



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:43 PM GMT

PDB ID : 1N4P
Title : Protein Geranylgeranyltransferasetype-I Complexed with Geranylgeranyl Diphosphate
Authors : Taylor, J.S.; Reid, T.S.; Casey, P.J.; Beese, L.S.
Deposited on : 2002-11-01
Resolution : 2.65 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

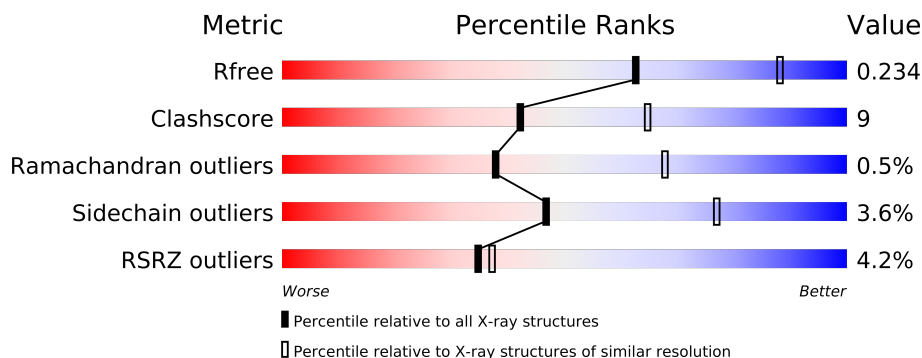
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.65 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}	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	377	
1	C	377	
1	E	377	
1	G	377	
1	I	377	
1	K	377	
2	B	377	
2	D	377	
2	F	377	
2	H	377	
2	J	377	
2	L	377	
3	M	11	
3	N	11	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	CL	C	1705	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33443 atoms, of which 0 are hydrogen and 0 are deuterium.

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 alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2629	1679	463	482	5			
1	C	314	Total	C	N	O	S	0	0	0
			2643	1689	461	488	5			
1	E	314	Total	C	N	O	S	0	0	0
			2642	1686	461	490	5			
1	G	314	Total	C	N	O	S	0	0	0
			2633	1683	459	486	5			
1	I	314	Total	C	N	O	S	0	0	0
			2656	1694	465	492	5			
1	K	314	Total	C	N	O	S	0	0	0
			2671	1703	467	496	5			

- Molecule 2 is a protein called geranyltransferase type-I beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2697	1707	467	499	24			
2	D	346	Total	C	N	O	S	0	0	0
			2713	1715	472	502	24			
2	F	346	Total	C	N	O	S	0	0	0
			2718	1717	474	503	24			
2	H	346	Total	C	N	O	S	0	0	0
			2694	1706	464	500	24			
2	J	346	Total	C	N	O	S	0	0	0
			2711	1713	471	503	24			
2	L	346	Total	C	N	O	S	0	0	0
			2723	1720	473	506	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	4	Total	C	N	O	S	0	0	0
			30	20	4	5	1			
3	N	4	Total	C	N	O	S	0	0	0
			30	20	4	5	1			

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

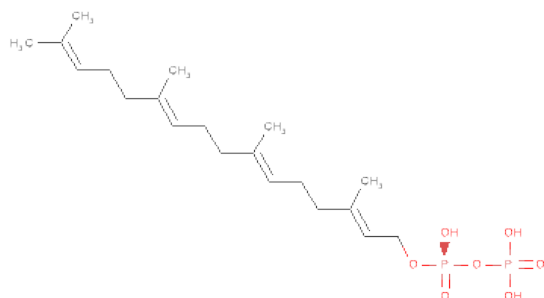
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Cl	0	0
			1	1		
5	J	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	K	1	Total	Cl	0	0
			1	1		
5	H	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		
5	L	1	Total	Cl	0	0
			1	1		
5	F	1	Total	Cl	0	0
			1	1		

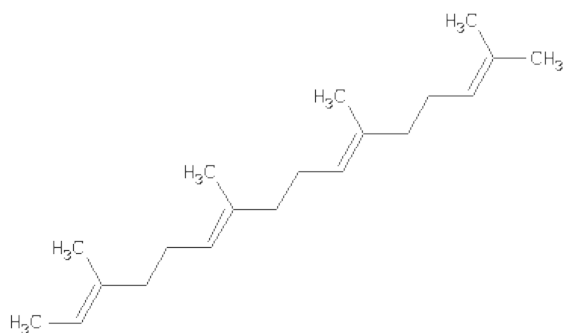
- Molecule 6 is GERANYLGERANYL DIPHOSPHATE (three-letter code: GRG) (formula:

C₂₀H₃₆O₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	P	0	0
			29	20	7	2		
6	D	1	Total	C	O	P	0	0
			29	20	7	2		
6	F	1	Total	C	O	P	0	0
			29	20	7	2		
6	H	1	Total	C	O	P	0	0
			29	20	7	2		
6	J	1	Total	C	O	P	0	0
			29	20	7	2		
6	L	1	Total	C	O	P	0	0
			29	20	7	2		

- Molecule 7 is GERAN-8-YL GERAN (three-letter code: GER) (formula: C₂₀H₃₄).



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

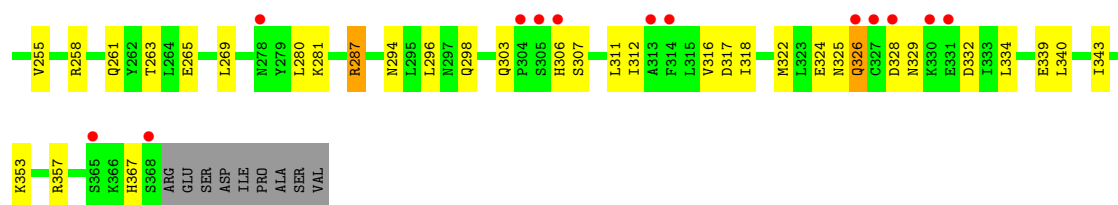
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	71	Total O 71 71	0	0
8	B	63	Total O 63 63	0	0
8	C	80	Total O 80 80	0	0
8	D	94	Total O 94 94	0	0
8	E	64	Total O 64 64	0	0
8	F	92	Total O 92 92	0	0
8	G	58	Total O 58 58	0	0
8	H	48	Total O 48 48	0	0
8	I	87	Total O 87 87	0	0
8	J	73	Total O 73 73	0	0

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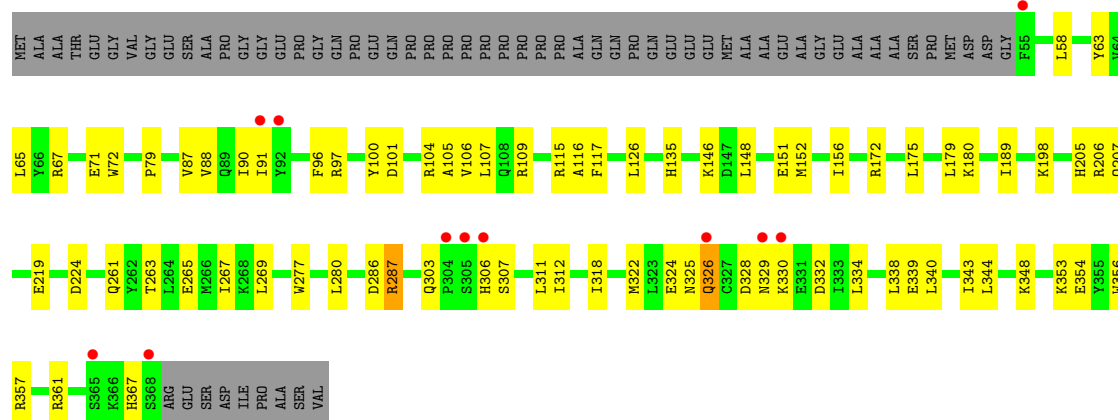
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	K	159	Total 159	O 159	0	0
8	L	134	Total 134	O 134	0	0
8	N	1	Total 1	O 1	0	0



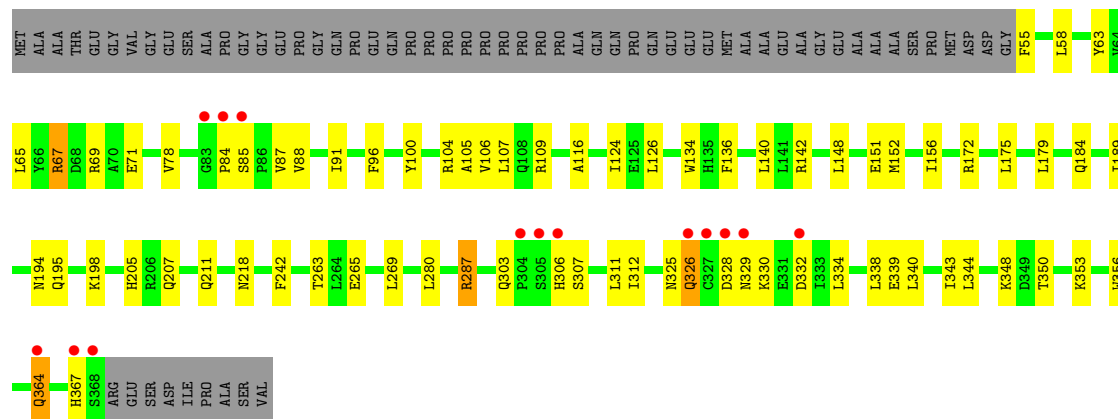
• Molecule 1: protein farnesyltransferase alpha subunit

Chain G:



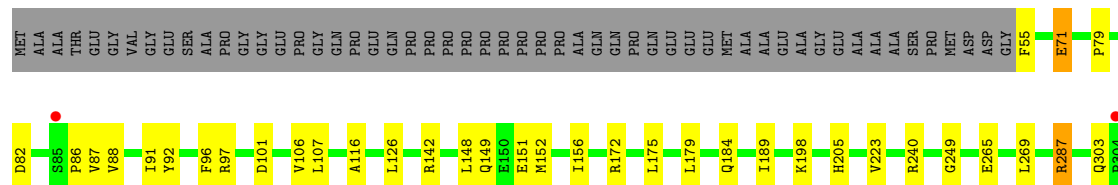
• Molecule 1: protein farnesyltransferase alpha subunit

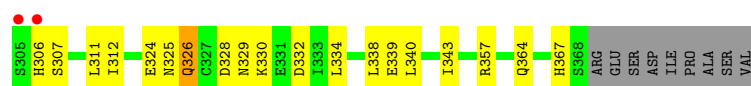
Chain I:



• Molecule 1: protein farnesyltransferase alpha subunit

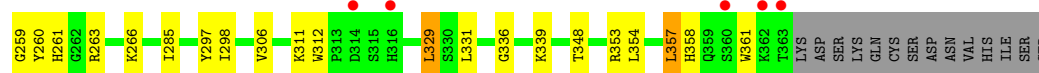
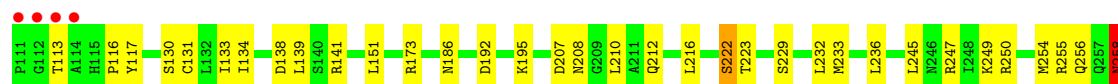
Chain K:





