



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 12:23 pm GMT

PDB ID : 1N4Q
Title : Protein Geranylgeranyltransferase type-I Complexed with a GGPP Analog and a KKKSSTKCVIL Peptide
Authors : Taylor, J.S.; Reid, T.S.; Casey, P.J.; Beese, L.S.
Deposited on : 2002-11-01
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

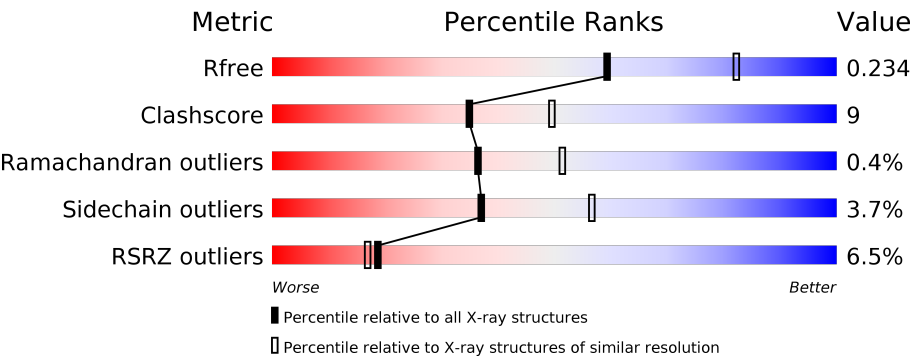
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	377	<div><div>3%</div><div><div></div><div>67%</div><div>15%</div><div>•</div><div>17%</div></div></div>
1	C	377	<div><div>2%</div><div><div></div><div>67%</div><div>15%</div><div>•</div><div>17%</div></div></div>
1	E	377	<div><div>3%</div><div><div></div><div>64%</div><div>18%</div><div>•</div><div>17%</div></div></div>
1	G	377	<div><div>3%</div><div><div></div><div>65%</div><div>18%</div><div>•</div><div>17%</div></div></div>
1	I	377	<div><div>3%</div><div><div></div><div>67%</div><div>15%</div><div>•</div><div>17%</div></div></div>
1	K	377	<div><div>%</div><div><div></div><div>69%</div><div>13%</div><div>•</div><div>17%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	B	377	
2	D	377	
2	F	377	
2	H	377	
2	J	377	
2	L	377	
3	M	11	
3	N	11	
3	O	11	
3	P	11	
3	Q	11	
3	R	11	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33546 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 Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2611	1672	458	476	5			
1	C	314	Total	C	N	O	S	0	0	0
			2630	1683	457	485	5			
1	E	314	Total	C	N	O	S	0	0	0
			2639	1685	461	488	5			
1	G	314	Total	C	N	O	S	0	0	0
			2621	1677	455	484	5			
1	I	314	Total	C	N	O	S	0	0	0
			2645	1690	460	490	5			
1	K	314	Total	C	N	O	S	0	0	0
			2667	1700	466	496	5			

- Molecule 2 is a protein called Geranylgeranyl transferase type-1 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2689	1702	467	496	24			
2	D	346	Total	C	N	O	S	0	0	0
			2690	1705	463	498	24			
2	F	346	Total	C	N	O	S	0	0	0
			2700	1708	468	500	24			
2	H	346	Total	C	N	O	S	0	0	0
			2680	1698	460	498	24			
2	J	346	Total	C	N	O	S	0	0	0
			2706	1710	471	501	24			
2	L	346	Total	C	N	O	S	0	0	0
			2710	1713	471	502	24			

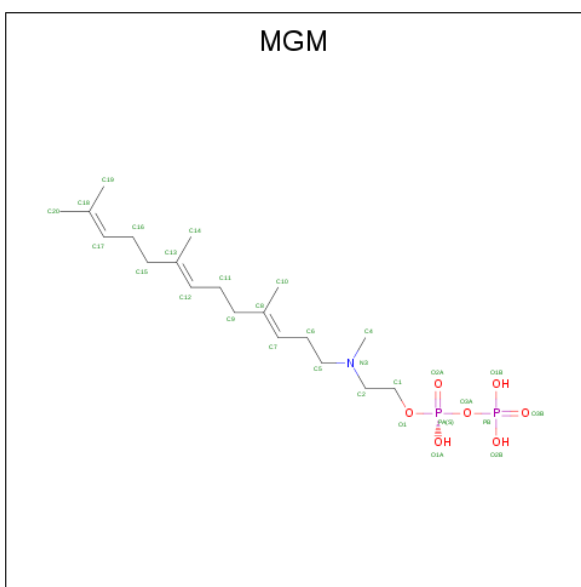
- Molecule 3 is a protein called Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			
3	N	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			
3	O	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			
3	P	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			
3	Q	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			
3	R	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 2-[METHYL-(5-GERANYL-4-METHYL-PENT-3-ENYL)-AMINO]-ETHYL-DIPHOSPHATE (three-letter code: MGM) (formula: C₁₉H₃₇NO₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 29	C 19	N 1	O 7	P 2	0	0
5	D	1	Total 29	C 19	N 1	O 7	P 2	0	0
5	F	1	Total 29	C 19	N 1	O 7	P 2	0	0
5	H	1	Total 29	C 19	N 1	O 7	P 2	0	0
5	J	1	Total 29	C 19	N 1	O 7	P 2	0	0
5	L	1	Total 29	C 19	N 1	O 7	P 2	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

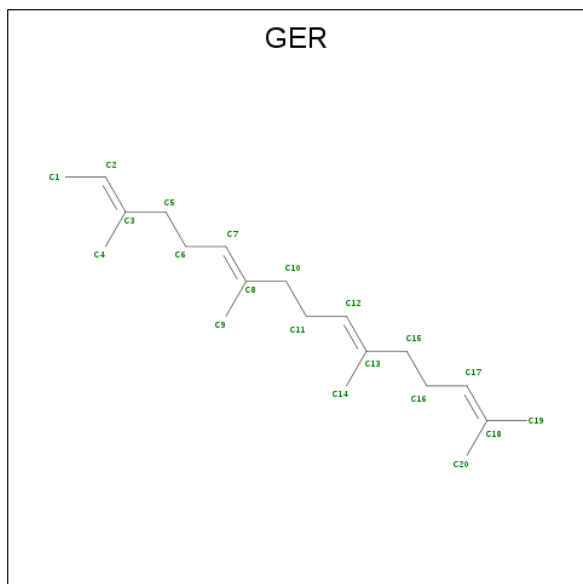
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total Cl 1 1	0	0
6	J	1	Total Cl 1 1	0	0
6	D	1	Total Cl 1 1	0	0
6	K	1	Total Cl 1 1	0	0
6	H	1	Total Cl 1 1	0	0
6	C	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Cl 1 1	0	0

- Molecule 7 is GERAN-8-YL GERAN (three-letter code: GER) (formula: $C_{20}H_{34}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	R	1	Total C 20 20	0	0

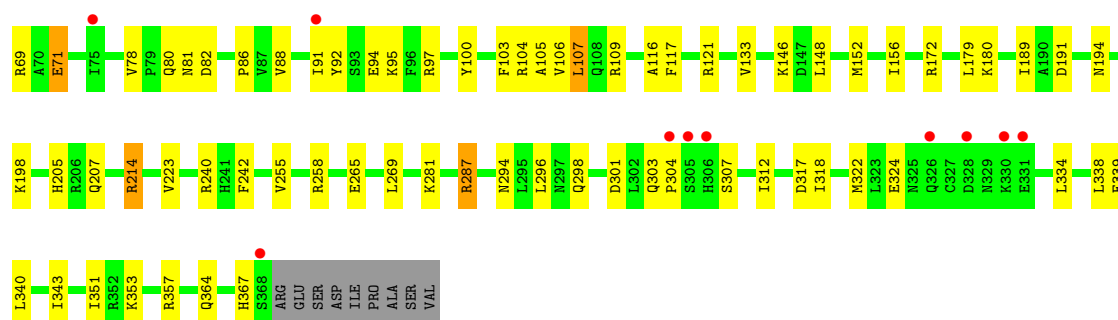
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	78	Total O 78 78	0	0
8	B	64	Total O 64 64	0	0
8	C	82	Total O 82 82	0	0
8	D	89	Total O 89 89	0	0
8	E	81	Total O 81 81	0	0
8	F	91	Total O 91 91	0	0
8	G	75	Total O 75 75	0	0

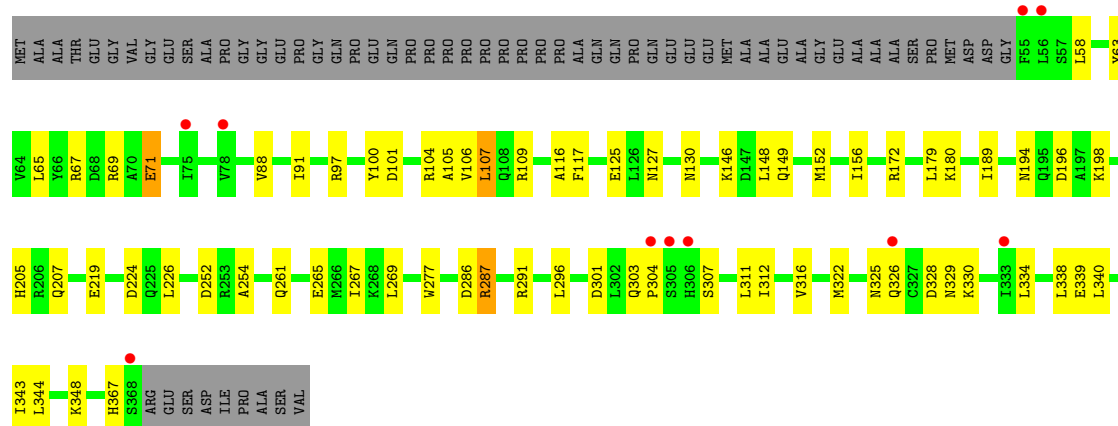
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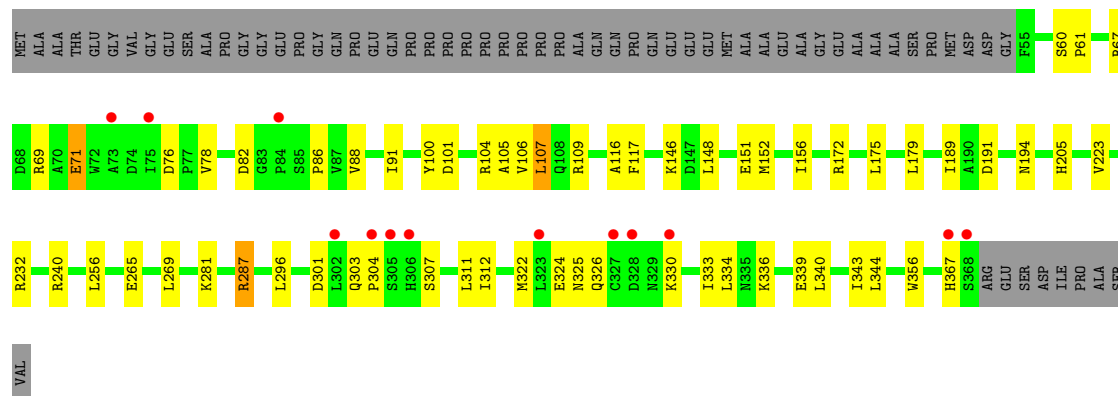
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	56	Total 56	O 56	0	0
8	I	104	Total 104	O 104	0	0
8	J	82	Total 82	O 82	0	0
8	K	169	Total 169	O 169	0	0
8	L	121	Total 121	O 121	0	0
8	M	7	Total 7	O 7	0	0
8	N	4	Total 4	O 4	0	0
8	O	4	Total 4	O 4	0	0
8	P	1	Total 1	O 1	0	0
8	Q	6	Total 6	O 6	0	0
8	R	3	Total 3	O 3	0	0



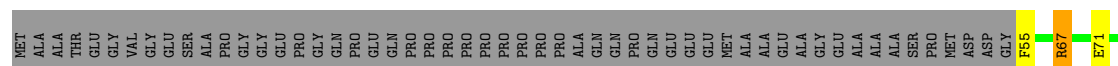
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

