	0
3	CO3	G	701	4/4	0.83	0.17	39,39,46,50	0
5	1PE	H	704	10/16	0.83	0.17	44,51,59,61	0
5	1PE	C	706	9/16	0.83	0.13	33,38,46,48	0
4	SO4	C	704	5/5	0.83	0.15	66,72,75,94	0
5	1PE	D	705	10/16	0.83	0.17	33,39,41,45	0
3	CO3	D	703	4/4	0.84	0.15	23,23,25,31	0
5	1PE	F	705	10/16	0.84	0.13	33,38,44,48	0
3	CO3	L	704	4/4	0.84	0.13	37,43,44,48	0
4	SO4	K	706	5/5	0.85	0.18	46,53,74,74	0
5	1PE	J	704	10/16	0.86	0.14	33,37,46,51	0
5	1PE	E	705	12/16	0.86	0.14	28,33,64,64	0
4	SO4	G	704	5/5	0.87	0.12	45,54,65,69	0
3	CO3	E	703	4/4	0.87	0.12	37,38,39,42	0
5	1PE	E	706	9/16	0.88	0.14	23,33,41,41	0
3	CO3	H	703	4/4	0.89	0.11	37,37,39,39	0
3	CO3	F	704	4/4	0.91	0.11	25,29,32,36	0
3	CO3	I	703	4/4	0.91	0.10	29,31,32,33	0
4	SO4	C	708	5/5	0.92	0.12	49,52,54,65	0
3	CO3	C	703	4/4	0.92	0.09	33,34,35,43	0
4	SO4	B	1004	5/5	0.93	0.11	33,33,33,37	0
3	CO3	K	703	4/4	0.94	0.09	26,29,34,42	0
3	CO3	B	1001	4/4	0.94	0.09	29,30,32,33	0
2	ZN	F	702	1/1	0.95	0.09	31,31,31,31	0
2	ZN	L	702	1/1	0.95	0.07	32,32,32,32	0
4	SO4	J	705	5/5	0.96	0.08	24,31,34,41	0
4	SO4	I	704	5/5	0.96	0.08	34,34,34,40	0
2	ZN	B	1003	1/1	0.97	0.08	35,35,35,35	0
2	ZN	F	703	1/1	0.97	0.05	24,24,24,24	0
2	ZN	C	701	1/1	0.97	0.10	29,29,29,29	0
2	ZN	J	701	1/1	0.98	0.10	30,30,30,30	0
2	ZN	A	701	1/1	0.98	0.04	32,32,32,32	0
2	ZN	L	703	1/1	0.98	0.05	28,28,28,28	0
2	ZN	D	701	1/1	0.98	0.06	25,25,25,25	0
2	ZN	G	703	1/1	0.98	0.07	34,34,34,34	0
2	ZN	H	702	1/1	0.98	0.04	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	F	701	5/5	0.98	0.05	20,24,29,33	0
2	ZN	I	701	1/1	0.98	0.09	29,29,29,29	0
2	ZN	I	702	1/1	0.98	0.09	29,29,29,29	0
2	ZN	B	1002	1/1	0.99	0.06	29,29,29,29	0
2	ZN	J	702	1/1	0.99	0.06	24,24,24,24	0
2	ZN	K	701	1/1	0.99	0.06	25,25,25,25	0
2	ZN	K	702	1/1	0.99	0.06	32,32,32,32	0
2	ZN	C	702	1/1	0.99	0.08	29,29,29,29	0
2	ZN	G	702	1/1	0.99	0.05	34,34,34,34	0
2	ZN	A	702	1/1	0.99	0.04	32,32,32,32	0
2	ZN	H	701	1/1	0.99	0.04	31,31,31,31	0
2	ZN	D	702	1/1	0.99	0.05	30,30,30,30	0
2	ZN	E	701	1/1	0.99	0.04	23,23,23,23	0
2	ZN	E	702	1/1	0.99	0.09	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.