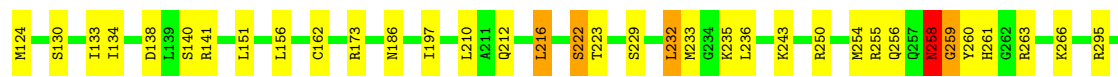
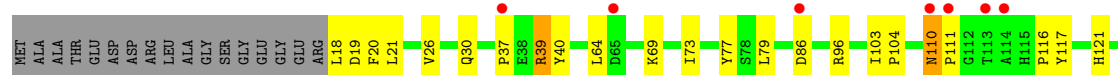
- Molecule 2: geranyltransferase type-I beta subunit

Chain B:



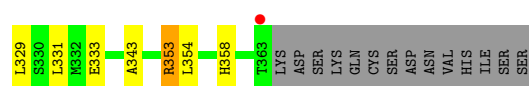
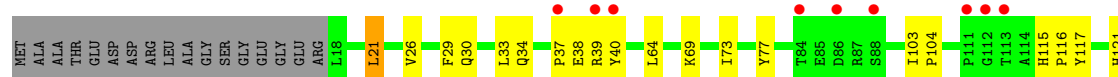
- Molecule 2: geranyltransferase type-I beta subunit

Chain D:



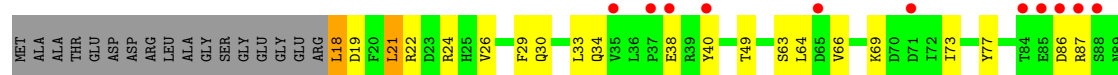
- Molecule 2: geranyltransferase type-I beta subunit

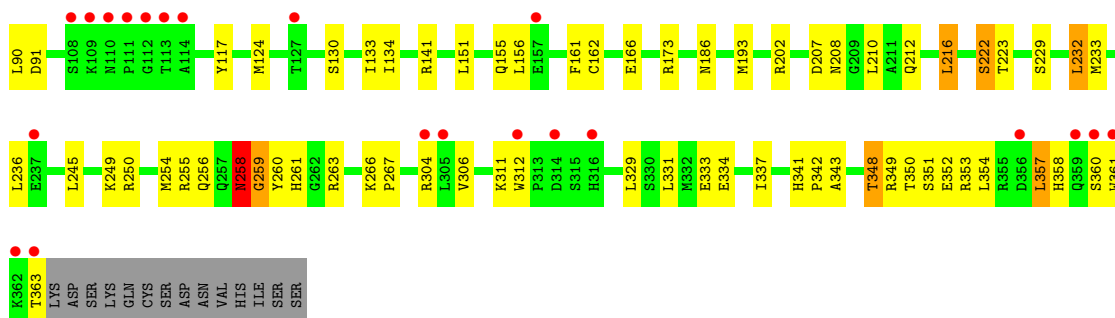
Chain F:



- Molecule 2: geranyltransferase type-I beta subunit

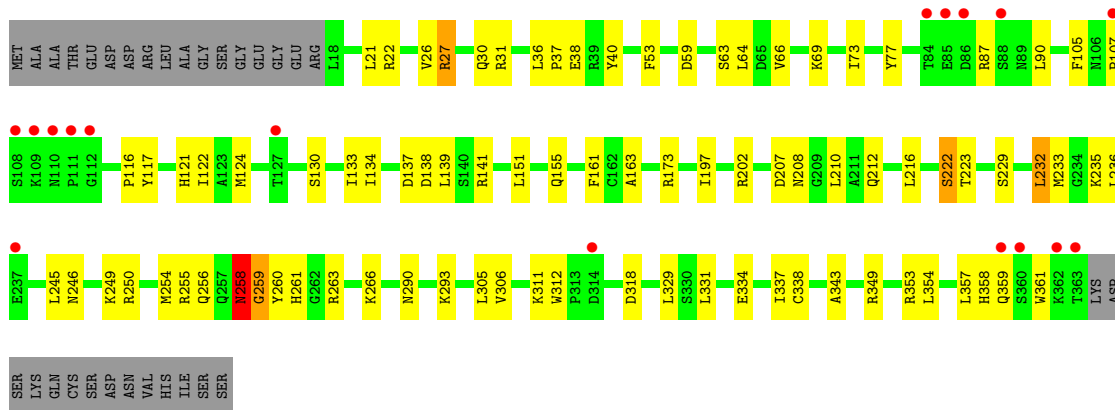
Chain H:





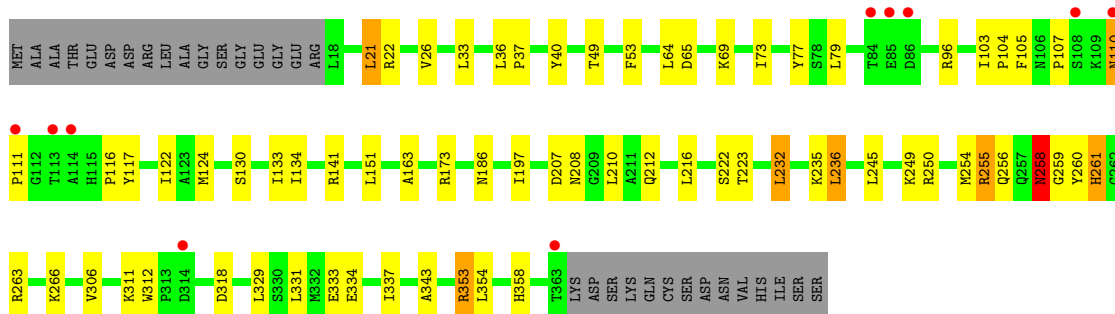
- Molecule 2: geranyltransferase type-I beta subunit

Chain J: 



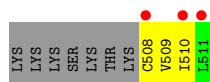
- Molecule 2: geranyltransferase type-I beta subunit

Chain L:



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

Chain M:



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

Chain N: 

LYS		
LYS		
LYS		
SER		
LYS		
THR		
LYS		
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	272.34Å 271.57Å 185.43Å 90.00° 131.56° 90.00°	Depositor
Resolution (Å)	29.92 – 2.65 29.92 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.92-2.65) 98.7 (29.92-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.64Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.204 , 0.228 0.212 , 0.234	Depositor DCC
R_{free} test set	14292 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.1	EDS
Estimated twinning fraction	0.080 for -h-2*1,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 286743 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33443	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GRG, ZN, CL, GER