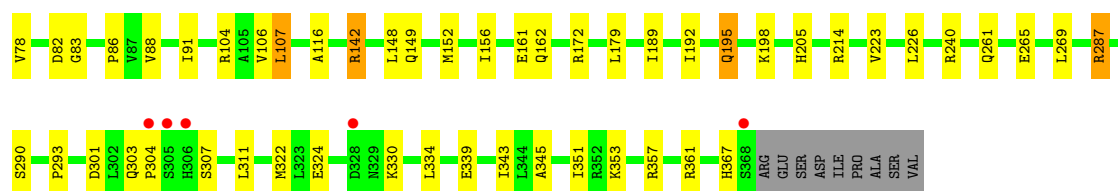


- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

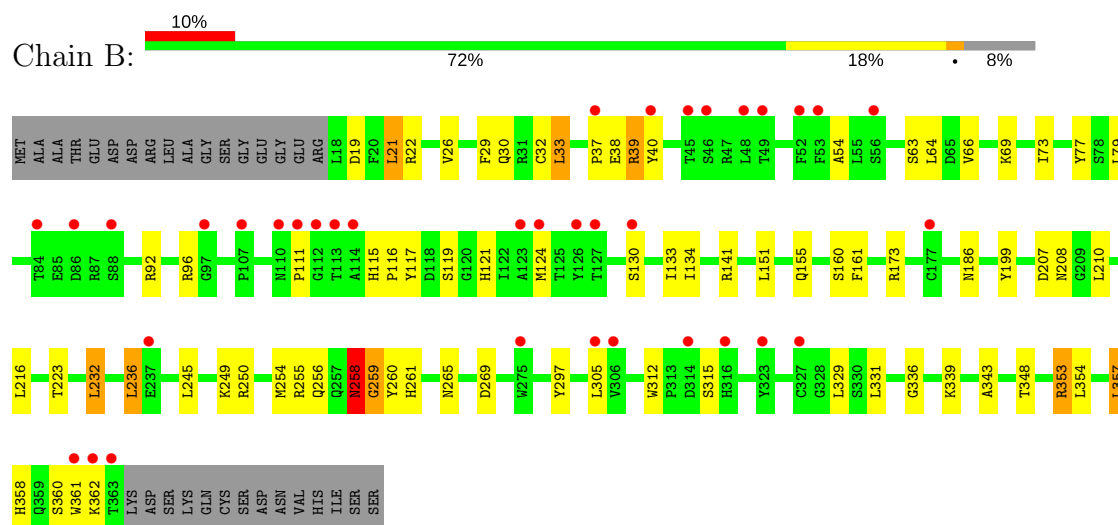


- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

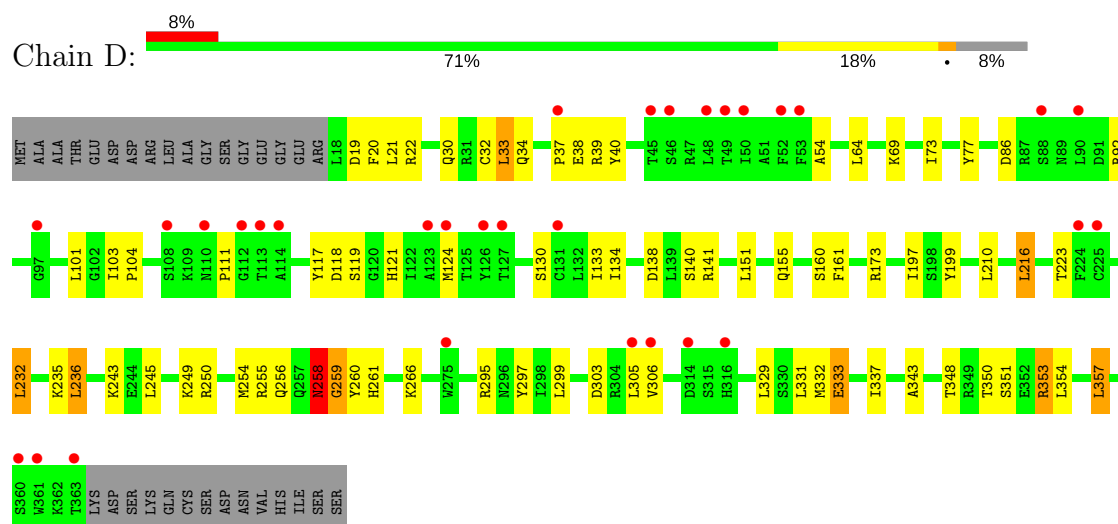




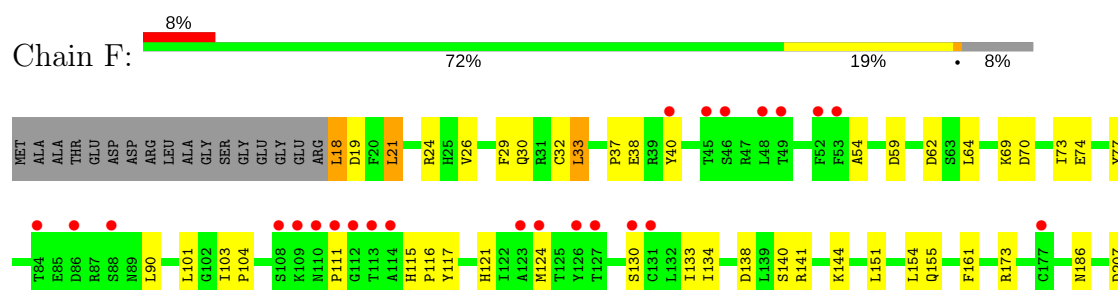
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

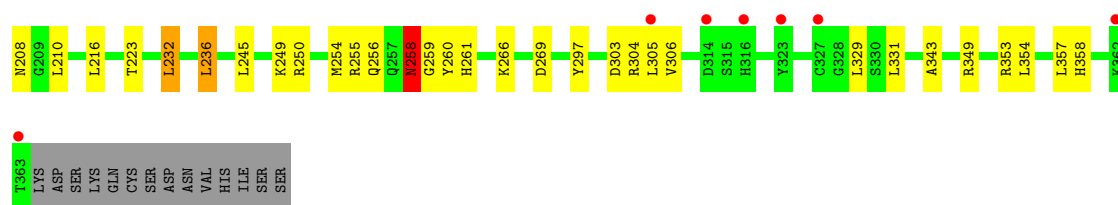


• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

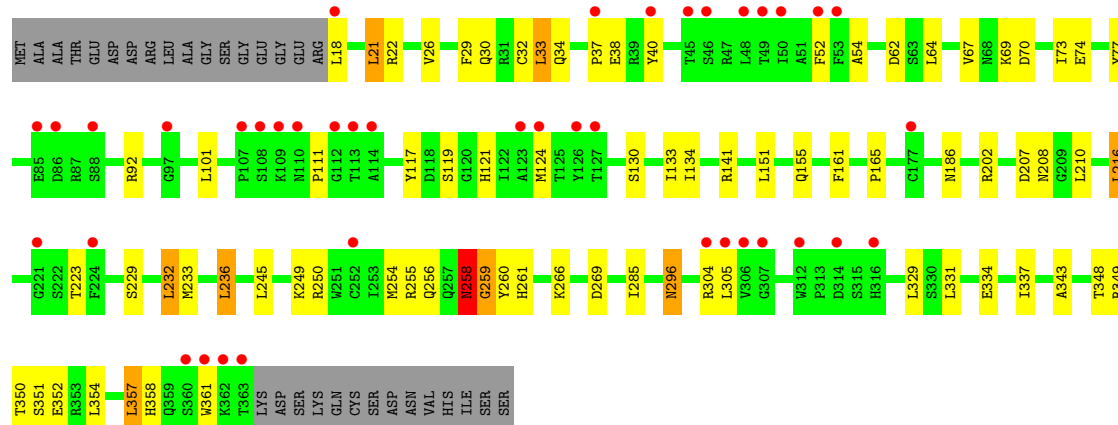


• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

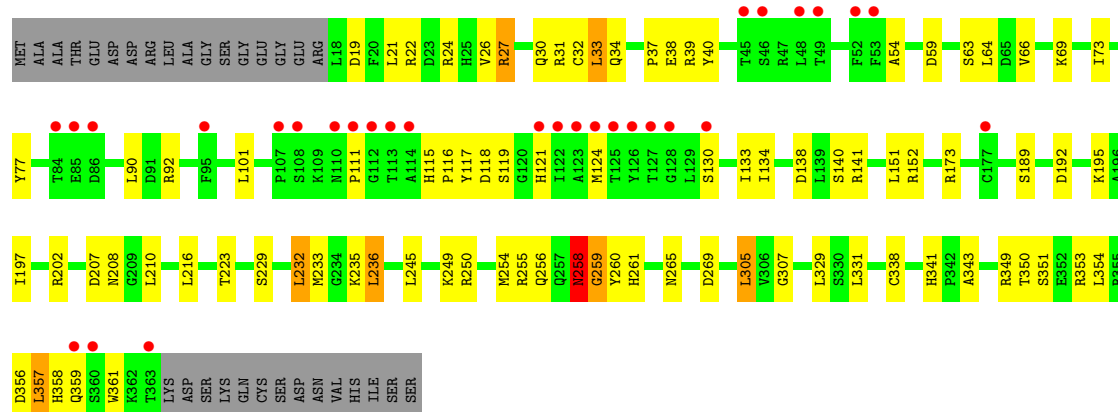




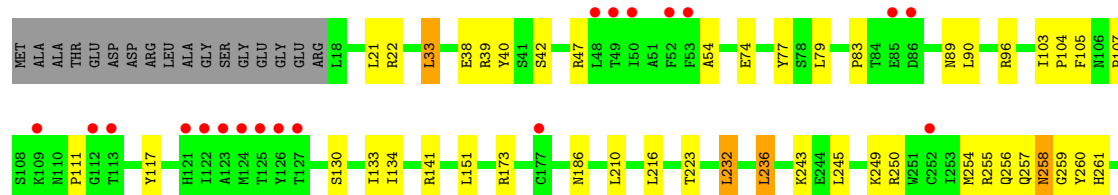
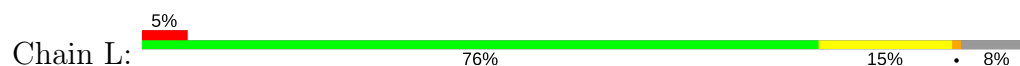
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

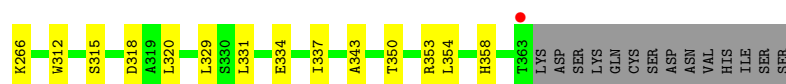


• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

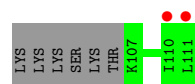


• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

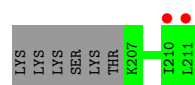




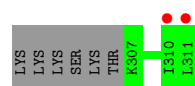
- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



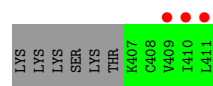
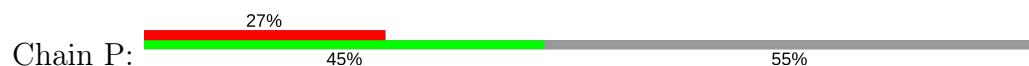
- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



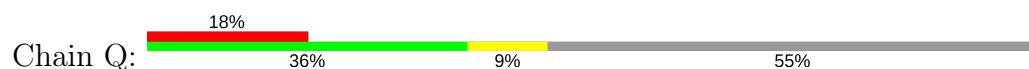
- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



LYS		
LYS		
LYS		
SER		
LYS		
THR		
K607		
C608		
V609		
I610		
L611		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	271.06Å 268.03Å 184.97Å 90.00° 131.73° 90.00°	Depositor
Resolution (Å)	29.99 – 2.40 33.12 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.8 (29.99-2.40) 92.6 (33.12-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.234 0.213 , 0.234	Depositor DCC
R_{free} test set	17766 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.087 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33546	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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: GER, ZN, MGM, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/2677	0.52	0/3645
1	C	0.35	0/2696	0.53	0/3668
1	E	0.33	0/2705	0.53	0/3680
1	G	0.34	0/2687	0.52	0/3658
1	I	0.35	0/2711	0.53	0/3686
1	K	0.39	0/2733	0.55	0/3713
2	B	0.35	0/2750	0.60	2/3720 (0.1%)
2	D	0.36	0/2751	0.60	2/3720 (0.1%)
2	F	0.37	0/2761	0.60	2/3733 (0.1%)
2	H	0.35	0/2741	0.59	2/3710 (0.1%)
2	J	0.36	0/2767	0.60	2/3741 (0.1%)
2	L	0.39	0/2771	0.62	2/3745 (0.1%)
3	M	0.56	0/38	0.52	0/48
3	N	0.53	0/38	0.54	0/48
3	O	0.57	0/38	0.54	0/48
3	P	0.53	0/38	0.51	0/48
3	Q	0.55	0/38	0.52	0/48
3	R	0.67	0/38	1.08	0/48
All	All	0.36	0/32978	0.57	12/44707 (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
2	B	0	1
2	D	0	1
2	F	0	1
All	All	0	3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	259	GLY	N-CA-C	-6.07	97.93	113.10
2	L	259	GLY	N-CA-C	-5.91	98.32	113.10
2	H	259	GLY	N-CA-C	-5.90	98.34	113.10
2	D	259	GLY	N-CA-C	-5.87	98.43	113.10
2	F	259	GLY	N-CA-C	-5.82	98.54	113.10
2	B	259	GLY	N-CA-C	-5.81	98.57	113.10
2	J	258	ASN	N-CA-C	-5.57	95.96	111.00
2	D	258	ASN	N-CA-C	-5.54	96.05	111.00
2	L	258	ASN	N-CA-C	-5.50	96.16	111.00
2	H	258	ASN	N-CA-C	-5.45	96.28	111.00
2	F	258	ASN	N-CA-C	-5.36	96.52	111.00
2	B	258	ASN	N-CA-C	-5.35	96.55	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	297	TYR	Sidechain
2	D	297	TYR	Sidechain
2	F	297	TYR	Sidechain