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	0.34	0/2695	0.52	0/3668
1	C	0.36	0/2709	0.53	0/3684
1	E	0.35	0/2708	0.53	0/3684
1	G	0.35	0/2699	0.53	0/3672
1	I	0.36	0/2722	0.53	0/3700
1	K	0.40	0/2737	0.55	0/3717
2	B	0.36	0/2759	0.60	2/3733 (0.1%)
2	D	0.37	0/2775	0.59	2/3752 (0.1%)
2	F	0.38	0/2780	0.60	2/3758 (0.1%)
2	H	0.35	0/2756	0.58	2/3729 (0.1%)
2	J	0.36	0/2773	0.59	2/3750 (0.1%)
2	L	0.40	0/2785	0.61	2/3764 (0.1%)
3	M	0.67	0/29	0.82	0/37
3	N	0.66	0/29	0.81	0/37
All	All	0.37	0/32956	0.56	12/44685 (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	F	0	1
All	All	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	259	GLY	N-CA-C	-6.01	98.07	113.10
2	F	259	GLY	N-CA-C	-5.96	98.20	113.10
2	D	259	GLY	N-CA-C	-5.84	98.49	113.10
2	J	259	GLY	N-CA-C	-5.83	98.51	113.10
2	L	259	GLY	N-CA-C	-5.77	98.68	113.10
2	B	259	GLY	N-CA-C	-5.76	98.70	113.10
2	L	258	ASN	N-CA-C	-5.46	96.25	111.00
2	J	258	ASN	N-CA-C	-5.42	96.36	111.00
2	B	258	ASN	N-CA-C	-5.32	96.63	111.00
2	D	258	ASN	N-CA-C	-5.31	96.67	111.00
2	H	258	ASN	N-CA-C	-5.29	96.72	111.00
2	F	258	ASN	N-CA-C	-5.25	96.84	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2629	0	2520	48	0
1	C	2643	0	2540	44	0
1	E	2642	0	2534	57	0
1	G	2633	0	2524	55	0
1	I	2656	0	2560	44	0
1	K	2671	0	2588	39	0
2	B	2697	0	2600	50	0
2	D	2713	0	2628	52	0
2	F	2718	0	2635	37	0
2	H	2694	0	2590	67	0
2	J	2711	0	2616	51	0
2	L	2723	0	2643	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	30	0	34	3	0
3	N	30	0	34	3	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	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	1	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	1	0
5	L	1	0	0	0	0
6	B	29	0	33	1	0
6	D	29	0	33	1	0
6	F	29	0	33	2	0
6	H	29	0	33	1	0
6	J	29	0	33	1	0
6	L	29	0	33	1	0
7	M	20	0	33	5	0
7	N	20	0	33	5	0
8	A	71	0	0	1	0
8	B	63	0	0	0	0
8	C	80	0	0	3	0
8	D	94	0	0	1	0
8	E	64	0	0	0	0
8	F	92	0	0	2	0
8	G	58	0	0	2	0
8	H	48	0	0	2	0
8	I	87	0	0	4	0
8	J	73	0	0	2	0
8	K	159	0	0	4	0
8	L	134	0	0	2	0
8	N	1	0	0	0	0
All	All	33443	0	31310	573	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (573) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.10	1.15
1:E:156:ILE:HG12	1:E:172:ARG:HH12	1.09	1.11
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.03	1.08
1:K:156:ILE:HG12	1:K:172:ARG:HH12	0.99	1.08
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.17	1.04
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.17	1.04
2:F:212:GLN:HE21	2:F:222:SER:HB3	1.21	1.01
2:J:212:GLN:HE21	2:J:222:SER:HB3	1.29	0.96
1:K:156:ILE:HG12	1:K:172:ARG:NH1	1.81	0.95
2:H:21:LEU:HD21	2:H:304:ARG:HG2	1.47	0.95
2:F:212:GLN:NE2	2:F:222:SER:HB3	1.86	0.90
1:A:156:ILE:HG12	1:A:172:ARG:NH1	1.86	0.90
1:E:353:LYS:HE2	1:E:357:ARG:HH12	1.38	0.87
5:G:1711:CL:CL	8:G:383:HOH:O	2.31	0.86
2:H:18:LEU:HA	2:H:304:ARG:NH2	1.91	0.85
2:D:173:ARG:HG2	6:D:1722:GRG:H112	1.59	0.84
2:D:212:GLN:HE21	2:D:222:SER:HB3	1.41	0.84
2:L:173:ARG:HG2	6:L:1726:GRG:H112	1.59	0.83
1:E:255:VAL:HG13	1:E:258:ARG:HH21	1.42	0.83
1:G:152:MET:O	1:G:156:ILE:HG13	1.79	0.83
2:B:212:GLN:HE21	2:B:222:SER:HB3	1.44	0.83
2:D:39:ARG:H	2:D:39:ARG:HD2	1.42	0.82
2:D:212:GLN:NE2	2:D:222:SER:HB3	1.95	0.82
2:B:212:GLN:NE2	2:B:222:SER:HB3	1.95	0.82
2:H:348:THR:O	2:H:352:GLU:HG2	1.80	0.81
2:J:173:ARG:HG2	6:J:1725:GRG:H112	1.60	0.81
2:D:37:PRO:HB2	2:D:39:ARG:CD	2.11	0.81
1:A:152:MET:O	1:A:156:ILE:HG13	1.80	0.81
2:B:173:ARG:HG2	6:B:1721:GRG:H112	1.63	0.80
2:F:173:ARG:HG2	6:F:1723:GRG:H112	1.62	0.80
1:I:152:MET:O	1:I:156:ILE:HG13	1.82	0.79
1:E:152:MET:O	1:E:156:ILE:HG13	1.81	0.79
1:E:318:ILE:HG22	1:E:322:MET:HE3	1.65	0.79
1:K:330:LYS:HE2	1:K:367:HIS:HB3	1.66	0.77
2:D:37:PRO:HB2	2:D:39:ARG:HD2	1.67	0.77
2:H:173:ARG:HG2	6:H:1724:GRG:H112	1.67	0.76
2:H:186:ASN:HB2	2:H:358:HIS:CE1	2.20	0.76
1:C:152:MET:O	1:C:156:ILE:HG13	1.83	0.76
1:K:152:MET:O	1:K:156:ILE:HG13	1.85	0.76
1:E:156:ILE:HG12	1:E:172:ARG:NH1	1.94	0.75
1:E:255:VAL:HG13	1:E:258:ARG:NH2	2.01	0.75
2:H:212:GLN:NE2	2:H:222:SER:HB3	2.03	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:609:VAL:HG23	3:N:610:ILE:HG23	1.71	0.73
1:I:156:ILE:HG12	1:I:172:ARG:NH1	1.95	0.73
2:J:212:GLN:NE2	2:J:222:SER:HB3	2.02	0.73
1:G:97:ARG:HG2	1:G:101:ASP:OD2	1.89	0.72
1:K:156:ILE:CG1	1:K:172:ARG:HH12	1.90	0.72
2:H:229:SER:O	2:H:233:MET:HG3	1.90	0.71
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.56	0.71
1:E:156:ILE:CG1	1:E:172:ARG:HH12	1.98	0.71
3:M:509:VAL:HG23	3:M:510:ILE:HG23	1.71	0.71
5:K:1717:CL:CL	8:K:391:HOH:O	2.43	0.71
2:F:133:ILE:HD13	2:F:354:LEU:HD13	1.72	0.70
1:C:318:ILE:HG22	1:C:322:MET:HE3	1.73	0.70
2:L:212:GLN:HE21	2:L:222:SER:HB3	1.56	0.70
1:E:189:ILE:HD11	1:E:205:HIS:HD2	1.57	0.69
1:A:214:ARG:HG2	1:G:180:LYS:HB2	1.73	0.69
1:G:189:ILE:HD11	1:G:205:HIS:HD2	1.57	0.69
1:C:189:ILE:HD11	1:C:205:HIS:HD2	1.58	0.69
2:B:133:ILE:HD13	2:B:354:LEU:HD13	1.75	0.68
2:D:69:LYS:O	2:D:73:ILE:HG13	1.93	0.68
1:G:312:ILE:HG23	1:G:340:LEU:HD22	1.76	0.68
2:B:69:LYS:O	2:B:73:ILE:HG13	1.93	0.67
2:L:133:ILE:HD13	2:L:354:LEU:HD13	1.75	0.67
1:C:87:VAL:HG12	1:C:88:VAL:HG23	1.75	0.67
2:H:19:ASP:HB2	8:H:1494:HOH:O	1.96	0.66
2:D:37:PRO:HB2	2:D:39:ARG:HD3	1.77	0.66
1:K:91:ILE:O	1:K:91:ILE:HD12	1.95	0.66
1:K:189:ILE:HD11	1:K:205:HIS:HD2	1.60	0.65
2:H:212:GLN:HE21	2:H:222:SER:HB3	1.61	0.65
2:H:69:LYS:O	2:H:73:ILE:HG13	1.97	0.65
2:H:18:LEU:N	2:H:18:LEU:HD22	2.11	0.65
1:I:91:ILE:HD12	1:I:91:ILE:O	1.96	0.65
2:B:245:LEU:O	2:B:249:LYS:HG3	1.97	0.64
2:J:263:ARG:HG3	2:J:266:LYS:HG3	1.78	0.64
1:G:91:ILE:HD12	1:G:91:ILE:O	1.97	0.64
2:B:186:ASN:HB2	2:B:358:HIS:CE1	2.32	0.64
2:H:334:GLU:HB3	2:H:337:ILE:HD12	1.79	0.63
1:E:312:ILE:HG23	1:E:340:LEU:HD22	1.80	0.63
1:K:87:VAL:HG12	1:K:88:VAL:HG23	1.80	0.63
1:I:156:ILE:CG1	1:I:172:ARG:HH12	2.00	0.63
1:E:91:ILE:O	1:E:91:ILE:HD12	1.98	0.63
1:G:87:VAL:HG12	1:G:88:VAL:HG23	1.79	0.63
1:G:261:GLN:O	1:G:265:GLU:HG2	1.99	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:353:ARG:HH11	2:B:353:ARG:HG2	1.62	0.63
1:I:189:ILE:HD11	1:I:205:HIS:HD2	1.62	0.63
1:I:87:VAL:HG12	1:I:88:VAL:HG23	1.80	0.63
2:D:263:ARG:HG3	2:D:266:LYS:HG3	1.80	0.62
2:H:21:LEU:CD2	2:H:304:ARG:HG2	2.25	0.62
2:D:295:ARG:CZ	2:D:299:LEU:HD11	2.29	0.62
2:F:69:LYS:O	2:F:73:ILE:HG13	1.99	0.62
1:A:91:ILE:O	1:A:91:ILE:HD12	2.00	0.62
2:H:263:ARG:HG3	2:H:266:LYS:HG3	1.81	0.62
2:B:39:ARG:HB3	2:B:39:ARG:HH11	1.65	0.62
1:E:353:LYS:CE	1:E:357:ARG:HH12	2.10	0.61
2:F:37:PRO:HD2	2:F:40:TYR:CD1	2.34	0.61
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.82	0.61
2:F:26:VAL:O	2:F:30:GLN:HG3	1.99	0.61
1:G:334:LEU:HD22	1:G:367:HIS:O	2.00	0.61
2:F:263:ARG:HG3	2:F:266:LYS:HG3	1.81	0.61
2:J:133:ILE:HD13	2:J:354:LEU:HD13	1.82	0.61
2:H:87:ARG:HH12	2:H:90:LEU:HD11	1.65	0.61
1:K:312:ILE:HG23	1:K:340:LEU:HD22	1.83	0.61
2:L:197:ILE:HD11	2:L:235:LYS:HD3	1.83	0.61
1:G:101:ASP:HA	1:G:104:ARG:NH1	2.15	0.60
1:G:100:TYR:O	1:G:104:ARG:HG3	2.01	0.60
1:G:198:LYS:HD3	2:H:266:LYS:HD3	1.81	0.60
1:C:91:ILE:O	1:C:91:ILE:HD12	2.01	0.60
1:C:330:LYS:HE2	1:C:367:HIS:HB3	1.83	0.60
2:B:263:ARG:HG3	2:B:266:LYS:HG3	1.82	0.60
1:A:78:VAL:O	1:A:104:ARG:HD2	2.01	0.60
1:G:357:ARG:O	1:G:361:ARG:HG3	2.01	0.60
2:H:232:LEU:HD13	2:H:343:ALA:HB1	1.84	0.60
1:I:156:ILE:HD11	1:I:172:ARG:HH22	1.67	0.59
2:H:21:LEU:HD23	2:H:24:ARG:HE	1.67	0.59
1:A:339:GLU:O	1:A:343:ILE:HG13	2.02	0.59
1:K:156:ILE:HD11	1:K:172:ARG:HH22	1.68	0.59
2:D:39:ARG:H	2:D:39:ARG:CD	2.14	0.59
2:H:193:MET:HE2	2:H:233:MET:HB3	1.85	0.59
2:B:26:VAL:O	2:B:30:GLN:HG3	2.01	0.59
1:A:97:ARG:HG2	1:A:101:ASP:OD2	2.02	0.59
1:K:107:LEU:HD22	2:L:117:TYR:CD2	2.37	0.59
1:C:303:GLN:O	1:C:307:SER:HB2	2.03	0.58
1:I:207:GLN:HG2	1:I:242:PHE:CE2	2.38	0.58
2:J:22:ARG:O	2:J:26:VAL:HG23	2.03	0.58
2:H:210:LEU:HB2	2:H:223:THR:HA	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:198:LYS:HD3	2:D:266:LYS:HD3	1.85	0.58
1:C:180:LYS:HB2	1:E:214:ARG:HG2	1.85	0.58
2:L:232:LEU:HD13	2:L:343:ALA:HB1	1.85	0.58
2:J:210:LEU:HB2	2:J:223:THR:HA	1.84	0.58
1:E:78:VAL:O	1:E:104:ARG:HD2	2.03	0.57
2:L:353:ARG:HD3	2:L:353:ARG:O	2.04	0.57
2:L:210:LEU:HB2	2:L:223:THR:HA	1.86	0.57
2:H:245:LEU:O	2:H:249:LYS:HG3	2.04	0.57
2:J:318:ASP:HB2	7:M:1727:GER:H71	1.87	0.57
1:G:334:LEU:O	1:G:338:LEU:HG	2.04	0.57
1:C:148:LEU:HB2	1:C:179:LEU:HD21	1.87	0.57
1:A:328:ASP:O	1:A:329:ASN:HB2	2.05	0.57
1:I:330:LYS:HE2	1:I:367:HIS:HB3	1.87	0.57
1:A:87:VAL:HG12	1:A:88:VAL:HG23	1.87	0.56
1:G:101:ASP:HA	1:G:104:ARG:HH11	1.69	0.56
1:A:214:ARG:O	1:A:214:ARG:HG3	2.05	0.56
2:H:22:ARG:HG2	2:H:22:ARG:HH11	1.70	0.56
2:D:210:LEU:HB2	2:D:223:THR:HA	1.86	0.56
2:J:338:CYS:SG	2:J:349:ARG:NH2	2.78	0.56
1:K:265:GLU:O	1:K:269:LEU:HD13	2.06	0.56
2:D:37:PRO:HB3	2:D:39:ARG:HH11	1.70	0.56
1:I:107:LEU:HD22	2:J:117:TYR:CD2	2.40	0.56
1:I:312:ILE:HG23	1:I:340:LEU:HD22	1.87	0.56
1:I:329:ASN:HB3	1:I:332:ASP:HB3	1.88	0.56
1:E:82:ASP:HB2	1:E:86:PRO:HB3	1.88	0.56
1:G:156:ILE:HG12	1:G:172:ARG:NH1	2.03	0.56
1:I:148:LEU:HB2	1:I:179:LEU:HD21	1.88	0.56
2:J:232:LEU:HD13	2:J:343:ALA:HB1	1.86	0.56
2:L:263:ARG:HG3	2:L:266:LYS:HG3	1.86	0.56
1:A:265:GLU:O	1:A:269:LEU:HD13	2.06	0.56
1:E:265:GLU:O	1:E:269:LEU:HD13	2.06	0.56
1:E:87:VAL:HG12	1:E:88:VAL:HG23	1.88	0.55
2:F:37:PRO:HD2	2:F:40:TYR:CE1	2.41	0.55
2:D:18:LEU:HD12	2:D:304:ARG:NH1	2.21	0.55
2:H:353:ARG:O	2:H:357:LEU:HB2	2.05	0.55
2:B:210:LEU:HB2	2:B:223:THR:HA	1.87	0.55
2:J:290:ASN:ND2	2:J:293:LYS:HD2	2.22	0.55
1:G:189:ILE:HD11	1:G:205:HIS:CD2	2.41	0.55
1:E:148:LEU:HB2	1:E:179:LEU:HD21	1.87	0.55
1:G:90:ILE:HD13	2:H:40:TYR:O	2.07	0.55
1:C:78:VAL:HB	1:C:104:ARG:HB3	1.89	0.55
1:G:148:LEU:HB2	1:G:179:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:64:LEU:HD11	2:H:134:ILE:HG22	1.88	0.55
1:C:334:LEU:HD22	1:C:367:HIS:O	2.07	0.55
2:F:210:LEU:HB2	2:F:223:THR:HA	1.88	0.55
2:B:336:GLY:HA2	2:J:305:LEU:HD13	1.89	0.55
1:E:261:GLN:O	1:E:265:GLU:HG2	2.06	0.55
1:C:82:ASP:HB2	1:C:86:PRO:HB3	1.89	0.55
1:C:261:GLN:O	1:C:265:GLU:HG2	2.07	0.55
1:E:353:LYS:HE2	1:E:357:ARG:NH1	2.17	0.55
2:D:133:ILE:HD13	2:D:354:LEU:HD13	1.89	0.55
1:K:97:ARG:HG2	1:K:101:ASP:OD2	2.07	0.55
1:E:121:ARG:NH1	1:E:121:ARG:HG3	2.21	0.55
2:F:186:ASN:HB2	2:F:358:HIS:NE2	2.22	0.54
1:E:353:LYS:HE3	1:E:357:ARG:HH22	1.73	0.54
1:A:357:ARG:HH11	1:A:357:ARG:HG3	1.72	0.54
2:L:212:GLN:NE2	2:L:222:SER:HB3	2.21	0.54
2:H:349:ARG:O	2:H:352:GLU:HB2	2.07	0.54
2:H:348:THR:HA	2:H:351:SER:OG	2.07	0.54
1:A:334:LEU:HD22	1:A:367:HIS:O	2.07	0.54
1:K:334:LEU:HD22	1:K:367:HIS:O	2.07	0.54
1:E:339:GLU:O	1:E:343:ILE:HG13	2.08	0.54
2:F:232:LEU:HD13	2:F:343:ALA:HB1	1.89	0.54
1:I:198:LYS:HD3	2:J:266:LYS:HD3	1.89	0.54
1:A:303:GLN:O	1:A:307:SER:HB2	2.08	0.54
2:B:250:ARG:O	2:B:254:MET:HG2	2.07	0.54
1:G:91:ILE:HD12	2:H:38:GLU:HB2	1.89	0.54
1:I:195:GLN:NE2	8:I:1500:HOH:O	2.41	0.53
2:J:197:ILE:HD11	2:J:235:LYS:HD3	1.91	0.53
2:D:212:GLN:HE21	2:D:222:SER:CB	2.18	0.53
1:K:198:LYS:HD3	2:L:266:LYS:HD3	1.90	0.53
1:I:344:LEU:HD13	1:I:356:TRP:CE2	2.44	0.53
1:E:294:ASN:O	1:E:298:GLN:HG3	2.08	0.53
1:C:339:GLU:O	1:C:343:ILE:HG13	2.09	0.53
2:H:186:ASN:HB2	2:H:358:HIS:NE2	2.24	0.53
2:L:318:ASP:HB2	7:N:1727:GER:H71	1.90	0.53
1:I:334:LEU:HD22	1:I:367:HIS:O	2.09	0.53
2:H:258:ASN:OD1	2:H:259:GLY:N	2.38	0.53
1:K:311:LEU:HD23	1:K:311:LEU:O	2.09	0.53
1:G:328:ASP:O	1:G:329:ASN:HB2	2.09	0.53
3:N:609:VAL:N	7:N:1727:GER:H11	2.23	0.52
1:C:328:ASP:O	1:C:329:ASN:HB2	2.09	0.52
1:I:339:GLU:O	1:I:343:ILE:HG13	2.08	0.52
2:J:202:ARG:HD2	8:J:384:HOH:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:339:LYS:O	2:B:348:THR:HG23	2.10	0.52
2:B:24:ARG:HD3	2:B:27:ARG:HH22	1.74	0.52
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.92	0.52
2:B:353:ARG:HG2	2:B:353:ARG:NH1	2.22	0.52
2:H:130:SER:O	2:H:134:ILE:HG13	2.10	0.52
2:B:229:SER:O	2:B:233:MET:HG3	2.09	0.52
1:G:303:GLN:O	1:G:307:SER:HB2	2.10	0.52
1:I:67:ARG:HD2	8:I:927:HOH:O	2.09	0.52
1:G:79:PRO:HA	1:G:101:ASP:OD1	2.11	0.51
1:K:338:LEU:HD11	1:K:364:GLN:HG2	1.92	0.51
2:J:87:ARG:HH12	2:J:90:LEU:HD11	1.75	0.51
1:K:148:LEU:HB2	1:K:179:LEU:HD21	1.92	0.51
1:E:198:LYS:HD3	2:F:266:LYS:HD3	1.92	0.51
1:C:78:VAL:O	1:C:104:ARG:HD2	2.11	0.51
1:I:265:GLU:O	1:I:269:LEU:HD13	2.10	0.51
1:A:189:ILE:HD11	1:A:205:HIS:CD2	2.41	0.51
1:I:328:ASP:O	1:I:329:ASN:HB2	2.10	0.51
1:K:311:LEU:HD23	1:K:311:LEU:C	2.30	0.51
2:H:267:PRO:HG2	8:H:1609:HOH:O	2.10	0.51
3:M:509:VAL:N	7:M:1727:GER:H11	2.25	0.51
2:J:105:PHE:CE2	2:J:107:PRO:HD3	2.46	0.51
2:J:77:TYR:CE1	2:J:141:ARG:HB2	2.45	0.51
1:I:106:VAL:HG11	1:I:116:ALA:HB1	1.93	0.51
1:G:343:ILE:HG22	1:G:348:LYS:HG3	1.93	0.51
2:L:334:GLU:HB3	2:L:337:ILE:HD12	1.93	0.51
1:E:318:ILE:HG22	1:E:322:MET:CE	2.38	0.51
2:J:63:SER:O	2:J:66:VAL:HG22	2.11	0.51
1:K:303:GLN:O	1:K:307:SER:HB2	2.11	0.51
2:F:250:ARG:O	2:F:254:MET:HG2	2.11	0.51
1:G:344:LEU:HD13	1:G:356:TRP:CE2	2.45	0.51
1:I:151:GLU:HG3	1:I:175:LEU:HD11	1.93	0.51
2:B:77:TYR:CZ	2:B:141:ARG:HB2	2.46	0.50
1:A:58:LEU:HD23	1:A:63:TYR:CZ	2.46	0.50
1:I:311:LEU:C	1:I:311:LEU:HD23	2.32	0.50
1:E:214:ARG:O	1:E:214:ARG:HG3	2.12	0.50
1:I:78:VAL:O	1:I:104:ARG:HD2	2.11	0.50
1:K:96:PHE:CE1	1:K:126:LEU:HB3	2.46	0.50
1:G:329:ASN:HB3	1:G:332:ASP:HB3	1.94	0.50
2:L:212:GLN:HE21	2:L:212:GLN:HA	1.76	0.50
2:D:232:LEU:HD13	2:D:343:ALA:HB1	1.92	0.50
1:C:69:ARG:HB3	1:C:71:GLU:OE1	2.12	0.50
1:E:92:TYR:O	1:E:97:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:311:LEU:HD23	1:G:311:LEU:C	2.32	0.50
2:F:207:ASP:O	2:F:208:ASN:HB2	2.11	0.49
2:D:333:GLU:HA	8:D:740:HOH:O	2.11	0.49
2:D:333:GLU:O	1:K:357:ARG:NH2	2.45	0.49
2:B:130:SER:O	2:B:134:ILE:HG13	2.11	0.49
2:F:256:GLN:HB2	2:F:260:TYR:CE2	2.47	0.49
2:J:27:ARG:HH12	2:J:30:GLN:NE2	2.09	0.49
2:H:202:ARG:HG3	2:H:202:ARG:HH11	1.77	0.49
2:F:130:SER:O	2:F:134:ILE:HG13	2.12	0.49
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.95	0.49
1:A:214:ARG:CG	1:A:214:ARG:O	2.59	0.49
2:F:38:GLU:O	2:F:38:GLU:HG2	2.13	0.49
1:C:100:TYR:HB3	1:C:104:ARG:HH21	1.78	0.49
2:J:334:GLU:HB3	2:J:337:ILE:HD12	1.93	0.49
2:B:29:PHE:O	2:B:33:LEU:HD22	2.12	0.49
2:D:250:ARG:O	2:D:254:MET:HG2	2.13	0.49
1:G:135:HIS:CD2	2:H:166:GLU:HG2	2.48	0.49
2:L:333:GLU:HA	8:L:1050:HOH:O	2.13	0.49
2:B:207:ASP:O	2:B:208:ASN:HB2	2.13	0.49
1:K:189:ILE:HD11	1:K:205:HIS:CD2	2.45	0.49
2:B:22:ARG:HH11	2:B:22:ARG:HG2	1.77	0.49
2:D:186:ASN:HB2	2:D:358:HIS:CE1	2.48	0.49
1:G:65:LEU:HD12	1:G:67:ARG:HH11	1.77	0.49
1:C:106:VAL:HG11	1:C:116:ALA:HB1	1.94	0.49
2:L:256:GLN:HB2	2:L:260:TYR:CE2	2.48	0.49
1:I:100:TYR:O	1:I:104:ARG:HG3	2.12	0.48
2:B:105:PHE:CE2	2:B:107:PRO:HD3	2.47	0.48
1:G:97:ARG:HH11	1:G:97:ARG:HB3	1.78	0.48
1:A:325:ASN:O	1:A:326:GLN:C	2.52	0.48
1:E:67:ARG:NH2	1:E:94:GLU:OE1	2.43	0.48
1:G:339:GLU:O	1:G:343:ILE:HG13	2.13	0.48
1:I:84:PRO:HG2	1:I:85:SER:H	1.79	0.48
1:E:303:GLN:O	1:E:307:SER:HB2	2.14	0.48
2:F:212:GLN:HE21	2:F:222:SER:CB	2.08	0.48
2:H:256:GLN:HB2	2:H:260:TYR:CE2	2.49	0.48
1:A:156:ILE:HD11	1:A:172:ARG:HH22	1.79	0.48
2:H:22:ARG:O	2:H:26:VAL:HG23	2.14	0.48
1:I:303:GLN:O	1:I:307:SER:HB2	2.14	0.48
1:C:265:GLU:O	1:C:269:LEU:HD13	2.13	0.48
1:I:338:LEU:HD11	1:I:364:GLN:HG2	1.96	0.48
2:J:358:HIS:O	2:J:361:TRP:HB2	2.14	0.48
2:B:38:GLU:HG2	2:B:38:GLU:O	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:69:ARG:HB3	1:E:71:GLU:OE1	2.14	0.48
1:A:117:PHE:CE2	1:A:146:LYS:HE2	2.49	0.48
2:H:193:MET:HE2	2:H:233:MET:CG	2.44	0.48
1:E:121:ARG:HH11	1:E:121:ARG:HG3	1.78	0.48
1:E:296:LEU:HD22	1:E:322:MET:CE	2.44	0.47
1:G:219:GLU:OE1	1:G:219:GLU:HA	2.14	0.47
2:D:79:LEU:O	2:D:96:ARG:HG3	2.14	0.47
2:J:130:SER:O	2:J:134:ILE:HG13	2.14	0.47
1:A:184:GLN:HB2	8:A:379:HOH:O	2.14	0.47
2:L:105:PHE:CE2	2:L:107:PRO:HD3	2.49	0.47
2:L:110:ASN:HB3	2:L:111:PRO:HD2	1.96	0.47
1:C:311:LEU:HD23	1:C:311:LEU:C	2.34	0.47
2:D:197:ILE:HD11	2:D:235:LYS:HD3	1.95	0.47
1:I:189:ILE:HD11	1:I:205:HIS:CD2	2.47	0.47
2:J:229:SER:O	2:J:233:MET:HG3	2.14	0.47
1:E:96:PHE:CE1	1:E:126:LEU:HB3	2.49	0.47
1:I:184:GLN:HB2	8:I:378:HOH:O	2.15	0.47
1:G:265:GLU:O	1:G:269:LEU:HD13	2.14	0.47
2:B:256:GLN:HB2	2:B:260:TYR:CE2	2.50	0.47
1:C:173:ARG:NH1	8:C:412:HOH:O	2.46	0.47
1:E:106:VAL:HG11	1:E:116:ALA:HB1	1.96	0.47
1:E:58:LEU:HD23	1:E:63:TYR:CE2	2.50	0.47
2:J:258:ASN:OD1	2:J:259:GLY:N	2.42	0.47
2:H:311:LYS:HG3	2:H:312:TRP:CD2	2.49	0.47
1:G:117:PHE:CE2	1:G:146:LYS:HE2	2.49	0.47
2:J:69:LYS:O	2:J:73:ILE:HG13	2.13	0.47
1:K:249:GLY:HA3	8:K:640:HOH:O	2.14	0.47
1:C:312:ILE:HG23	1:C:340:LEU:HD22	1.97	0.47
1:G:156:ILE:HD11	1:G:172:ARG:HH22	1.80	0.47
2:F:311:LYS:HG3	2:F:312:TRP:CD2	2.50	0.47
2:D:37:PRO:CB	2:D:39:ARG:HH11	2.27	0.47
1:E:312:ILE:O	1:E:316:VAL:HG23	2.15	0.46
1:E:156:ILE:HD11	1:E:172:ARG:HH22	1.79	0.46
1:C:214:ARG:HG2	1:C:214:ARG:O	2.14	0.46
2:H:250:ARG:O	2:H:254:MET:HG2	2.16	0.46
2:D:130:SER:O	2:D:134:ILE:HG13	2.15	0.46
2:B:212:GLN:HE21	2:B:222:SER:CB	2.20	0.46
2:L:53:PHE:HE1	7:N:1727:GER:H42	1.80	0.46
2:H:30:GLN:OE1	2:H:66:VAL:HB	2.16	0.46
1:I:65:LEU:O	1:I:69:ARG:HG3	2.15	0.46
1:E:334:LEU:HD22	1:E:367:HIS:O	2.15	0.46
1:C:96:PHE:CE1	1:C:126:LEU:HB3	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:22:ARG:O	2:B:26:VAL:HG23	2.16	0.46
2:H:29:PHE:O	2:H:33:LEU:HD22	2.15	0.46
1:K:71:GLU:H	1:K:71:GLU:CD	2.18	0.46
1:G:325:ASN:O	1:G:326:GLN:C	2.54	0.46
1:C:189:ILE:HD11	1:C:205:HIS:CD2	2.44	0.46
2:L:133:ILE:CD1	2:L:354:LEU:HD13	2.42	0.46
2:D:311:LYS:HG3	2:D:312:TRP:CD2	2.50	0.46
1:G:106:VAL:HG11	1:G:116:ALA:HB1	1.97	0.46
2:H:22:ARG:HG2	2:H:22:ARG:NH1	2.29	0.46
2:D:138:ASP:OD1	2:D:140:SER:HB3	2.15	0.46
2:B:357:LEU:HD22	2:B:361:TRP:CE2	2.51	0.46
2:H:193:MET:HE2	2:H:233:MET:CB	2.46	0.46
1:A:198:LYS:HD3	2:B:266:LYS:HD3	1.97	0.46
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.51	0.46
1:E:263:THR:HG21	1:E:280:LEU:HB2	1.98	0.46
2:B:311:LYS:HG3	2:B:312:TRP:CD2	2.51	0.46
1:C:80:GLN:N	1:C:104:ARG:NH1	2.64	0.46
1:A:106:VAL:HG11	1:A:116:ALA:HB1	1.97	0.46
1:K:106:VAL:HG11	1:K:116:ALA:HB1	1.98	0.45
1:A:285:GLN:NE2	2:B:247:ARG:NH1	2.63	0.45
1:C:219:GLU:HA	1:C:219:GLU:OE1	2.16	0.45
2:L:22:ARG:NH1	2:L:22:ARG:HG2	2.30	0.45
2:B:37:PRO:HD2	2:B:40:TYR:CE1	2.51	0.45
1:I:263:THR:HG21	1:I:280:LEU:HB2	1.98	0.45
1:G:96:PHE:CE1	1:G:126:LEU:HB3	2.51	0.45
2:H:26:VAL:O	2:H:30:GLN:HG3	2.17	0.45
1:I:325:ASN:O	1:I:326:GLN:C	2.54	0.45
1:C:97:ARG:HG2	1:C:101:ASP:OD2	2.15	0.45
2:L:77:TYR:CZ	2:L:141:ARG:HB2	2.51	0.45
2:J:77:TYR:CZ	2:J:141:ARG:HB2	2.51	0.45
1:G:58:LEU:HD23	1:G:63:TYR:CZ	2.51	0.45
2:F:245:LEU:O	2:F:249:LYS:HG3	2.16	0.45
1:A:357:ARG:NH1	1:A:357:ARG:HG3	2.31	0.45
1:E:287:ARG:HG2	1:E:287:ARG:H	1.49	0.45
1:A:263:THR:HG21	1:A:280:LEU:HB2	1.98	0.45
2:J:311:LYS:HE2	2:J:312:TRP:CZ2	2.52	0.45
2:J:38:GLU:O	2:J:38:GLU:HG2	2.17	0.45
2:D:64:LEU:HD11	2:D:134:ILE:HG22	1.98	0.45
2:L:22:ARG:HH11	2:L:22:ARG:HG2	1.81	0.45
1:A:96:PHE:CE1	1:A:126:LEU:HB3	2.52	0.45