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	2611	0	2497	46	0
1	C	2630	0	2521	41	0
1	E	2639	0	2532	56	0
1	G	2621	0	2502	58	0
1	I	2645	0	2543	40	0
1	K	2667	0	2577	45	0
2	B	2689	0	2585	50	0
2	D	2690	0	2588	50	0
2	F	2700	0	2602	48	0
2	H	2680	0	2562	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	2706	0	2608	54	0
2	L	2710	0	2617	38	0
3	M	39	0	47	0	0
3	N	39	0	47	0	0
3	O	39	0	47	0	0
3	P	39	0	47	0	0
3	Q	39	0	47	1	0
3	R	39	0	47	6	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
5	B	29	0	34	3	0
5	D	29	0	34	3	0
5	F	29	0	34	2	0
5	H	29	0	34	2	0
5	J	29	0	34	3	0
5	L	29	0	34	4	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	1	0
6	H	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	1	0
7	R	20	0	33	7	0
8	A	78	0	0	3	0
8	B	64	0	0	1	0
8	C	82	0	0	2	0
8	D	89	0	0	1	0
8	E	81	0	0	0	0
8	F	91	0	0	3	0
8	G	75	0	0	5	0
8	H	56	0	0	1	0
8	I	104	0	0	1	0
8	J	82	0	0	3	0
8	K	169	0	0	7	0
8	L	121	0	0	3	0
8	M	7	0	0	0	0
8	N	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	O	4	0	0	0	0
8	P	1	0	0	0	0
8	Q	6	0	0	1	0
8	R	3	0	0	0	0
All	All	33546	0	31253	569	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (569) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:156:ILE:HG12	1:K:172:ARG:HH12	1.03	1.15
1:E:156:ILE:HG12	1:E:172:ARG:HH12	1.08	1.13
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.13	1.12
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.14	1.07
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.14	1.05
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.16	1.04
1:K:156:ILE:HG12	1:K:172:ARG:NH1	1.84	0.91
2:L:318:ASP:HB2	7:R:1300:GER:H71	1.53	0.88
6:G:1311:CL:CL	8:G:1323:HOH:O	2.31	0.84
1:A:156:ILE:HG12	1:A:172:ARG:NH1	1.94	0.83
1:E:156:ILE:HG12	1:E:172:ARG:NH1	1.93	0.83
6:K:1317:CL:CL	8:K:1332:HOH:O	2.33	0.82
1:A:152:MET:O	1:A:156:ILE:HG13	1.80	0.81
2:B:92:ARG:NH1	2:B:119:SER:HB3	1.96	0.81
2:B:39:ARG:HB3	2:B:39:ARG:HH11	1.44	0.80
1:G:152:MET:O	1:G:156:ILE:HG13	1.82	0.79
1:I:156:ILE:HG12	1:I:172:ARG:NH1	1.96	0.79
1:K:152:MET:O	1:K:156:ILE:HG13	1.82	0.78
2:H:348:THR:O	2:H:352:GLU:HG2	1.84	0.78
1:E:152:MET:O	1:E:156:ILE:HG13	1.84	0.77
1:E:353:LYS:HE2	1:E:357:ARG:HH12	1.47	0.77
1:I:152:MET:O	1:I:156:ILE:HG13	1.84	0.77
2:B:92:ARG:HH11	2:B:119:SER:HB3	1.48	0.77
1:C:152:MET:O	1:C:156:ILE:HG13	1.85	0.76
2:D:39:ARG:HG3	2:D:40:TYR:CE1	2.20	0.76
1:G:101:ASP:HA	1:G:104:ARG:NH1	2.00	0.76
2:L:42:SER:HG	3:R:607:LYS:N	1.88	0.72
2:D:295:ARG:CZ	2:D:299:LEU:HD11	2.21	0.71
1:G:156:ILE:HG12	1:G:172:ARG:NH1	2.00	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ILE:HG12	1:C:172:ARG:NH1	1.99	0.70
2:D:69:LYS:O	2:D:73:ILE:HG13	1.92	0.70
2:F:19:ASP:HB3	8:F:1433:HOH:O	1.90	0.69
1:E:353:LYS:CE	1:E:357:ARG:HH12	2.06	0.69
1:K:156:ILE:CG1	1:K:172:ARG:HH12	1.94	0.69
2:H:92:ARG:HG2	2:H:165:PRO:HG3	1.75	0.68
2:B:353:ARG:HH11	2:B:353:ARG:HG2	1.59	0.68
1:I:334:LEU:HD22	1:I:367:HIS:O	1.93	0.68
3:R:609:VAL:HG23	3:R:610:ILE:HG23	1.76	0.66
2:F:133:ILE:HD13	2:F:354:LEU:HD13	1.78	0.65
1:G:334:LEU:HD22	1:G:367:HIS:O	1.96	0.65
2:F:69:LYS:O	2:F:73:ILE:HG13	1.96	0.65
2:H:349:ARG:O	2:H:352:GLU:HB2	1.95	0.65
1:K:107:LEU:HD22	2:L:117:TYR:CD2	2.32	0.65
1:G:97:ARG:HG2	1:G:101:ASP:OD2	1.97	0.65
2:H:133:ILE:HG22	2:H:350:THR:HG23	1.78	0.64
1:G:100:TYR:O	1:G:104:ARG:HG3	1.97	0.64
2:L:133:ILE:HD13	2:L:354:LEU:HD13	1.79	0.64
2:H:18:LEU:N	2:H:18:LEU:HD22	2.13	0.64
1:E:312:ILE:HG23	1:E:340:LEU:HD22	1.80	0.64
2:J:92:ARG:HH11	2:J:119:SER:HB3	1.62	0.64
2:J:195:LYS:NZ	8:J:1444:HOH:O	2.30	0.63
2:B:39:ARG:HH11	2:B:39:ARG:CB	2.09	0.63
1:A:214:ARG:HG2	1:G:180:LYS:HB2	1.79	0.63
2:J:92:ARG:NH1	2:J:119:SER:HB3	2.14	0.63
1:C:334:LEU:HD22	1:C:367:HIS:O	1.98	0.63
1:E:69:ARG:HB3	1:E:71:GLU:OE1	1.98	0.63
2:D:37:PRO:HB2	2:D:39:ARG:HG2	1.81	0.63
1:G:261:GLN:O	1:G:265:GLU:HG2	1.99	0.63
2:H:296:ASN:HD22	2:H:296:ASN:C	2.02	0.63
2:B:69:LYS:O	2:B:73:ILE:HG13	1.99	0.62
2:F:37:PRO:HD2	2:F:40:TYR:CD1	2.33	0.62
2:H:69:LYS:O	2:H:73:ILE:HG13	1.99	0.62
2:B:258:ASN:OD1	2:B:259:GLY:N	2.30	0.62
1:E:78:VAL:O	1:E:104:ARG:HD2	1.99	0.62
1:I:69:ARG:HB3	1:I:71:GLU:OE1	2.00	0.61
1:E:353:LYS:HE3	1:E:357:ARG:HH22	1.65	0.61
2:D:37:PRO:HD2	2:D:40:TYR:CD1	2.35	0.61
2:B:133:ILE:HD13	2:B:354:LEU:HD13	1.81	0.61
1:I:107:LEU:HD22	2:J:117:TYR:CD2	2.36	0.61
1:G:328:ASP:O	1:G:329:ASN:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:LEU:HD11	1:E:364:GLN:HG3	1.83	0.60
1:G:101:ASP:HA	1:G:104:ARG:HH11	1.65	0.60
2:L:232:LEU:HD13	2:L:343:ALA:HB1	1.82	0.60
1:A:301:ASP:O	1:A:304:PRO:HD2	2.01	0.60
2:B:186:ASN:HB2	2:B:358:HIS:CE1	2.37	0.60
1:G:343:ILE:HG22	1:G:348:LYS:HG3	1.83	0.60
2:J:258:ASN:OD1	2:J:259:GLY:N	2.31	0.59
3:R:608:CYS:HA	7:R:1300:GER:C2	2.32	0.59
2:J:133:ILE:HD13	2:J:354:LEU:HD13	1.83	0.59
1:E:214:ARG:O	1:E:214:ARG:HG3	2.02	0.59
1:G:189:ILE:HD11	1:G:205:HIS:HD2	1.68	0.59
1:G:58:LEU:HD12	1:G:125:GLU:OE2	2.03	0.59
2:L:334:GLU:HB3	2:L:337:ILE:HD12	1.85	0.59
1:A:91:ILE:HD11	2:B:38:GLU:H	1.68	0.59
1:C:91:ILE:HD11	2:D:38:GLU:H	1.68	0.58
1:C:303:GLN:O	1:C:307:SER:HB2	2.02	0.58
2:J:210:LEU:HB2	2:J:223:THR:HA	1.84	0.58
3:R:608:CYS:HA	7:R:1300:GER:H21	1.84	0.58
1:A:214:ARG:O	1:A:214:ARG:HG3	2.03	0.58
2:J:232:LEU:HD13	2:J:343:ALA:HB1	1.86	0.58
2:F:210:LEU:HB2	2:F:223:THR:HA	1.85	0.58
1:I:91:ILE:HD12	1:I:91:ILE:O	2.03	0.58
2:H:210:LEU:HB2	2:H:223:THR:HA	1.85	0.58
2:L:210:LEU:HB2	2:L:223:THR:HA	1.86	0.57
1:A:303:GLN:O	1:A:307:SER:HB2	2.04	0.57
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.70	0.57
2:H:334:GLU:HB3	2:H:337:ILE:HD12	1.87	0.57
1:A:339:GLU:O	1:A:343:ILE:HG13	2.03	0.57
1:E:303:GLN:O	1:E:307:SER:HB2	2.05	0.57
1:A:261:GLN:O	1:A:265:GLU:HG2	2.04	0.57
1:A:334:LEU:HD22	1:A:367:HIS:O	2.04	0.57
1:C:148:LEU:HB2	1:C:179:LEU:HD21	1.87	0.57
1:K:334:LEU:HD22	1:K:367:HIS:O	2.04	0.57
2:F:130:SER:O	2:F:134:ILE:HG13	2.05	0.57
1:I:106:VAL:HG11	1:I:116:ALA:HB1	1.87	0.57
1:I:301:ASP:O	1:I:304:PRO:HD2	2.05	0.57
1:A:104:ARG:NH2	8:A:394:HOH:O	2.37	0.57
2:H:245:LEU:O	2:H:249:LYS:HG3	2.05	0.57
2:B:353:ARG:HG2	2:B:353:ARG:NH1	2.20	0.57
1:C:69:ARG:HB3	1:C:71:GLU:OE1	2.04	0.57
1:G:312:ILE:HG23	1:G:340:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:330:LYS:HE2	1:K:367:HIS:HB3	1.87	0.56
1:K:91:ILE:O	1:K:91:ILE:HD12	2.06	0.56
2:B:210:LEU:HB2	2:B:223:THR:HA	1.86	0.56
2:B:26:VAL:O	2:B:30:GLN:HG3	2.05	0.56
2:D:92:ARG:HH11	2:D:119:SER:HB3	1.68	0.56
2:H:26:VAL:O	2:H:30:GLN:HG3	2.06	0.56
1:G:91:ILE:HD11	2:H:38:GLU:H	1.70	0.56
1:A:265:GLU:O	1:A:269:LEU:HD13	2.06	0.56
1:E:148:LEU:HB2	1:E:179:LEU:HD21	1.87	0.56
1:E:265:GLU:O	1:E:269:LEU:HD13	2.05	0.56
1:I:100:TYR:O	1:I:104:ARG:HG3	2.05	0.56
5:L:1406:MGM:HC42	8:L:1499:HOH:O	2.05	0.56
2:D:210:LEU:HB2	2:D:223:THR:HA	1.87	0.56
2:D:133:ILE:HG22	2:D:350:THR:HG23	1.86	0.56
1:E:117:PHE:CE2	1:E:146:LYS:HE2	2.41	0.56
1:C:82:ASP:HB2	1:C:86:PRO:HB3	1.87	0.55
1:I:148:LEU:HB2	1:I:179:LEU:HD21	1.88	0.55
1:G:303:GLN:O	1:G:307:SER:HB2	2.07	0.55
1:E:156:ILE:CG1	1:E:172:ARG:HH12	2.00	0.55
1:E:334:LEU:HD22	1:E:367:HIS:O	2.06	0.55
1:G:148:LEU:HB2	1:G:179:LEU:HD21	1.89	0.55
1:G:91:ILE:HD12	1:G:91:ILE:O	2.07	0.55
2:H:21:LEU:HD21	2:H:304:ARG:HG2	1.89	0.55
2:H:18:LEU:HB3	2:H:304:ARG:HH21	1.71	0.55
1:K:301:ASP:O	1:K:304:PRO:HD2	2.06	0.55
1:C:180:LYS:HB2	1:E:214:ARG:HG2	1.88	0.55
1:I:156:ILE:CG1	1:I:172:ARG:HH12	2.04	0.54
1:C:88:VAL:HG12	2:D:32:CYS:O	2.07	0.54
1:C:189:ILE:HD11	1:C:205:HIS:HD2	1.73	0.54
2:J:63:SER:O	2:J:66:VAL:HG22	2.06	0.54
1:K:214:ARG:HH11	1:K:214:ARG:HG3	1.71	0.54
1:C:312:ILE:HG23	1:C:340:LEU:HD22	1.89	0.54
2:D:197:ILE:HD11	2:D:235:LYS:HD3	1.88	0.54
1:G:97:ARG:HH11	1:G:97:ARG:HB3	1.72	0.54
1:G:334:LEU:O	1:G:338:LEU:HG	2.08	0.54
1:E:105:ALA:O	1:E:109:ARG:HG3	2.07	0.54
1:E:91:ILE:O	1:E:91:ILE:HD12	2.08	0.54
1:I:88:VAL:HG12	2:J:32:CYS:O	2.07	0.54
1:I:91:ILE:HD11	2:J:38:GLU:H	1.72	0.54
1:K:265:GLU:O	1:K:269:LEU:HD13	2.08	0.54
1:E:91:ILE:HD11	2:F:38:GLU:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:LEU:HB3	2:H:304:ARG:NH2	2.23	0.54
1:I:339:GLU:O	1:I:343:ILE:HG13	2.08	0.54
1:C:106:VAL:HG11	1:C:116:ALA:HB1	1.90	0.53
1:C:328:ASP:O	1:C:329:ASN:HB2	2.08	0.53
1:E:106:VAL:HG11	1:E:116:ALA:HB1	1.90	0.53
2:H:130:SER:O	2:H:134:ILE:HG13	2.08	0.53
1:E:301:ASP:O	1:E:304:PRO:HD2	2.08	0.53
1:K:189:ILE:HD11	1:K:205:HIS:HD2	1.73	0.53
1:K:293:PRO:HD3	8:K:1464:HOH:O	2.08	0.53
5:L:1406:MGM:O1	5:L:1406:MGM:HC41	2.06	0.53
2:D:133:ILE:HD13	2:D:354:LEU:HD13	1.91	0.53
1:G:265:GLU:O	1:G:269:LEU:HD13	2.09	0.53
1:I:232:ARG:HD3	2:J:265:ASN:ND2	2.24	0.53
1:A:287:ARG:O	1:A:291:ARG:HD3	2.09	0.53
1:K:303:GLN:O	1:K:307:SER:HB2	2.09	0.53
1:A:91:ILE:O	1:A:91:ILE:HD12	2.08	0.53
2:B:339:LYS:O	2:B:348:THR:HG23	2.08	0.53
1:E:189:ILE:HD11	1:E:205:HIS:HD2	1.73	0.53
2:F:37:PRO:HD2	2:F:40:TYR:CE1	2.44	0.53
2:J:59:ASP:OD2	2:J:349:ARG:NH1	2.42	0.53
2:B:37:PRO:HD2	2:B:40:TYR:CD1	2.44	0.53
1:C:149:GLN:HG3	8:C:1375:HOH:O	2.08	0.53
1:C:311:LEU:HD23	1:C:311:LEU:C	2.29	0.53
2:J:69:LYS:O	2:J:73:ILE:HG13	2.09	0.53
2:B:22:ARG:HG2	2:B:22:ARG:HH11	1.73	0.52
2:F:26:VAL:O	2:F:30:GLN:HG3	2.09	0.52
1:G:88:VAL:HG12	2:H:32:CYS:O	2.08	0.52
2:H:77:TYR:CZ	2:H:141:ARG:HB2	2.44	0.52
2:L:74:GLU:CD	2:L:141:ARG:HH22	2.11	0.52
5:B:1401:MGM:HC42	8:B:1452:HOH:O	2.08	0.52
2:H:92:ARG:HD2	2:H:119:SER:HB3	1.90	0.52
1:I:265:GLU:O	1:I:269:LEU:HD13	2.08	0.52
1:E:88:VAL:HG12	2:F:32:CYS:O	2.09	0.52
2:F:357:LEU:O	2:F:357:LEU:HD23	2.10	0.52
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.92	0.52
1:K:149:GLN:HG3	8:K:1459:HOH:O	2.09	0.52
2:L:22:ARG:HH11	2:L:22:ARG:HG2	1.73	0.52
1:A:340:LEU:HD23	1:A:343:ILE:HD12	1.91	0.52
1:E:92:TYR:O	1:E:97:ARG:NH2	2.43	0.52
1:E:58:LEU:HD22	1:E:95:LYS:HD3	1.92	0.52
1:I:303:GLN:O	1:I:307:SER:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:311:LEU:HD23	1:K:311:LEU:O	2.10	0.52
1:G:106:VAL:HG11	1:G:116:ALA:HB1	1.92	0.52
2:J:245:LEU:O	2:J:249:LYS:HG3	2.10	0.52
1:K:83:GLY:HA3	2:L:105:PHE:CD1	2.45	0.52
2:B:29:PHE:O	2:B:33:LEU:HD22	2.10	0.51
1:C:265:GLU:O	1:C:269:LEU:HD13	2.10	0.51
1:E:255:VAL:HG13	1:E:258:ARG:NH2	2.24	0.51
2:F:186:ASN:HB2	2:F:358:HIS:NE2	2.25	0.51
1:G:69:ARG:HB3	1:G:71:GLU:OE1	2.09	0.51
2:H:348:THR:HA	2:H:351:SER:OG	2.10	0.51
2:J:338:CYS:SG	2:J:349:ARG:NH2	2.82	0.51
1:A:78:VAL:O	1:A:104:ARG:HD2	2.11	0.51
1:E:281:LYS:NZ	1:E:317:ASP:OD1	2.33	0.51
2:H:296:ASN:C	2:H:296:ASN:ND2	2.64	0.51
1:C:97:ARG:HG2	1:C:101:ASP:OD2	2.11	0.51
2:D:64:LEU:HD11	2:D:134:ILE:HG22	1.93	0.51
1:G:339:GLU:O	1:G:343:ILE:HG13	2.10	0.51
2:H:64:LEU:HD11	2:H:134:ILE:HG22	1.93	0.51
1:I:330:LYS:HE2	1:I:367:HIS:HB3	1.93	0.51
2:L:40:TYR:CE2	7:R:1300:GER:H101	2.46	0.51
1:K:106:VAL:HG11	1:K:116:ALA:HB1	1.92	0.51
1:C:286:ASP:HB2	8:C:1368:HOH:O	2.10	0.51
2:D:37:PRO:HD2	2:D:40:TYR:CE1	2.45	0.51
1:A:106:VAL:HG11	1:A:116:ALA:HB1	1.91	0.51
2:B:250:ARG:O	2:B:254:MET:HG2	2.10	0.51
1:C:91:ILE:HD12	1:C:91:ILE:O	2.11	0.51
1:E:318:ILE:HG22	1:E:322:MET:CE	2.42	0.51
2:H:70:ASP:O	2:H:74:GLU:HG2	2.11	0.50
2:H:22:ARG:HG2	2:H:22:ARG:HH11	1.75	0.50
2:J:39:ARG:NH2	2:J:40:TYR:OH	2.44	0.50
2:H:133:ILE:HD13	2:H:354:LEU:HD13	1.92	0.50
2:H:33:LEU:HD22	2:H:54:ALA:HB1	1.92	0.50
2:J:197:ILE:HD11	2:J:235:LYS:HD3	1.92	0.50
1:K:156:ILE:HD11	1:K:172:ARG:HH22	1.76	0.50
1:C:301:ASP:O	1:C:304:PRO:HD2	2.11	0.50
1:K:311:LEU:HD23	1:K:311:LEU:C	2.31	0.50
2:L:79:LEU:O	2:L:96:ARG:HG3	2.11	0.50
1:A:214:ARG:CG	1:A:214:ARG:O	2.59	0.50
1:C:296:LEU:HD22	1:C:322:MET:HE1	1.92	0.50
2:H:52:PHE:HE1	2:H:130:SER:HG	1.57	0.50
1:K:104:ARG:NH2	8:K:1336:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:ARG:HG2	5:B:1401:MGM:H112	1.94	0.50
2:D:173:ARG:HG2	5:D:1402:MGM:H112	1.93	0.50
1:I:189:ILE:HD11	1:I:205:HIS:HD2	1.77	0.50
2:L:22:ARG:NH1	2:L:22:ARG:HG2	2.27	0.50
2:F:186:ASN:HB2	2:F:358:HIS:CE1	2.47	0.50
2:H:232:LEU:HD13	2:H:343:ALA:HB1	1.92	0.50
2:L:173:ARG:HG2	5:L:1406:MGM:H112	1.94	0.50
1:A:117:PHE:CE2	1:A:146:LYS:HE2	2.46	0.49
1:K:214:ARG:NH1	1:K:214:ARG:HG3	2.27	0.49
5:J:1405:MGM:O1	5:J:1405:MGM:HC41	2.12	0.49
2:J:27:ARG:HH11	2:J:27:ARG:HG3	1.77	0.49
1:G:301:ASP:O	1:G:304:PRO:HD2	2.12	0.49
2:D:232:LEU:HD13	2:D:343:ALA:HB1	1.93	0.49
2:F:303:ASP:OD1	2:F:306:VAL:HG13	2.12	0.49
2:J:33:LEU:HD22	2:J:54:ALA:HB1	1.94	0.49
2:D:138:ASP:OD1	2:D:140:SER:HB3	2.12	0.49
1:I:311:LEU:C	1:I:311:LEU:HD23	2.33	0.49
2:J:38:GLU:O	2:J:38:GLU:HG2	2.13	0.49
1:K:345:ALA:O	1:K:353:LYS:HE3	2.13	0.49
1:A:218:ASN:HA	8:A:424:HOH:O	2.12	0.49
2:F:62:ASP:OD1	2:F:349:ARG:NH2	2.46	0.49
1:E:82:ASP:HB2	1:E:86:PRO:HB3	1.94	0.49
2:L:245:LEU:O	2:L:249:LYS:HG3	2.13	0.49
2:B:258:ASN:CG	2:B:259:GLY:H	2.16	0.49
1:E:121:ARG:HG3	1:E:121:ARG:NH1	2.26	0.49
2:F:173:ARG:HG2	5:F:1403:MGM:H112	1.94	0.49
2:F:138:ASP:HA	2:F:357:LEU:HD11	1.95	0.49
2:H:202:ARG:HG3	2:H:202:ARG:HH11	1.78	0.49
2:H:256:GLN:HB2	2:H:260:TYR:CE2	2.48	0.49
2:H:22:ARG:HG2	2:H:22:ARG:NH1	2.28	0.48
2:B:130:SER:O	2:B:134:ILE:HG13	2.12	0.48
2:D:130:SER:O	2:D:134:ILE:HG13	2.13	0.48
3:R:609:VAL:N	7:R:1300:GER:H11	2.29	0.48
2:F:64:LEU:HD11	2:F:134:ILE:HG22	1.96	0.48
2:F:250:ARG:O	2:F:254:MET:HG2	2.13	0.48
1:K:148:LEU:HB2	1:K:179:LEU:HD21	1.96	0.48
2:L:133:ILE:CD1	2:L:354:LEU:HD13	2.44	0.48
2:D:77:TYR:CZ	2:D:141:ARG:HB2	2.48	0.48
1:E:107:LEU:HD22	2:F:117:TYR:CD2	2.49	0.48
1:K:91:ILE:HD11	2:L:38:GLU:H	1.77	0.48
2:B:37:PRO:HD2	2:B:40:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:GLN:O	1:C:265:GLU:HG2	2.13	0.48
1:C:207:GLN:OE1	2:D:216:LEU:HD13	2.13	0.48
2:J:77:TYR:CZ	2:J:141:ARG:HB2	2.49	0.48
2:D:20:PHE:CZ	2:D:337:ILE:HD11	2.49	0.48
2:D:295:ARG:NH1	2:D:299:LEU:CD1	2.77	0.48