2:L:103:ILE:HG23	2:L:104:PRO:HD2	1.98	0.45
1:G:105:ALA:O	1:G:109:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:21:LEU:CD1	2:H:21:LEU:N	2.79	0.45
1:I:218:ASN:HB3	8:I:1242:HOH:O	2.16	0.45
1:E:281:LYS:NZ	1:E:317:ASP:OD1	2.37	0.45
2:B:311:LYS:HE2	2:B:312:TRP:CZ2	2.51	0.45
1:E:107:LEU:HD22	2:F:117:TYR:CD2	2.52	0.45
2:H:156:LEU:HD21	2:H:162:CYS:SG	2.57	0.45
1:G:286:ASP:HB2	8:G:618:HOH:O	2.16	0.45
1:K:325:ASN:O	1:K:326:GLN:C	2.55	0.45
1:G:318:ILE:HG22	1:G:322:MET:CE	2.47	0.45
1:E:91:ILE:HD12	2:F:38:GLU:HB2	1.99	0.45
1:A:91:ILE:HD11	2:B:38:GLU:H	1.81	0.45
2:B:103:ILE:HG23	2:B:104:PRO:HD2	1.99	0.44
1:A:71:GLU:O	1:A:115:ARG:NH1	2.50	0.44
1:I:105:ALA:O	1:I:109:ARG:HG3	2.17	0.44
1:A:198:LYS:CD	2:B:266:LYS:HD3	2.47	0.44
2:D:133:ILE:HG22	2:D:350:THR:HG23	1.98	0.44
1:A:58:LEU:HD23	1:A:63:TYR:CE2	2.52	0.44
2:J:256:GLN:HB2	2:J:260:TYR:CE2	2.52	0.44
1:E:189:ILE:HD11	1:E:205:HIS:CD2	2.44	0.44
1:C:344:LEU:HD13	1:C:356:TRP:CE2	2.52	0.44
1:E:328:ASP:O	1:E:329:ASN:HB2	2.18	0.44
2:D:19:ASP:OD2	2:D:19:ASP:N	2.44	0.44
2:D:295:ARG:NH2	2:D:299:LEU:HD11	2.33	0.44
2:J:207:ASP:O	2:J:208:ASN:HB2	2.18	0.44
1:C:263:THR:HG21	1:C:280:LEU:HB2	1.98	0.44
3:N:608:CYS:HA	7:N:1727:GER:C2	2.48	0.44
2:D:103:ILE:HG23	2:D:104:PRO:HD2	1.99	0.44
2:D:229:SER:O	2:D:233:MET:HG3	2.18	0.44
1:I:58:LEU:HD23	1:I:63:TYR:CZ	2.52	0.44
1:G:353:LYS:HG2	1:G:354:GLU:N	2.32	0.44
3:M:508:CYS:HA	7:M:1727:GER:C2	2.48	0.44
2:L:212:GLN:NE2	2:L:212:GLN:HA	2.33	0.44
2:H:24:ARG:HG3	2:H:24:ARG:HH11	1.83	0.44
2:J:116:PRO:HB2	2:J:117:TYR:CD2	2.53	0.44
1:A:334:LEU:O	1:A:338:LEU:HG	2.18	0.44
2:H:311:LYS:HE2	2:H:312:TRP:CZ2	2.52	0.44
2:H:77:TYR:CZ	2:H:141:ARG:HB2	2.53	0.44
2:H:360:SER:O	2:H:363:THR:HG23	2.18	0.44
2:L:207:ASP:O	2:L:208:ASN:HB2	2.18	0.44
1:G:107:LEU:HD22	2:H:117:TYR:CD2	2.53	0.44
2:H:24:ARG:NH1	2:H:24:ARG:HG3	2.32	0.43
2:D:295:ARG:NH1	2:D:299:LEU:CD1	2.81	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:92:TYR:O	1:K:97:ARG:NH2	2.52	0.43
2:B:116:PRO:HB2	2:B:117:TYR:CD2	2.53	0.43
1:C:207:GLN:OE1	2:D:216:LEU:HD13	2.18	0.43
1:K:79:PRO:HA	1:K:101:ASP:OD1	2.19	0.43
2:L:130:SER:O	2:L:134:ILE:HG13	2.18	0.43
2:J:311:LYS:HG3	2:J:312:TRP:CD2	2.53	0.43
1:I:96:PHE:CE1	1:I:126:LEU:HB3	2.53	0.43
1:G:263:THR:HG21	1:G:280:LEU:HB2	2.00	0.43
1:E:121:ARG:HH11	1:E:121:ARG:CG	2.32	0.43
2:F:29:PHE:O	2:F:33:LEU:HD22	2.19	0.43
2:H:207:ASP:O	2:H:208:ASN:HB2	2.18	0.43
1:K:328:ASP:O	1:K:329:ASN:HB2	2.18	0.43
1:E:117:PHE:CE2	1:E:146:LYS:HE2	2.54	0.43
2:F:333:GLU:HA	8:F:875:HOH:O	2.18	0.43
1:G:330:LYS:HE2	1:G:367:HIS:HB3	2.00	0.43
2:B:22:ARG:HG2	2:B:22:ARG:NH1	2.34	0.43
2:L:245:LEU:O	2:L:249:LYS:HG3	2.19	0.43
2:D:116:PRO:HB2	2:D:117:TYR:CD2	2.53	0.43
1:K:151:GLU:HG3	1:K:175:LEU:HD11	2.00	0.43
1:E:296:LEU:HD22	1:E:322:MET:HE1	2.00	0.43
2:F:30:GLN:O	2:F:34:GLN:HG3	2.19	0.43
2:D:110:ASN:HB3	2:D:111:PRO:HD2	2.01	0.43
2:L:311:LYS:HG3	2:L:312:TRP:CD2	2.54	0.43
1:K:223:VAL:HG11	1:K:240:ARG:HB2	2.01	0.43
2:F:21:LEU:N	2:F:21:LEU:CD1	2.82	0.43
2:H:18:LEU:N	2:H:18:LEU:CD2	2.81	0.43
2:J:53:PHE:HE1	7:M:1727:GER:H42	1.84	0.43
2:B:64:LEU:HD11	2:B:134:ILE:HG22	2.01	0.43
1:A:340:LEU:HD23	1:A:343:ILE:HD12	2.01	0.43
1:G:72:TRP:CZ2	1:G:115:ARG:HB2	2.53	0.43
2:L:250:ARG:O	2:L:254:MET:HG2	2.19	0.43
2:H:193:MET:HG3	2:H:233:MET:HE1	2.01	0.43
2:L:21:LEU:HG	8:L:632:HOH:O	2.19	0.43
2:F:103:ILE:HG23	2:F:104:PRO:HD2	2.00	0.43
2:B:192:ASP:OD1	2:B:195:LYS:HE3	2.18	0.43
1:K:339:GLU:O	1:K:343:ILE:HG13	2.19	0.43
2:L:122:ILE:HG22	2:L:163:ALA:HA	2.01	0.43
1:E:97:ARG:HG2	1:E:101:ASP:OD2	2.18	0.43
1:C:361:ARG:HD3	8:C:1272:HOH:O	2.19	0.43
1:C:296:LEU:HD22	1:C:322:MET:CE	2.49	0.42
2:D:311:LYS:HE2	2:D:312:TRP:CZ2	2.54	0.42
2:F:116:PRO:HB2	2:F:117:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:267:ILE:HD13	1:G:277:TRP:CE2	2.54	0.42
2:D:77:TYR:CZ	2:D:141:ARG:HB2	2.54	0.42
1:E:325:ASN:O	1:E:326:GLN:C	2.56	0.42
1:C:286:ASP:HB2	8:C:621:HOH:O	2.18	0.42
2:H:354:LEU:HD11	2:H:358:HIS:NE2	2.34	0.42
1:E:329:ASN:HB3	1:E:332:ASP:HB3	2.00	0.42
2:D:86:ASP:N	2:D:86:ASP:OD2	2.48	0.42
2:J:36:LEU:HA	2:J:37:PRO:HD3	1.89	0.42
2:L:22:ARG:O	2:L:26:VAL:HG23	2.18	0.42
1:C:107:LEU:HD22	2:D:117:TYR:CD2	2.53	0.42
2:D:256:GLN:HB2	2:D:260:TYR:CE2	2.53	0.42
2:D:243:LYS:HE2	2:D:243:LYS:HB3	1.87	0.42
1:C:156:ILE:HD11	1:C:172:ARG:HH22	1.84	0.42
6:F:1723:GRG:HC62	6:F:1723:GRG:H101	1.91	0.42
1:K:329:ASN:HB3	1:K:332:ASP:HB3	2.02	0.42
1:G:318:ILE:HG22	1:G:322:MET:HE3	2.02	0.42
1:A:71:GLU:CD	1:A:71:GLU:H	2.17	0.42
2:L:186:ASN:HB2	2:L:358:HIS:CE1	2.55	0.42
1:A:267:ILE:HD13	1:A:277:TRP:CE2	2.55	0.42
2:L:79:LEU:O	2:L:96:ARG:HG3	2.19	0.42
1:I:287:ARG:H	1:I:287:ARG:HG2	1.59	0.42
1:A:348:LYS:HA	1:A:348:LYS:HD3	1.82	0.42
2:F:311:LYS:HE2	2:F:312:TRP:CZ2	2.54	0.42
2:D:121:HIS:HB3	2:D:124:MET:HG2	2.02	0.42
2:D:20:PHE:CZ	2:D:337:ILE:HD11	2.55	0.42
2:F:121:HIS:HB3	2:F:124:MET:HG2	2.02	0.42
2:F:353:ARG:NE	8:F:739:HOH:O	2.52	0.42
2:B:21:LEU:CD1	2:B:21:LEU:N	2.83	0.42
2:L:311:LYS:HE2	2:L:312:TRP:CZ2	2.55	0.42
1:A:311:LEU:HD23	1:A:311:LEU:C	2.40	0.42
2:H:87:ARG:HB3	2:H:87:ARG:NH1	2.35	0.42
2:H:63:SER:O	2:H:66:VAL:HG22	2.20	0.42
2:F:115:HIS:HA	2:F:116:PRO:HD3	1.91	0.42
2:J:122:ILE:HG22	2:J:163:ALA:HA	2.01	0.42
1:A:359:ILE:HD13	1:A:359:ILE:HA	1.92	0.42
2:J:59:ASP:OD2	2:J:349:ARG:NH1	2.53	0.41
2:F:77:TYR:CZ	2:F:141:ARG:HB2	2.54	0.41
2:D:37:PRO:HD2	2:D:40:TYR:CE1	2.55	0.41
2:L:69:LYS:O	2:L:73:ILE:HG13	2.20	0.41
1:E:219:GLU:HA	1:E:219:GLU:OE1	2.19	0.41
1:E:214:ARG:O	1:E:214:ARG:CG	2.68	0.41
2:J:138:ASP:O	2:J:139:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:82:ASP:HB2	1:K:86:PRO:HB3	2.03	0.41
2:F:37:PRO:HD2	2:F:40:TYR:HD1	1.85	0.41
1:G:287:ARG:HG2	1:G:287:ARG:H	1.54	0.41
2:B:77:TYR:CE1	2:B:141:ARG:HB2	2.55	0.41
2:B:37:PRO:HD2	2:B:40:TYR:CD1	2.55	0.41
1:C:325:ASN:O	1:C:326:GLN:C	2.59	0.41
2:J:246:ASN:ND2	8:J:395:HOH:O	2.54	0.41
2:J:155:GLN:HB2	2:J:161:PHE:CE2	2.56	0.41
1:E:311:LEU:HD23	1:E:311:LEU:C	2.41	0.41
7:M:1727:GER:H112	7:M:1727:GER:H91	1.88	0.41
2:D:26:VAL:O	2:D:30:GLN:HG3	2.21	0.41
2:D:353:ARG:NH1	2:D:357:LEU:HG	2.35	0.41
2:L:116:PRO:HB2	2:L:117:TYR:CD2	2.56	0.41
1:I:344:LEU:HA	1:I:348:LYS:HB2	2.02	0.41
1:C:329:ASN:HB3	1:C:332:ASP:HB3	2.01	0.41
2:J:359:GLN:C	2:J:361:TRP:H	2.24	0.41
2:J:37:PRO:HD2	2:J:40:TYR:CE1	2.55	0.41
1:I:136:PHE:CE2	1:I:140:LEU:HD11	2.55	0.41
1:K:149:GLN:HG3	8:K:1048:HOH:O	2.20	0.41
1:E:155:ILE:HD12	1:E:155:ILE:HA	1.94	0.41
2:L:37:PRO:HD2	2:L:40:TYR:CD1	2.56	0.41
1:A:92:TYR:O	1:A:97:ARG:NH2	2.54	0.41
1:C:100:TYR:HB3	1:C:104:ARG:NH2	2.36	0.41
2:J:121:HIS:HB3	2:J:124:MET:HG2	2.03	0.41
2:H:49:THR:HG23	2:H:124:MET:SD	2.61	0.41
1:E:353:LYS:CE	1:E:357:ARG:HH22	2.34	0.41
2:D:37:PRO:HD2	2:D:40:TYR:CD1	2.55	0.41
2:H:352:GLU:HA	2:H:352:GLU:OE2	2.20	0.41
2:L:36:LEU:HA	2:L:37:PRO:HD3	1.93	0.41
2:L:40:TYR:CE2	7:N:1727:GER:H101	2.56	0.41
1:G:189:ILE:HG21	1:G:206:ARG:HB2	2.03	0.41
2:H:30:GLN:O	2:H:34:GLN:HG3	2.21	0.41
2:F:64:LEU:HD23	2:F:64:LEU:HA	1.84	0.41
2:L:236:LEU:HD22	2:L:245:LEU:HD21	2.03	0.41
1:C:353:LYS:HE3	1:K:339:GLU:HG3	2.03	0.41
2:B:138:ASP:O	2:B:139:LEU:HB2	2.20	0.41
2:H:341:HIS:HA	2:H:342:PRO:HD2	1.81	0.41
2:H:133:ILE:HG22	2:H:350:THR:HG23	2.02	0.41
2:J:250:ARG:O	2:J:254:MET:HG2	2.20	0.41
2:L:255:ARG:HD3	2:L:261:HIS:CD2	2.55	0.41
2:J:77:TYR:HE2	2:J:137:ASP:OD2	2.04	0.41
1:A:331:GLU:O	1:A:335:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:245:LEU:O	2:J:249:LYS:HG3	2.21	0.41
1:K:184:GLN:HB2	8:K:382:HOH:O	2.20	0.41
2:B:52:PHE:HA	2:B:131:CYS:SG	2.61	0.41
2:B:249:LYS:HB3	2:B:285:ILE:HD13	2.03	0.40
2:D:156:LEU:HD21	2:D:162:CYS:SG	2.61	0.40
1:G:207:GLN:OE1	2:H:216:LEU:HD13	2.21	0.40
2:L:49:THR:HG23	2:L:124:MET:SD	2.61	0.40
2:D:258:ASN:OD1	2:D:259:GLY:N	2.42	0.40
1:C:287:ARG:H	1:C:287:ARG:HG2	1.64	0.40
1:K:287:ARG:HG2	1:K:287:ARG:H	1.63	0.40
2:B:64:LEU:HB3	2:B:69:LYS:HE2	2.03	0.40
2:J:133:ILE:CD1	2:J:354:LEU:HD13	2.49	0.40
1:G:58:LEU:HD23	1:G:63:TYR:CE2	2.56	0.40
1:I:350:THR:O	1:I:353:LYS:HB3	2.21	0.40
2:L:64:LEU:HD23	2:L:64:LEU:HA	1.90	0.40
1:A:156:ILE:CD1	1:A:172:ARG:HH22	2.35	0.40
2:B:298:ILE:HD12	2:B:329:LEU:HD13	2.04	0.40
1:G:151:GLU:HG3	1:G:175:LEU:HD11	2.02	0.40
2:H:357:LEU:HD22	2:H:361:TRP:CZ2	2.56	0.40
2:J:30:GLN:HE21	2:J:30:GLN:HB3	1.65	0.40
2:F:64:LEU:HD11	2:F:134:ILE:HG22	2.04	0.40
2:J:64:LEU:HB3	2:J:69:LYS:HE2	2.03	0.40
1:A:107:LEU:HD22	2:B:117:TYR:CD2	2.56	0.40
2:J:37:PRO:HD2	2:J:40:TYR:CD1	2.57	0.40
1:I:124:ILE:HD13	1:I:134:TRP:CH2	2.57	0.40
2:H:155:GLN:HB2	2:H:161:PHE:CE2	2.56	0.40
2:H:86:ASP:N	2:H:86:ASP:OD2	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	312/377 (83%)	287 (92%)	23 (7%)	2 (1%)	33 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	312/377 (83%)	289 (93%)	22 (7%)	1 (0%)	50	80
1	E	312/377 (83%)	289 (93%)	21 (7%)	2 (1%)	33	63
1	G	312/377 (83%)	291 (93%)	19 (6%)	2 (1%)	33	63
1	I	312/377 (83%)	289 (93%)	21 (7%)	2 (1%)	33	63
1	K	312/377 (83%)	293 (94%)	17 (5%)	2 (1%)	33	63
2	B	344/377 (91%)	329 (96%)	14 (4%)	1 (0%)	50	80
2	D	344/377 (91%)	329 (96%)	13 (4%)	2 (1%)	33	63
2	F	344/377 (91%)	328 (95%)	15 (4%)	1 (0%)	50	80
2	H	344/377 (91%)	323 (94%)	19 (6%)	2 (1%)	33	63
2	J	344/377 (91%)	324 (94%)	19 (6%)	1 (0%)	50	80
2	L	344/377 (91%)	330 (96%)	13 (4%)	1 (0%)	50	80
3	M	2/11 (18%)	2 (100%)	0	0	100	100
3	N	2/11 (18%)	2 (100%)	0	0	100	100
All	All	3940/4546 (87%)	3705 (94%)	216 (6%)	19 (0%)	38	68

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	258	ASN
1	G	306	HIS
1	G	326	GLN
2	H	258	ASN
1	I	306	HIS
2	J	258	ASN
1	K	306	HIS
2	L	258	ASN
1	A	306	HIS
1	A	326	GLN
2	D	258	ASN
2	F	258	ASN
1	I	326	GLN
1	K	326	GLN
1	C	306	HIS
2	D	333	GLU
1	E	306	HIS
2	H	333	GLU
1	E	326	GLN

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	280/338 (83%)	276 (99%)	4 (1%)	78	94
1	C	283/338 (84%)	275 (97%)	8 (3%)	56	84
1	E	284/338 (84%)	276 (97%)	8 (3%)	56	84
1	G	281/338 (83%)	277 (99%)	4 (1%)	78	94
1	I	287/338 (85%)	279 (97%)	8 (3%)	56	84
1	K	291/338 (86%)	286 (98%)	5 (2%)	73	93
2	B	289/326 (89%)	275 (95%)	14 (5%)	35	65
2	D	293/326 (90%)	278 (95%)	15 (5%)	33	62
2	F	294/326 (90%)	281 (96%)	13 (4%)	39	69
2	H	288/326 (88%)	272 (94%)	16 (6%)	30	56
2	J	292/326 (90%)	276 (94%)	16 (6%)	30	57
2	L	296/326 (91%)	281 (95%)	15 (5%)	33	62
3	M	4/11 (36%)	4 (100%)	0	100	100
3	N	4/11 (36%)	4 (100%)	0	100	100
All	All	3466/4006 (86%)	3340 (96%)	126 (4%)	47	77