1:E:198:LYS:HD3	2:F:266:LYS:HD3	1.96	0.48
1:E:294:ASN:O	1:E:298:GLN:HG3	2.14	0.48
2:F:77:TYR:CZ	2:F:141:ARG:HB2	2.48	0.48
2:J:130:SER:O	2:J:134:ILE:HG13	2.14	0.48
1:G:58:LEU:HD23	1:G:63:TYR:CZ	2.48	0.47
2:D:250:ARG:O	2:D:254:MET:HG2	2.14	0.47
1:G:330:LYS:HE2	1:G:367:HIS:HB3	1.96	0.47
2:H:30:GLN:O	2:H:34:GLN:HG3	2.13	0.47
1:K:198:LYS:HD3	2:L:266:LYS:HD3	1.97	0.47
2:H:250:ARG:O	2:H:254:MET:HG2	2.14	0.47
2:J:138:ASP:OD1	2:J:140:SER:HB3	2.14	0.47
1:A:274:GLU:HG2	1:A:278:ASN:HD21	1.80	0.47
1:E:339:GLU:O	1:E:343:ILE:HG13	2.14	0.47
2:F:21:LEU:HD11	2:F:304:ARG:NH2	2.29	0.47
1:G:117:PHE:CE2	1:G:146:LYS:HE2	2.49	0.47
2:H:37:PRO:HD2	2:H:40:TYR:CD1	2.49	0.47
5:H:1404:MGM:HC41	5:H:1404:MGM:O1	2.15	0.47
2:F:59:ASP:OD2	2:F:349:ARG:NH1	2.47	0.47
1:G:207:GLN:OE1	2:H:216:LEU:HD13	2.13	0.47
2:D:295:ARG:NH2	2:D:299:LEU:HD11	2.29	0.47
2:F:138:ASP:OD1	2:F:140:SER:HB3	2.15	0.47
2:L:318:ASP:HB2	7:R:1300:GER:C7	2.33	0.47
1:E:103:PHE:CZ	1:E:133:VAL:HG22	2.50	0.47
2:F:144:LYS:HG3	8:F:1453:HOH:O	2.15	0.47
2:J:173:ARG:HG2	5:J:1405:MGM:H112	1.95	0.47
2:B:22:ARG:NH1	2:B:22:ARG:HG2	2.31	0.47
2:B:33:LEU:HD22	2:B:54:ALA:HB1	1.96	0.47
2:D:86:ASP:N	2:D:86:ASP:OD2	2.46	0.47
1:I:106:VAL:HG11	1:I:116:ALA:CB	2.45	0.47
2:J:202:ARG:HD2	8:J:1442:HOH:O	2.15	0.47
1:E:287:ARG:HG2	1:E:287:ARG:H	1.50	0.46
1:G:296:LEU:HD22	1:G:322:MET:HE1	1.97	0.46
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.97	0.46
1:A:88:VAL:HG12	2:B:32:CYS:O	2.15	0.46
1:C:78:VAL:O	1:C:104:ARG:HD2	2.16	0.46
2:J:92:ARG:NH1	2:J:118:ASP:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HD22	1:A:322:MET:HE3	1.98	0.46
2:D:121:HIS:HB3	2:D:124:MET:HG2	1.97	0.46
5:D:1402:MGM:HC42	8:D:1477:HOH:O	2.16	0.46
1:G:156:ILE:HD11	1:G:172:ARG:HH22	1.81	0.46
2:B:357:LEU:HD22	2:B:361:TRP:CE2	2.51	0.46
1:C:311:LEU:O	1:C:311:LEU:HD23	2.15	0.46
2:H:155:GLN:HB2	2:H:161:PHE:CE2	2.50	0.46
1:A:92:TYR:O	1:A:97:ARG:NH2	2.48	0.46
2:B:21:LEU:CD1	2:B:21:LEU:N	2.79	0.46
2:B:245:LEU:O	2:B:249:LYS:HG3	2.15	0.46
5:D:1402:MGM:O1	5:D:1402:MGM:HC41	2.16	0.46
1:G:149:GLN:HG3	8:G:1378:HOH:O	2.15	0.46
2:D:348:THR:HA	2:D:351:SER:OG	2.16	0.46
2:F:256:GLN:HB2	2:F:260:TYR:CE2	2.51	0.46
2:F:33:LEU:HD22	2:F:54:ALA:HB1	1.98	0.46
1:I:344:LEU:HD13	1:I:356:TRP:CE2	2.51	0.46
2:J:207:ASP:O	2:J:208:ASN:HB2	2.16	0.46
2:B:256:GLN:HB2	2:B:260:TYR:CE2	2.52	0.46
1:C:339:GLU:O	1:C:343:ILE:HG13	2.15	0.46
5:H:1404:MGM:HC42	8:H:1447:HOH:O	2.16	0.46
5:B:1401:MGM:O1	5:B:1401:MGM:HC41	2.16	0.45
1:C:334:LEU:O	1:C:338:LEU:HG	2.16	0.45
1:G:107:LEU:HD22	2:H:117:TYR:CD2	2.50	0.45
2:J:121:HIS:HB3	2:J:124:MET:HG2	1.98	0.45
2:B:64:LEU:HD11	2:B:134:ILE:HG22	1.98	0.45
2:F:21:LEU:HD23	2:F:304:ARG:HA	1.98	0.45
1:I:60:SER:OG	1:I:61:PRO:HD2	2.17	0.45
2:J:138:ASP:HA	2:J:357:LEU:HD11	1.97	0.45
2:J:19:ASP:OD2	2:J:19:ASP:N	2.48	0.45
1:G:296:LEU:HD22	1:G:322:MET:CE	2.47	0.45
1:I:312:ILE:HG23	1:I:340:LEU:HD22	1.99	0.45
2:J:27:ARG:NH1	2:J:27:ARG:HG3	2.32	0.45
2:B:207:ASP:O	2:B:208:ASN:HB2	2.16	0.45
2:D:353:ARG:NH1	2:D:357:LEU:HG	2.31	0.45
1:G:291:ARG:NH2	8:G:1323:HOH:O	2.45	0.45
2:J:229:SER:O	2:J:233:MET:HG3	2.17	0.45
1:K:223:VAL:HG11	1:K:240:ARG:HB2	1.98	0.45
1:A:334:LEU:O	1:A:338:LEU:HG	2.16	0.45
1:E:180:LYS:HD3	1:E:180:LYS:HA	1.82	0.45
1:G:189:ILE:HD11	1:G:205:HIS:CD2	2.51	0.45
2:D:92:ARG:NH1	2:D:118:ASP:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ASN:HB3	1:C:332:ASP:HB3	1.99	0.45
2:D:332:MET:O	2:D:333:GLU:HB2	2.17	0.45
1:E:121:ARG:HH11	1:E:121:ARG:HG3	1.81	0.45
1:E:191:ASP:O	1:E:194:ASN:HB2	2.17	0.45
2:H:207:ASP:O	2:H:208:ASN:HB2	2.16	0.45
2:J:22:ARG:O	2:J:26:VAL:HG23	2.17	0.45
2:L:256:GLN:HB2	2:L:260:TYR:CE2	2.52	0.45
2:B:236:LEU:HD22	2:B:245:LEU:HD21	1.99	0.45
2:F:121:HIS:HB3	2:F:124:MET:HG2	1.99	0.45
2:F:232:LEU:HD13	2:F:343:ALA:HB1	1.98	0.45
1:A:189:ILE:HD11	1:A:205:HIS:CD2	2.52	0.44
1:C:251:SER:HA	1:C:287:ARG:HH12	1.82	0.44
2:D:155:GLN:HB2	2:D:161:PHE:CE2	2.52	0.44
1:K:303:GLN:HB3	1:K:304:PRO:HD3	1.98	0.44
1:E:58:LEU:HD23	1:E:63:TYR:CE2	2.52	0.44
2:J:256:GLN:HB2	2:J:260:TYR:CE2	2.52	0.44
1:K:82:ASP:HB2	1:K:86:PRO:HB3	1.99	0.44
1:A:107:LEU:HD22	2:B:117:TYR:CD2	2.52	0.44
1:A:255:VAL:HG13	1:A:258:ARG:HH12	1.82	0.44
2:F:18:LEU:HB2	2:F:19:ASP:H	1.43	0.44
1:I:296:LEU:HD22	1:I:322:MET:HE3	1.99	0.44
1:I:82:ASP:HB2	1:I:86:PRO:HB3	1.99	0.44
2:J:250:ARG:O	2:J:254:MET:HG2	2.17	0.44
1:E:207:GLN:HG2	1:E:242:PHE:CE2	2.53	0.44
2:F:33:LEU:CD2	2:F:54:ALA:HB1	2.47	0.44
2:B:269:ASP:C	2:B:269:ASP:OD1	2.56	0.44
2:F:207:ASP:O	2:F:208:ASN:HB2	2.17	0.44
2:F:64:LEU:HD23	2:F:64:LEU:HA	1.83	0.44
2:H:40:TYR:N	2:H:40:TYR:CD1	2.85	0.44
2:H:33:LEU:CD2	2:H:54:ALA:HB1	2.48	0.44
1:I:105:ALA:O	1:I:109:ARG:HG3	2.17	0.44
2:J:351:SER:O	2:J:354:LEU:HB3	2.18	0.44
1:K:287:ARG:HG2	1:K:287:ARG:H	1.68	0.44
2:H:21:LEU:CD2	2:H:304:ARG:HG2	2.47	0.44
1:K:339:GLU:O	1:K:343:ILE:HG13	2.18	0.44
3:Q:507:LYS:NZ	8:Q:422:HOH:O	2.46	0.44
1:A:57:SER:HB3	8:K:1468:HOH:O	2.18	0.44
1:C:107:LEU:HD22	2:D:117:TYR:CD2	2.52	0.44
5:F:1403:MGM:O1	5:F:1403:MGM:HC41	2.17	0.44
1:G:311:LEU:HD23	1:G:311:LEU:C	2.38	0.44
2:D:92:ARG:NH1	2:D:119:SER:HB3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:351:ILE:CD1	2:F:256:GLN:HG2	2.47	0.44
1:G:219:GLU:OE1	1:G:219:GLU:HA	2.17	0.44
2:H:258:ASN:OD1	2:H:259:GLY:N	2.44	0.44
1:I:191:ASP:O	1:I:194:ASN:HB2	2.17	0.44
1:I:256:LEU:HD22	1:I:287:ARG:NH2	2.33	0.44
2:L:33:LEU:HD22	2:L:54:ALA:HB1	2.00	0.44
1:A:156:ILE:HD11	1:A:172:ARG:HH22	1.83	0.44
2:B:77:TYR:CZ	2:B:141:ARG:HB2	2.53	0.44
1:C:212:GLU:O	1:E:180:LYS:HE3	2.17	0.44
2:D:33:LEU:HD22	2:D:54:ALA:HB1	2.00	0.44
2:H:29:PHE:O	2:H:33:LEU:HD22	2.18	0.44
2:L:250:ARG:O	2:L:254:MET:HG2	2.18	0.44
2:D:19:ASP:OD2	2:D:19:ASP:N	2.42	0.43
1:G:107:LEU:HD12	2:H:101:LEU:HD22	1.99	0.43
2:H:269:ASP:OD1	2:H:269:ASP:C	2.56	0.43
1:I:287:ARG:H	1:I:287:ARG:HG2	1.59	0.43
2:B:232:LEU:HD13	2:B:343:ALA:HB1	2.01	0.43
1:C:87:VAL:CG1	2:D:33:LEU:HD12	2.48	0.43
1:G:252:ASP:OD2	1:G:254:ALA:HB3	2.18	0.43
2:H:18:LEU:N	2:H:18:LEU:CD2	2.80	0.43
1:I:117:PHE:CE2	1:I:146:LYS:HE2	2.53	0.43
1:K:78:VAL:O	1:K:104:ARG:HD2	2.18	0.43
1:A:151:GLU:HG3	1:A:175:LEU:HD11	2.01	0.43
1:G:105:ALA:O	1:G:109:ARG:HG3	2.17	0.43
1:K:261:GLN:NE2	1:K:265:GLU:OE2	2.51	0.43
2:D:303:ASP:OD1	2:D:306:VAL:HG13	2.18	0.43
2:J:77:TYR:CE1	2:J:141:ARG:HB2	2.54	0.43
1:K:361:ARG:NH1	8:K:1390:HOH:O	2.35	0.43
2:L:103:ILE:HG23	2:L:104:PRO:HD2	1.99	0.43
2:D:236:LEU:HD22	2:D:245:LEU:HD21	1.99	0.43
2:D:39:ARG:HG3	2:D:40:TYR:CD1	2.54	0.43
2:H:249:LYS:HB3	2:H:285:ILE:HD13	2.01	0.43
2:B:37:PRO:O	2:B:40:TYR:HD1	2.01	0.43
2:D:243:LYS:HE2	2:D:243:LYS:HB3	1.85	0.43
2:D:256:GLN:HB2	2:D:260:TYR:CE2	2.52	0.43
1:E:223:VAL:HG11	1:E:240:ARG:HB2	2.00	0.43
1:E:100:TYR:O	1:E:104:ARG:HG3	2.19	0.43
2:H:229:SER:O	2:H:233:MET:HG3	2.18	0.43
1:A:97:ARG:HD3	8:A:448:HOH:O	2.18	0.43
2:L:133:ILE:HG22	2:L:350:THR:HG23	2.00	0.43
2:B:33:LEU:CD2	2:B:54:ALA:HB1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:LEU:HD12	2:F:101:LEU:HD22	2.00	0.43
2:F:70:ASP:O	2:F:74:GLU:HG2	2.18	0.43
2:J:236:LEU:HD22	2:J:245:LEU:HD21	2.00	0.43
1:I:281:LYS:HD3	8:I:407:HOH:O	2.19	0.42
1:I:333:ILE:HD13	1:I:336:LYS:HD2	1.99	0.42
2:J:133:ILE:HG22	2:J:350:THR:HG23	2.01	0.42
2:J:269:ASP:OD1	2:J:269:ASP:C	2.58	0.42
2:L:130:SER:O	2:L:134:ILE:HG13	2.19	0.42
2:D:37:PRO:HB2	2:D:39:ARG:CG	2.47	0.42
2:H:186:ASN:HB2	2:H:358:HIS:CE1	2.54	0.42
1:K:290:SER:HB2	1:K:322:MET:HG2	2.01	0.42
2:F:115:HIS:HA	2:F:116:PRO:HD3	1.90	0.42
1:G:196:ASP:HB3	8:G:1379:HOH:O	2.19	0.42
2:H:357:LEU:HD22	2:H:361:TRP:CZ2	2.54	0.42
2:J:356:ASP:O	2:J:359:GLN:HB2	2.18	0.42
1:K:192:ILE:O	1:K:195:GLN:HG3	2.20	0.42
2:B:63:SER:O	2:B:66:VAL:HG22	2.20	0.42
1:C:223:VAL:HG11	1:C:240:ARG:HB2	2.00	0.42
2:F:236:LEU:HD22	2:F:245:LEU:HD21	2.02	0.42
1:I:151:GLU:HG3	1:I:175:LEU:HD11	2.02	0.42
2:B:312:TRP:O	2:B:315:SER:HB3	2.19	0.42
1:E:214:ARG:O	1:E:214:ARG:CG	2.65	0.42
1:E:71:GLU:N	1:E:71:GLU:OE1	2.45	0.42
2:F:90:LEU:HD23	2:F:90:LEU:HA	1.91	0.42
1:G:312:ILE:O	1:G:316:VAL:HG23	2.20	0.42
1:G:65:LEU:O	1:G:69:ARG:HG3	2.19	0.42
2:H:92:ARG:HG2	2:H:165:PRO:CG	2.47	0.42
2:L:236:LEU:HD22	2:L:245:LEU:HD21	2.01	0.42
2:B:155:GLN:HB2	2:B:161:PHE:CE2	2.55	0.42
2:F:40:TYR:CD1	2:F:40:TYR:N	2.87	0.42
1:G:325:ASN:O	1:G:326:GLN:C	2.58	0.42
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.55	0.42
2:H:121:HIS:HB3	2:H:124:MET:HG2	2.01	0.42
2:L:77:TYR:CZ	2:L:141:ARG:HB2	2.54	0.42
2:L:186:ASN:HB2	2:L:358:HIS:CE1	2.55	0.42
1:A:348:LYS:HA	1:A:348:LYS:HD3	1.69	0.42
2:D:258:ASN:OD1	2:D:259:GLY:N	2.41	0.42
1:E:318:ILE:HG22	1:E:322:MET:HE1	2.01	0.42
2:B:160:SER:HB3	2:B:199:TYR:CE1	2.55	0.42
2:B:357:LEU:HD22	2:B:361:TRP:NE1	2.35	0.42
1:E:156:ILE:HD11	1:E:172:ARG:HH22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:269:ASP:C	2:F:269:ASP:OD1	2.58	0.42
2:J:64:LEU:HB3	2:J:69:LYS:HE2	2.02	0.42
1:K:142:ARG:HD3	1:K:142:ARG:HA	1.75	0.42
1:A:312:ILE:O	1:A:316:VAL:HG23	2.20	0.41
1:C:219:GLU:HA	1:C:219:GLU:OE1	2.20	0.41
1:C:244:ILE:HD11	1:C:259:GLU:OE1	2.19	0.41
2:F:155:GLN:HB2	2:F:161:PHE:CE2	2.55	0.41
1:I:101:ASP:HA	1:I:104:ARG:HH11	1.85	0.41
1:A:267:ILE:HD13	1:A:277:TRP:CE2	2.55	0.41
1:A:311:LEU:HD23	1:A:311:LEU:C	2.40	0.41
1:C:106:VAL:HG11	1:C:116:ALA:CB	2.50	0.41
1:E:334:LEU:O	1:E:338:LEU:HG	2.20	0.41
2:J:90:LEU:HA	2:J:90:LEU:HD23	1.91	0.41
1:K:330:LYS:CE	1:K:367:HIS:HB3	2.50	0.41
1:K:351:ILE:CD1	2:L:256:GLN:HG2	2.50	0.41
2:L:38:GLU:HG2	2:L:38:GLU:O	2.20	0.41
1:A:226:LEU:HA	1:A:226:LEU:HD23	1.91	0.41
1:A:232:ARG:HD3	2:B:265:ASN:ND2	2.35	0.41
1:G:286:ASP:HB2	8:G:1372:HOH:O	2.20	0.41
2:L:105:PHE:CE2	2:L:107:PRO:HD3	2.55	0.41
2:L:257:GLN:HG3	8:L:1497:HOH:O	2.19	0.41
3:R:608:CYS:C	7:R:1300:GER:H11	2.41	0.41
1:C:107:LEU:HD12	2:D:101:LEU:HD22	2.01	0.41
2:D:103:ILE:HG23	2:D:104:PRO:HD2	2.02	0.41
2:F:29:PHE:O	2:F:33:LEU:HD22	2.21	0.41
1:A:106:VAL:HG11	1:A:116:ALA:CB	2.50	0.41
1:A:207:GLN:HG2	1:A:242:PHE:CE2	2.55	0.41
2:B:115:HIS:HA	2:B:116:PRO:HD3	1.89	0.41
1:C:92:TYR:O	1:C:97:ARG:NH2	2.53	0.41
2:H:62:ASP:OD1	2:H:349:ARG:NH2	2.53	0.41
2:J:115:HIS:HA	2:J:116:PRO:HD3	1.93	0.41
2:B:121:HIS:HB3	2:B:124:MET:HG2	2.03	0.41
2:D:245:LEU:O	2:D:249:LYS:HG3	2.20	0.41
2:D:266:LYS:HB3	2:D:266:LYS:HE3	1.95	0.41
1:E:106:VAL:HG11	1:E:116:ALA:CB	2.50	0.41
1:E:318:ILE:HG22	1:E:322:MET:HE3	2.03	0.41
1:G:226:LEU:HD23	1:G:226:LEU:HA	1.92	0.41
1:G:267:ILE:HD13	1:G:277:TRP:CE2	2.56	0.41
2:H:352:GLU:HA	2:H:352:GLU:OE2	2.21	0.41
2:J:358:HIS:O	2:J:361:TRP:HB2	2.21	0.41
1:A:103:PHE:CZ	1:A:133:VAL:HG22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:21:LEU:N	2:H:21:LEU:HD13	2.36	0.41
2:H:357:LEU:HD22	2:H:361:TRP:CE2	2.56	0.41
2:H:64:LEU:O	2:H:67:VAL:HG22	2.20	0.41
1:I:223:VAL:HG11	1:I:240:ARG:HB2	2.03	0.41
5:J:1405:MGM:HC42	8:J:1469:HOH:O	2.21	0.41
2:L:90:LEU:HD23	2:L:90:LEU:HA	1.88	0.41
2:B:19:ASP:N	2:B:19:ASP:OD2	2.46	0.41
1:K:67:ARG:HD2	8:K:1397:HOH:O	2.21	0.41
2:F:245:LEU:O	2:F:249:LYS:HG3	2.21	0.41
2:J:192:ASP:OD1	2:J:195:LYS:HE3	2.21	0.41
2:J:26:VAL:O	2:J:30:GLN:HG3	2.21	0.41
1:C:105:ALA:O	1:C:109:ARG:HG3	2.21	0.41
2:D:160:SER:HB3	2:D:199:TYR:CE1	2.56	0.41
2:F:103:ILE:HG23	2:F:104:PRO:HD2	2.02	0.41
1:I:107:LEU:HD12	2:J:101:LEU:HD22	2.03	0.41
1:I:78:VAL:O	1:I:104:ARG:HD2	2.20	0.41
2:J:24:ARG:HG3	2:J:307:GLY:CA	2.51	0.41
2:L:312:TRP:O	2:L:315:SER:HB3	2.20	0.41
2:L:83:PRO:HA	2:L:89:ASN:OD1	2.20	0.41
2:F:154:LEU:HD11	8:F:1427:HOH:O	2.20	0.41
1:G:198:LYS:HD3	2:H:266:LYS:HD3	2.03	0.41
1:G:344:LEU:HA	1:G:348:LYS:HB2	2.03	0.41
2:H:236:LEU:HD22	2:H:245:LEU:HD21	2.03	0.41
1:K:353:LYS:HB2	1:K:353:LYS:HE3	1.85	0.41
2:D:22:ARG:HH11	2:D:22:ARG:HG2	1.85	0.40
1:E:296:LEU:HD12	1:E:296:LEU:O	2.21	0.40
2:B:64:LEU:HD23	2:B:64:LEU:HA	1.84	0.40
2:B:79:LEU:O	2:B:96:ARG:HG3	2.22	0.40
1:G:287:ARG:O	1:G:291:ARG:HD3	2.20	0.40
2:H:64:LEU:HA	2:H:64:LEU:HD23	1.87	0.40
2:B:336:GLY:HA2	2:J:305:LEU:CD1	2.52	0.40
1:K:161:GLU:C	1:K:162:GLN:HG3	2.42	0.40
1:K:226:LEU:HA	1:K:226:LEU:HD23	1.90	0.40
1:K:88:VAL:CG2	2:L:47:ARG:HB3	2.52	0.40
2:D:30:GLN:O	2:D:34:GLN:HG3	2.22	0.40
1:G:101:ASP:CA	1:G:104:ARG:NH1	2.80	0.40
1:G:127:ASN:ND2	1:G:130:ASN:HB2	2.37	0.40
1:I:325:ASN:O	1:I:326:GLN:C	2.59	0.40
2:J:37:PRO:HD2	2:J:40:TYR:CE1	2.57	0.40
2:L:39:ARG:HG3	2:L:40:TYR:CE1	2.56	0.40
1:G:106:VAL:HG11	1:G:116:ALA:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:LEU:HD12	1:G:67:ARG:NH1	2.37	0.40
1:G:97:ARG:NH1	1:G:97:ARG:CB	2.84	0.40
2:J:152:ARG:HD3	2:J:189:SER:O	2.21	0.40
2:J:33:LEU:CD2	2:J:54:ALA:HB1	2.52	0.40
5:L:1406:MGM:HC61	8:L:1476:HOH:O	2.22	0.40
2:L:320:LEU:C	2:L:320:LEU:HD23	2.42	0.40
1:K:106:VAL:HG11	1:K:116:ALA:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/377 (83%)	289 (93%)	23 (7%)	0	100	100
1	C	312/377 (83%)	292 (94%)	20 (6%)	0	100	100
1	E	312/377 (83%)	290 (93%)	22 (7%)	0	100	100
1	G	312/377 (83%)	291 (93%)	21 (7%)	0	100	100
1	I	312/377 (83%)	293 (94%)	19 (6%)	0	100	100
1	K	312/377 (83%)	294 (94%)	18 (6%)	0	100	100
2	B	344/377 (91%)	329 (96%)	12 (4%)	3 (1%)	19	27
2	D	344/377 (91%)	329 (96%)	12 (4%)	3 (1%)	19	27
2	F	344/377 (91%)	329 (96%)	13 (4%)	2 (1%)	27	39
2	H	344/377 (91%)	330 (96%)	12 (4%)	2 (1%)	27	39
2	J	344/377 (91%)	327 (95%)	14 (4%)	3 (1%)	19	27
2	L	344/377 (91%)	331 (96%)	11 (3%)	2 (1%)	27	39
3	M	3/11 (27%)	3 (100%)	0	0	100	100
3	N	3/11 (27%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	3/11 (27%)	3 (100%)	0	0	100	100
3	P	3/11 (27%)	3 (100%)	0	0	100	100
3	Q	3/11 (27%)	3 (100%)	0	0	100	100
3	R	3/11 (27%)	3 (100%)	0	0	100	100
All	All	3954/4590 (86%)	3742 (95%)	197 (5%)	15 (0%)	36	51

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	258	ASN
2	H	258	ASN
2	B	362	LYS
2	D	258	ASN
2	F	258	ASN
2	J	34	GLN
2	J	258	ASN
2	L	258	ASN
2	B	111	PRO
2	D	111	PRO
2	F	111	PRO
2	H	111	PRO
2	J	111	PRO
2	L	111	PRO
2	D	333	GLU

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	275/338 (81%)	269 (98%)	6 (2%)	55	74
1	C	280/338 (83%)	272 (97%)	8 (3%)	45	66
1	E	283/338 (84%)	274 (97%)	9 (3%)	42	62
1	G	278/338 (82%)	273 (98%)	5 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	284/338 (84%)	278 (98%)	6 (2%)	56	75
1	K	290/338 (86%)	281 (97%)	9 (3%)	43	64
2	B	286/326 (88%)	271 (95%)	15 (5%)	25	41
2	D	286/326 (88%)	272 (95%)	14 (5%)	27	44
2	F	289/326 (89%)	274 (95%)	15 (5%)	25	41
2	H	284/326 (87%)	270 (95%)	14 (5%)	27	44
2	J	290/326 (89%)	274 (94%)	16 (6%)	24	37
2	L	291/326 (89%)	279 (96%)	12 (4%)	33	52
3	M	5/11 (46%)	5 (100%)	0	100	100
3	N	5/11 (46%)	5 (100%)	0	100	100
3	O	5/11 (46%)	5 (100%)	0	100	100
3	P	5/11 (46%)	5 (100%)	0	100	100
3	Q	5/11 (46%)	5 (100%)	0	100	100
3	R	5/11 (46%)	5 (100%)	0	100	100
All	All	3446/4050 (85%)	3317 (96%)	129 (4%)	37	56