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	PHE
1	A	71	GLU
1	A	214	ARG
1	A	287	ARG
2	B	39	ARG
2	B	113	THR
2	B	151	LEU
2	B	216	LEU
2	B	222	SER
2	B	232	LEU
2	B	236	LEU
2	B	255	ARG

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Mol	Chain	Res	Type
2	B	258	ASN
2	B	261	HIS
2	B	306	VAL
2	B	329	LEU
2	B	331	LEU
2	B	357	LEU
1	C	55	PHE
1	C	59	ASP
1	C	71	GLU
1	C	81	ASN
1	C	182	PRO
1	C	287	ARG
1	C	324	GLU
1	C	364	GLN
2	D	21	LEU
2	D	39	ARG
2	D	110	ASN
2	D	151	LEU
2	D	216	LEU
2	D	222	SER
2	D	232	LEU
2	D	236	LEU
2	D	255	ARG
2	D	258	ASN
2	D	261	HIS
2	D	306	VAL
2	D	329	LEU
2	D	331	LEU
2	D	353	ARG
1	E	55	PHE
1	E	67	ARG
1	E	71	GLU
1	E	121	ARG
1	E	211	GLN
1	E	214	ARG
1	E	287	ARG
1	E	324	GLU
2	F	21	LEU
2	F	39	ARG
2	F	151	LEU
2	F	216	LEU
2	F	232	LEU

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Mol	Chain	Res	Type
2	F	236	LEU
2	F	255	ARG
2	F	258	ASN
2	F	261	HIS
2	F	306	VAL
2	F	329	LEU
2	F	331	LEU
2	F	353	ARG
1	G	71	GLU
1	G	224	ASP
1	G	287	ARG
1	G	324	GLU
2	H	18	LEU
2	H	21	LEU
2	H	91	ASP
2	H	151	LEU
2	H	216	LEU
2	H	222	SER
2	H	232	LEU
2	H	236	LEU
2	H	255	ARG
2	H	258	ASN
2	H	261	HIS
2	H	306	VAL
2	H	329	LEU
2	H	331	LEU
2	H	348	THR
2	H	357	LEU
1	I	55	PHE
1	I	67	ARG
1	I	71	GLU
1	I	142	ARG
1	I	194	ASN
1	I	211	GLN
1	I	287	ARG
1	I	364	GLN
2	J	21	LEU
2	J	27	ARG
2	J	31	ARG
2	J	151	LEU
2	J	216	LEU
2	J	222	SER

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Mol	Chain	Res	Type
2	J	232	LEU
2	J	236	LEU
2	J	255	ARG
2	J	258	ASN
2	J	261	HIS
2	J	306	VAL
2	J	329	LEU
2	J	331	LEU
2	J	353	ARG
2	J	357	LEU
1	K	55	PHE
1	K	71	GLU
1	K	142	ARG
1	K	287	ARG
1	K	324	GLU
2	L	21	LEU
2	L	33	LEU
2	L	65	ASP
2	L	110	ASN
2	L	151	LEU
2	L	216	LEU
2	L	232	LEU
2	L	236	LEU
2	L	255	ARG
2	L	258	ASN
2	L	261	HIS
2	L	306	VAL
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 (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	201	HIS
1	A	278	ASN
1	A	329	ASN
1	A	335	ASN
2	B	212	GLN
1	C	108	GLN
1	C	184	GLN