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	PHE
1	A	71	GLU
1	A	107	LEU
1	A	211	GLN
1	A	214	ARG
1	A	287	ARG
2	B	21	LEU
2	B	33	LEU
2	B	39	ARG
2	B	151	LEU
2	B	216	LEU
2	B	232	LEU
2	B	236	LEU
2	B	255	ARG
2	B	261	HIS
2	B	305	LEU
2	B	329	LEU
2	B	331	LEU

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Mol	Chain	Res	Type
2	B	353	ARG
2	B	357	LEU
2	B	360	SER
1	C	59	ASP
1	C	71	GLU
1	C	107	LEU
1	C	182	PRO
1	C	194	ASN
1	C	287	ARG
1	C	324	GLU
1	C	364	GLN
2	D	21	LEU
2	D	33	LEU
2	D	151	LEU
2	D	216	LEU
2	D	232	LEU
2	D	236	LEU
2	D	255	ARG
2	D	258	ASN
2	D	261	HIS
2	D	305	LEU
2	D	329	LEU
2	D	331	LEU
2	D	353	ARG
2	D	357	LEU
1	E	55	PHE
1	E	71	GLU
1	E	80	GLN
1	E	81	ASN
1	E	94	GLU
1	E	107	LEU
1	E	214	ARG
1	E	287	ARG
1	E	324	GLU
2	F	18	LEU
2	F	21	LEU
2	F	24	ARG
2	F	33	LEU
2	F	151	LEU
2	F	216	LEU
2	F	232	LEU
2	F	236	LEU

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Mol	Chain	Res	Type
2	F	255	ARG
2	F	258	ASN
2	F	261	HIS
2	F	305	LEU
2	F	329	LEU
2	F	331	LEU
2	F	353	ARG
1	G	71	GLU
1	G	107	LEU
1	G	194	ASN
1	G	224	ASP
1	G	287	ARG
2	H	21	LEU
2	H	33	LEU
2	H	151	LEU
2	H	216	LEU
2	H	232	LEU
2	H	236	LEU
2	H	255	ARG
2	H	258	ASN
2	H	261	HIS
2	H	296	ASN
2	H	305	LEU
2	H	329	LEU
2	H	331	LEU
2	H	357	LEU
1	I	67	ARG
1	I	71	GLU
1	I	76	ASP
1	I	107	LEU
1	I	287	ARG
1	I	324	GLU
2	J	21	LEU
2	J	27	ARG
2	J	31	ARG
2	J	33	LEU
2	J	151	LEU
2	J	216	LEU
2	J	232	LEU
2	J	236	LEU
2	J	255	ARG
2	J	261	HIS

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Mol	Chain	Res	Type
2	J	305	LEU
2	J	329	LEU
2	J	331	LEU
2	J	341	HIS
2	J	353	ARG
2	J	357	LEU
1	K	55	PHE
1	K	67	ARG
1	K	71	GLU
1	K	107	LEU
1	K	142	ARG
1	K	195	GLN
1	K	287	ARG
1	K	324	GLU
1	K	357	ARG
2	L	21	LEU
2	L	33	LEU
2	L	151	LEU
2	L	216	LEU
2	L	232	LEU
2	L	236	LEU
2	L	243	LYS
2	L	255	ARG
2	L	261	HIS
2	L	329	LEU
2	L	331	LEU
2	L	353	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	201	HIS
1	A	278	ASN
1	A	285	GLN
2	B	208	ASN
2	B	265	ASN
1	C	108	GLN
1	C	184	GLN
1	C	297	ASN
1	C	298	GLN
1	C	364	GLN

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Mol	Chain	Res	Type
2	D	246	ASN
2	D	265	ASN
1	E	145	GLN
1	E	149	GLN
1	E	162	GLN
1	E	184	GLN
1	E	201	HIS
1	E	298	GLN
2	F	246	ASN
2	F	265	ASN
1	G	80	GLN
1	G	81	ASN
1	G	89	GLN
1	G	149	GLN
1	G	162	GLN
1	G	184	GLN
1	G	201	HIS
1	G	297	ASN
1	G	325	ASN
2	H	246	ASN
2	H	296	ASN
1	I	89	GLN
1	I	184	GLN
1	I	201	HIS
1	I	285	GLN
2	J	30	GLN
2	J	208	ASN
2	J	246	ASN
2	J	265	ASN
1	K	184	GLN
1	K	298	GLN
2	L	246	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 13 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	MGM	B	1401	-	27,28,28	0.80	0	30,37,37	1.85	4 (13%)
5	MGM	D	1402	-	27,28,28	0.84	0	30,37,37	1.84	4 (13%)
5	MGM	F	1403	-	27,28,28	0.81	0	30,37,37	1.86	4 (13%)
5	MGM	H	1404	-	27,28,28	0.78	0	30,37,37	1.82	4 (13%)
5	MGM	J	1405	-	27,28,28	0.79	0	30,37,37	1.80	4 (13%)
5	MGM	L	1406	-	27,28,28	0.79	0	30,37,37	1.74	4 (13%)
7	GER	R	1300	3	19,19,19	0.94	0	22,22,22	0.67	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	MGM	B	1401	-	-	0/31/31/31	0/0/0/0
5	MGM	D	1402	-	-	0/31/31/31	0/0/0/0
5	MGM	F	1403	-	-	0/31/31/31	0/0/0/0
5	MGM	H	1404	-	-	0/31/31/31	0/0/0/0
5	MGM	J	1405	-	-	0/31/31/31	0/0/0/0
5	MGM	L	1406	-	-	0/31/31/31	0/0/0/0
7	GER	R	1300	3	-	0/20/20/20	0/0/0/0

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1406	MGM	O1-C1-C2	2.14	112.26	107.56
5	J	1405	MGM	O1-C1-C2	2.43	112.90	107.56
5	D	1402	MGM	C2-N3-C5	2.43	121.92	111.94
5	F	1403	MGM	C2-N3-C5	2.44	121.94	111.94
5	B	1401	MGM	C2-N3-C5	2.44	121.97	111.94
5	J	1405	MGM	C2-N3-C5	2.45	121.99	111.94
5	H	1404	MGM	C2-N3-C5	2.47	122.09	111.94
5	F	1403	MGM	O1-C1-C2	2.63	113.34	107.56
5	H	1404	MGM	O1-C1-C2	2.66	113.41	107.56
5	L	1406	MGM	C2-N3-C5	2.69	122.99	111.94
5	D	1402	MGM	O1-C1-C2	2.75	113.60	107.56
5	B	1401	MGM	O1-C1-C2	2.78	113.68	107.56
5	L	1406	MGM	C4-N3-C2	5.10	124.84	110.62
5	H	1404	MGM	C4-N3-C2	5.25	125.25	110.62
5	J	1405	MGM	C4-N3-C2	5.26	125.29	110.62
5	B	1401	MGM	C4-N3-C2	5.26	125.30	110.62
5	D	1402	MGM	C4-N3-C2	5.33	125.48	110.62
5	F	1403	MGM	C4-N3-C2	5.35	125.53	110.62
5	L	1406	MGM	C1-C2-N3	5.95	127.82	113.31
5	J	1405	MGM	C1-C2-N3	6.41	128.94	113.31
5	H	1404	MGM	C1-C2-N3	6.55	129.27	113.31
5	D	1402	MGM	C1-C2-N3	6.58	129.35	113.31
5	B	1401	MGM	C1-C2-N3	6.66	129.54	113.31
5	F	1403	MGM	C1-C2-N3	6.72	129.69	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1401	MGM	3	0
5	D	1402	MGM	3	0
5	F	1403	MGM	2	0
5	H	1404	MGM	2	0
5	J	1405	MGM	3	0
5	L	1406	MGM	4	0
7	R	1300	GER	7	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	314/377 (83%)	0.01	13 (4%) 37 36	42, 63, 91, 106	0
1	C	314/377 (83%)	-0.09	7 (2%) 62 59	41, 59, 87, 138	0
1	E	314/377 (83%)	0.01	11 (3%) 44 42	40, 63, 86, 105	0
1	G	314/377 (83%)	0.04	10 (3%) 47 46	42, 62, 89, 140	0
1	I	314/377 (83%)	-0.02	13 (4%) 37 36	35, 60, 88, 100	0
1	K	314/377 (83%)	-0.26	5 (1%) 72 69	30, 48, 71, 87	0
2	B	346/377 (91%)	0.34	36 (10%) 6 6	41, 57, 81, 103	0
2	D	346/377 (91%)	0.26	31 (8%) 9 8	37, 51, 84, 101	0
2	F	346/377 (91%)	0.32	31 (8%) 9 8	36, 51, 83, 105	0
2	H	346/377 (91%)	0.52	40 (11%) 4 4	43, 64, 90, 112	0
2	J	346/377 (91%)	0.31	30 (8%) 10 9	36, 55, 83, 103	0
2	L	346/377 (91%)	0.17	20 (5%) 23 21	32, 46, 72, 95	0
3	M	5/11 (45%)	1.57	2 (40%) 0 0	52, 53, 60, 71	0
3	N	5/11 (45%)	1.82	2 (40%) 0 0	51, 55, 60, 73	0
3	O	5/11 (45%)	1.94	2 (40%) 0 0	53, 56, 60, 74	0
3	P	5/11 (45%)	2.35	3 (60%) 0 0	62, 62, 73, 83	0
3	Q	5/11 (45%)	1.71	2 (40%) 0 0	51, 51, 67, 78	0
3	R	5/11 (45%)	2.06	2 (40%) 0 0	50, 52, 78, 79	0
All	All	3990/4590 (86%)	0.16	260 (6%) 19 17	30, 57, 86, 140	0

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	55	PHE	8.3
2	J	108	SER	6.5
2	B	363	THR	6.0

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Mol	Chain	Res	Type	RSRZ
1	G	306	HIS	5.8
1	C	55	PHE	5.7
2	H	305	LEU	5.7
2	F	112	GLY	5.5
2	F	363	THR	5.3
2	H	363	THR	5.2
2	L	363	THR	5.0
1	I	304	PRO	4.9
1	C	306	HIS	4.9
2	H	127	THR	4.7
3	P	410	ILE	4.6
2	J	363	THR	4.5
2	H	108	SER	4.4
2	H	304	ARG	4.3
1	I	305	SER	4.3
1	I	368	SER	4.3
2	B	113	THR	4.3
2	J	112	GLY	4.3
1	E	304	PRO	4.3
2	H	112	GLY	4.2
2	D	363	THR	4.2
1	C	304	PRO	4.2
2	F	108	SER	4.2
2	B	110	ASN	4.2
2	H	123	ALA	4.2
3	O	311	LEU	4.1
2	F	127	THR	4.0
2	B	127	THR	4.0
2	F	126	TYR	4.0
2	F	113	THR	3.9
1	I	306	HIS	3.9
1	A	304	PRO	3.9
2	B	53	PHE	3.8
2	H	361	TRP	3.9
2	B	123	ALA	3.8
2	L	126	TYR	3.8
1	A	368	SER	3.8
3	P	411	LEU	3.7
2	J	123	ALA	3.7
2	H	113	THR	3.7
3	O	310	ILE	3.7
3	N	211	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	49	THR	3.7
2	H	48	LEU	3.6
3	Q	511	LEU	3.6
2	J	113	THR	3.6
2	L	113	THR	3.6
2	F	110	ASN	3.6
2	F	314	ASP	3.6
3	N	210	ILE	3.6
2	B	305	LEU	3.6
2	H	306	VAL	3.6
2	L	112	GLY	3.6
2	F	123	ALA	3.5
1	E	306	HIS	3.5
2	L	49	THR	3.5
1	G	304	PRO	3.5
3	M	111	LEU	3.5
3	R	611	LEU	3.5
2	D	113	THR	3.5
1	G	305	SER	3.5
3	M	110	ILE	3.4
2	D	49	THR	3.4
2	D	305	LEU	3.4
2	F	49	THR	3.4
2	J	127	THR	3.4
1	K	306	HIS	3.4
2	J	126	TYR	3.3
2	H	360	SER	3.3
1	G	56	LEU	3.3
2	D	48	LEU	3.3
2	D	123	ALA	3.3
2	H	110	ASN	3.3
2	B	52	PHE	3.3
2	D	126	TYR	3.3
2	B	112	GLY	3.2
2	L	123	ALA	3.2
2	J	124	MET	3.2
2	F	40	TYR	3.2
2	H	126	TYR	3.2
2	J	86	ASP	3.2
2	D	52	PHE	3.2
2	B	126	TYR	3.2
2	L	48	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	40	TYR	3.2
2	D	127	THR	3.2
2	F	52	PHE	3.1
2	B	124	MET	3.1
2	H	114	ALA	3.1
2	B	362	LYS	3.1
2	H	50	ILE	3.1
2	J	85	GLU	3.1
1	A	330	LYS	3.1
2	H	45	THR	3.1
2	H	49	THR	3.1
2	J	49	THR	3.1
2	B	48	LEU	3.1
2	L	127	THR	3.1
2	B	86	ASP	3.0
2	L	124	MET	3.0
1	A	367	HIS	3.0
2	D	88	SER	3.0
2	F	130	SER	3.0
2	J	360	SER	3.0
2	H	314	ASP	3.0
2	H	52	PHE	3.0
2	F	88	SER	3.0
2	J	110	ASN	3.0
1	E	55	PHE	3.0
2	J	46	SER	2.9
1	C	329	ASN	2.9
1	E	91	ILE	2.9
2	B	46	SER	2.9
2	B	114	ALA	2.9
2	F	362	LYS	2.9
2	H	53	PHE	2.8
1	G	368	SER	2.8
2	B	40	TYR	2.8
2	D	114	ALA	2.8
2	F	84	THR	2.8
2	F	305	LEU	2.8
2	F	86	ASP	2.8
1	I	328	ASP	2.8
2	D	314	ASP	2.8
2	D	124	MET	2.8
2	D	45	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	48	LEU	2.8
3	Q	510	ILE	2.8
2	J	84	THR	2.7
2	J	48	LEU	2.7
2	H	86	ASP	2.7
3	R	610	ILE	2.7
2	J	177	CYS	2.7
1	I	302	LEU	2.7
2	D	53	PHE	2.7
1	A	331	GLU	2.7
2	L	122	ILE	2.7
2	D	110	ASN	2.7
2	F	124	MET	2.7
2	F	46	SER	2.6
2	J	125	THR	2.6
1	A	329	ASN	2.6
2	H	307	GLY	2.6
2	B	111	PRO	2.6
1	E	305	SER	2.6
1	K	305	SER	2.6
2	H	97	GLY	2.6
2	L	52	PHE	2.6
1	E	368	SER	2.6
1	A	306	HIS	2.6
2	J	111	PRO	2.6
2	L	50	ILE	2.6
1	E	331	GLU	2.6
1	G	78	VAL	2.6
1	E	328	ASP	2.6
2	B	306	VAL	2.5
1	A	332	ASP	2.5
2	B	45	THR	2.5
1	I	367	HIS	2.5
2	F	111	PRO	2.5
2	D	97	GLY	2.5
2	F	327	CYS	2.5
2	H	124	MET	2.5
2	J	114	ALA	2.5
1	A	334	LEU	2.5
2	B	88	SER	2.5
2	B	361	TRP	2.5
2	F	53	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	304	PRO	2.5
2	J	359	GLN	2.5
2	D	46	SER	2.5
2	H	362	LYS	2.4
2	H	46	SER	2.4
2	H	88	SER	2.4
2	D	112	GLY	2.4
1	G	333	ILE	2.4
2	L	125	THR	2.4
1	C	305	SER	2.4
1	G	75	ILE	2.4
1	A	327	CYS	2.4
2	D	131	CYS	2.4
2	J	45	THR	2.4
2	H	109	LYS	2.3
1	I	84	PRO	2.3
2	D	37	PRO	2.3
2	D	50	ILE	2.3
2	H	37	PRO	2.3
1	K	328	ASP	2.3
1	A	326	GLN	2.3
2	L	53	PHE	2.3
2	J	128	GLY	2.3
2	F	316	HIS	2.3
2	H	316	HIS	2.3
2	L	85	GLU	2.3
2	L	121	HIS	2.3
2	F	177	CYS	2.3
1	C	75	ILE	2.3
2	J	95	PHE	2.3
1	E	330	LYS	2.3
1	I	330	LYS	2.3
2	J	121	HIS	2.3
2	B	177	CYS	2.3
2	J	52	PHE	2.3
1	C	332	ASP	2.3
2	H	18	LEU	2.3
1	I	327	CYS	2.3
2	H	107	PRO	2.3
2	H	85	GLU	2.3
2	L	109	LYS	2.3
2	F	114	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	90	LEU	2.3
2	B	316	HIS	2.2
2	H	177	CYS	2.2
2	J	107	PRO	2.2
2	B	327	CYS	2.2
2	D	275	TRP	2.2
2	F	323	TYR	2.2
2	J	122	ILE	2.2
2	D	316	HIS	2.2
2	H	221	GLY	2.2
2	B	130	SER	2.2
2	D	360	SER	2.2
1	I	73	ALA	2.2
2	F	131	CYS	2.2
2	F	109	LYS	2.1
2	D	361	TRP	2.1
2	B	84	THR	2.1
2	F	45	THR	2.1
1	I	75	ILE	2.1
2	B	107	PRO	2.1
2	B	314	ASP	2.1
2	B	323	TYR	2.1
2	H	252	CYS	2.1
1	E	326	GLN	2.1
2	H	312	TRP	2.1
2	J	53	PHE	2.1
2	L	86	ASP	2.1
2	D	306	VAL	2.1
3	P	409	VAL	2.1
1	A	333	ILE	2.1
2	D	225	CYS	2.1
2	J	130	SER	2.1
1	G	326	GLN	2.1
2	B	37	PRO	2.1
1	E	75	ILE	2.1
1	I	323	LEU	2.0
2	L	252	CYS	2.0
1	K	368	SER	2.0
2	B	56	SER	2.0
1	A	323	LEU	2.0
2	B	97	GLY	2.0
2	D	224	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	224	PHE	2.0
2	B	237	GLU	2.0
2	B	275	TRP	2.0
2	L	177	CYS	2.0
2	D	108	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GER	R	1300	20/20	0.78	0.30	66,71,80,81	0
5	MGM	F	1403	29/29	0.88	0.34	46,58,81,83	0
5	MGM	H	1404	29/29	0.88	0.39	59,69,91,94	0
5	MGM	B	1401	29/29	0.88	0.37	46,66,88,88	0
5	MGM	D	1402	29/29	0.89	0.33	43,59,80,80	0
5	MGM	L	1406	29/29	0.90	0.34	39,54,79,80	0
5	MGM	J	1405	29/29	0.91	0.35	41,58,81,82	0
6	CL	J	1315	1/1	0.93	0.10	60,60,60,60	0
6	CL	G	1311	1/1	0.96	0.22	59,59,59,59	0
6	CL	K	1317	1/1	0.96	0.17	61,61,61,61	0
6	CL	C	1301	1/1	0.96	0.25	65,65,65,65	0
6	CL	H	1312	1/1	0.97	0.10	59,59,59,59	0
6	CL	D	1306	1/1	0.98	0.11	45,45,45,45	0
4	ZN	H	378	1/1	0.98	0.12	60,60,60,60	0
4	ZN	D	378	1/1	0.99	0.11	39,39,39,39	0
6	CL	F	1309	1/1	0.99	0.12	51,51,51,51	0
4	ZN	F	378	1/1	1.00	0.12	45,45,45,45	0
4	ZN	J	378	1/1	1.00	0.13	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ZN	L	378	1/1	1.00	0.14	36,36,36,36	0
4	ZN	B	378	1/1	1.00	0.12	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.