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Mol	Chain	Res	Type
1	C	218	ASN
1	C	298	GLN
1	C	335	ASN
1	C	364	GLN
2	D	212	GLN
2	D	246	ASN
1	E	184	GLN
1	E	201	HIS
1	E	298	GLN
2	F	212	GLN
2	F	246	ASN
1	G	80	GLN
1	G	89	GLN
1	G	162	GLN
1	G	201	HIS
1	G	297	ASN
1	G	325	ASN
2	H	212	GLN
2	H	296	ASN
1	I	89	GLN
1	I	135	HIS
1	I	285	GLN
1	I	364	GLN
2	J	30	GLN
2	J	208	ASN
2	J	212	GLN
2	J	246	ASN
1	K	135	HIS
1	K	218	ASN
1	K	298	GLN
2	L	212	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 23 ligands modelled in this entry, 15 are monoatomic - leaving 8 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
6	GRG	B	1721	-	28,28,28	0.91	1 (3%)	37,37,37	0.85	0
6	GRG	D	1722	-	28,28,28	0.90	1 (3%)	37,37,37	0.84	0
6	GRG	F	1723	-	28,28,28	0.90	1 (3%)	37,37,37	0.82	0
6	GRG	H	1724	-	28,28,28	0.83	1 (3%)	37,37,37	0.86	1 (2%)
6	GRG	J	1725	-	28,28,28	0.87	2 (7%)	37,37,37	0.84	1 (2%)
6	GRG	L	1726	-	28,28,28	0.91	1 (3%)	37,37,37	0.84	0
7	GER	M	1727	-	19,19,19	0.86	1 (5%)	22,22,22	0.72	0
7	GER	N	1727	-	19,19,19	0.89	2 (10%)	22,22,22	0.74	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
6	GRG	B	1721	-	-	0/31/31/31	0/0/0/0
6	GRG	D	1722	-	-	0/31/31/31	0/0/0/0
6	GRG	F	1723	-	-	0/31/31/31	0/0/0/0
6	GRG	H	1724	-	-	0/31/31/31	0/0/0/0
6	GRG	J	1725	-	-	0/31/31/31	0/0/0/0
6	GRG	L	1726	-	-	0/31/31/31	0/0/0/0
7	GER	M	1727	-	-	0/20/20/20	0/0/0/0
7	GER	N	1727	-	-	0/20/20/20	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1726	GRG	PB-O3A	-2.65	1.55	1.60
6	F	1723	GRG	PB-O3A	-2.39	1.56	1.60
6	B	1721	GRG	PB-O3A	-2.36	1.56	1.60
6	J	1725	GRG	PB-O3A	-2.17	1.56	1.60
7	N	1727	GER	C12-C13	2.11	1.37	1.32
7	M	1727	GER	C12-C13	2.09	1.37	1.32
6	H	1724	GRG	PB-O3A	-2.07	1.56	1.60
7	N	1727	GER	C7-C8	2.04	1.37	1.32
6	D	1722	GRG	C7-C8	2.01	1.37	1.32
6	J	1725	GRG	C7-C8	2.01	1.37	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	1725	GRG	PA-O1-C1	-2.05	117.08	120.36
6	H	1724	GRG	PA-O1-C1	-2.04	117.09	120.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	0.02	13 (4%) 35 38	35, 57, 92, 110	0
1	C	314/377 (83%)	-0.03	9 (2%) 49 53	33, 54, 80, 97	0
1	E	314/377 (83%)	0.16	15 (4%) 29 31	35, 59, 86, 103	0
1	G	314/377 (83%)	0.14	11 (3%) 42 45	35, 59, 87, 102	0
1	I	314/377 (83%)	-0.02	14 (4%) 32 34	29, 52, 84, 95	0
1	K	314/377 (83%)	-0.25	4 (1%) 74 78	23, 41, 67, 81	0
2	B	346/377 (91%)	0.02	16 (4%) 31 33	35, 52, 75, 100	0
2	D	346/377 (91%)	-0.01	11 (3%) 45 48	32, 46, 71, 95	0
2	F	346/377 (91%)	-0.00	12 (3%) 42 45	34, 47, 74, 101	0
2	H	346/377 (91%)	0.42	32 (9%) 9 8	36, 65, 95, 112	0
2	J	346/377 (91%)	0.09	17 (4%) 28 30	30, 50, 80, 104	0
2	L	346/377 (91%)	-0.07	10 (2%) 49 53	25, 40, 65, 93	0
3	M	4/11 (36%)	2.53	3 (75%) 0 0	60, 65, 73, 79	4 (100%)
3	N	4/11 (36%)	2.20	2 (50%) 0 0	59, 65, 74, 80	4 (100%)
All	All	3968/4546 (87%)	0.04	169 (4%) 35 36	23, 52, 84, 112	8 (0%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	306	HIS	5.7
2	J	108	SER	5.0
2	H	363	THR	5.0
1	G	306	HIS	5.0
2	D	363	THR	4.9
2	H	112	GLY	4.7
1	E	91	ILE	4.7
1	E	306	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	304	PRO	4.6
1	G	55	PHE	4.6
1	G	305	SER	4.5
2	B	363	THR	4.4
2	H	361	TRP	4.4
1	G	304	PRO	4.3
2	J	86	ASP	4.2
1	A	304	PRO	4.1
2	F	112	GLY	4.0
2	H	111	PRO	4.0
2	H	65	ASP	4.0
1	I	328	ASP	3.9
2	H	304	ARG	3.9
2	J	111	PRO	3.9
2	H	86	ASP	3.7
2	F	113	THR	3.7
2	J	84	THR	3.7
2	B	113	THR	3.6
1	C	305	SER	3.6
2	B	37	PRO	3.6
1	E	304	PRO	3.6
3	M	508	CYS	3.6
2	H	38	GLU	3.6
2	F	363	THR	3.5
1	A	328	ASP	3.5
2	D	110	ASN	3.5
2	H	362	LYS	3.5
2	H	360	SER	3.5
2	L	363	THR	3.5
1	I	306	HIS	3.4
1	A	306	HIS	3.3
1	E	328	ASP	3.3
2	L	86	ASP	3.3
1	E	368	SER	3.3
2	H	314	ASP	3.3
2	H	88	SER	3.2
1	I	368	SER	3.2
2	B	111	PRO	3.1
2	B	110	ASN	3.1
2	F	37	PRO	3.1
2	H	108	SER	3.1
2	L	108	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	55	PHE	3.1
2	F	88	SER	3.1
2	D	111	PRO	3.1
1	I	304	PRO	3.1
1	A	91	ILE	3.1
3	N	608	CYS	3.0
2	H	305	LEU	3.0
2	L	113	THR	3.0
1	I	305	SER	3.0
3	M	510	ILE	3.0
2	B	86	ASP	3.0
2	H	114	ALA	2.9
1	E	55	PHE	2.9
2	H	71	ASP	2.9
2	D	362	LYS	2.9
2	J	363	THR	2.9
1	K	306	HIS	2.9
2	B	362	LYS	2.9
1	E	331	GLU	2.8
2	J	88	SER	2.8
1	G	329	ASN	2.8
2	F	111	PRO	2.8
2	J	112	GLY	2.8
1	E	314	PHE	2.8
2	J	85	GLU	2.8
2	L	110	ASN	2.8
2	H	84	THR	2.7
1	E	305	SER	2.7
1	A	301	ASP	2.7
2	L	111	PRO	2.7
1	K	305	SER	2.7
1	G	330	LYS	2.7
2	J	110	ASN	2.7
2	L	84	THR	2.7
1	G	91	ILE	2.7
2	H	316	HIS	2.7
1	I	84	PRO	2.6
2	H	110	ASN	2.6
1	E	326	GLN	2.6
2	H	35	VAL	2.6
1	A	329	ASN	2.6
2	D	113	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	329	ASN	2.6
2	H	40	TYR	2.6
2	H	127	THR	2.6
2	H	87	ARG	2.6
2	H	85	GLU	2.5
2	B	114	ALA	2.5
1	I	329	ASN	2.5
3	N	609	VAL	2.5
1	C	330	LYS	2.5
3	M	511	LEU	2.5
1	A	330	LYS	2.5
2	B	84	THR	2.5
2	D	314	ASP	2.5
1	A	314	PHE	2.4
2	F	39	ARG	2.4
1	E	313	ALA	2.4
2	J	360	SER	2.4
1	E	330	LYS	2.4
2	H	356	ASP	2.4
1	I	326	GLN	2.4
2	D	65	ASP	2.4
1	C	331	GLU	2.4
2	F	84	THR	2.4
2	D	305	LEU	2.4
2	H	359	GLN	2.4
1	E	365	SER	2.4
1	I	364	GLN	2.3
2	B	112	GLY	2.3
2	H	37	PRO	2.3
2	D	114	ALA	2.3
1	A	326	GLN	2.3
2	H	109	LYS	2.3
1	A	331	GLU	2.3
2	H	113	THR	2.3
2	F	314	ASP	2.3
2	J	359	GLN	2.3
2	B	316	HIS	2.3
1	G	368	SER	2.3
2	J	314	ASP	2.2
1	A	305	SER	2.2
1	C	347	GLU	2.2
1	G	92	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	86	ASP	2.2
2	H	237	GLU	2.2
2	H	157	GLU	2.2
2	J	237	GLU	2.2
1	G	326	GLN	2.2
1	G	365	SER	2.2
2	J	107	PRO	2.2
1	I	85	SER	2.2
2	B	360	SER	2.2
2	B	38	GLU	2.2
1	K	304	PRO	2.2
1	C	327	CYS	2.2
1	I	332	ASP	2.2
1	A	368	SER	2.1
1	I	83	GLY	2.1
2	B	109	LYS	2.1
2	F	305	LEU	2.1
2	B	87	ARG	2.1
1	K	85	SER	2.1
2	J	127	THR	2.1
2	D	86	ASP	2.1
1	E	327	CYS	2.1
2	D	37	PRO	2.1
2	J	109	LYS	2.1
2	L	85	GLU	2.1
2	L	114	ALA	2.1
2	H	312	TRP	2.1
2	F	40	TYR	2.1
2	B	314	ASP	2.0
2	L	314	ASP	2.0
1	E	278	ASN	2.0
1	A	367	HIS	2.0
1	I	327	CYS	2.0
2	J	362	LYS	2.0
1	I	367	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	CL	C	1705	1/1	0.23	4.39	55,55,55,55	0
7	GER	N	1727	20/20	0.36	1.94	63,70,82,82	20
7	GER	M	1727	20/20	0.32	1.18	67,74,81,82	20
5	CL	G	1711	1/1	0.18	1.16	55,55,55,55	0
6	GRG	L	1726	29/29	0.21	0.25	37,42,53,58	0
6	GRG	B	1721	29/29	0.17	0.16	48,53,59,60	0
6	GRG	F	1723	29/29	0.16	0.07	47,52,59,59	0
6	GRG	J	1725	29/29	0.20	-0.11	38,44,55,58	0
6	GRG	D	1722	29/29	0.16	-0.16	42,48,55,57	0
6	GRG	H	1724	29/29	0.17	-0.21	52,57,72,73	0
4	ZN	B	378	1/1	0.09	-1.33	38,38,38,38	0
4	ZN	D	378	1/1	0.08	-1.42	37,37,37,37	0
4	ZN	H	378	1/1	0.09	-1.45	54,54,54,54	0
5	CL	D	1706	1/1	0.06	-1.59	41,41,41,41	0
4	ZN	F	378	1/1	0.07	-1.75	40,40,40,40	0
5	CL	L	1718	1/1	0.05	-1.96	43,43,43,43	0
5	CL	K	1717	1/1	0.09	-1.97	55,55,55,55	0
4	ZN	J	378	1/1	0.10	-2.07	35,35,35,35	0
5	CL	F	1709	1/1	0.08	-2.11	46,46,46,46	0
5	CL	B	1702	1/1	0.06	-2.14	64,64,64,64	0
5	CL	J	1715	1/1	0.06	-2.18	58,58,58,58	0
4	ZN	L	378	1/1	0.09	-2.65	27,27,27,27	0
5	CL	H	1712	1/1	0.06	-2.74	58,58,58,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.