



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:06 PM UTC

PDB ID : 3EMJ / pdb_00003emj
Title : 2.2 Å crystal structure of inorganic pyrophosphatase from rickettsia prowazekii (p21 form)
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2008-09-24
Resolution : 2.20 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

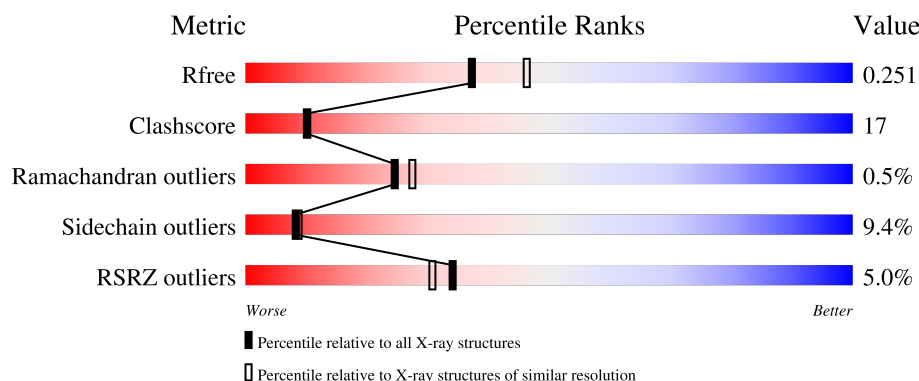
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	173	7% 68% 25% • •
1	B	173	7% 60% 31% 5% •
1	C	173	6% 68% 26% • •
1	D	173	7% 58% 30% 8% • •
1	E	173	8% 55% 32% • • 9%

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Mol	Chain	Length	Quality of chain
1	F	173	3% 51% 37% 8%
1	G	173	6% 65% 28%
1	H	173	7% 58% 35% 5%
1	I	173	5% 60% 27% 5% 8%
1	J	173	2% 71% 22%
1	K	173	2% 64% 27% 6%
1	L	173	3% 60% 25% 6% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16189 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 Inorganic pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	1	0
			1329	851	217	252	9			
1	B	166	Total	C	N	O	S	0	0	0
			1315	843	215	248	9			
1	C	168	Total	C	N	O	S	0	2	0
			1345	862	221	253	9			
1	D	170	Total	C	N	O	S	0	2	0
			1365	880	224	252	9			
1	E	158	Total	C	N	O	S	0	0	0
			1255	807	202	237	9			
1	F	160	Total	C	N	O	S	0	1	0
			1274	817	206	241	10			
1	G	166	Total	C	N	O	S	0	1	0
			1321	847	215	250	9			
1	H	170	Total	C	N	O	S	0	0	0
			1352	870	221	252	9			
1	I	160	Total	C	N	O	S	0	0	0
			1271	815	206	241	9			
1	J	167	Total	C	N	O	S	0	0	0
			1323	847	217	250	9			
1	K	168	Total	C	N	O	S	0	1	0
			1338	857	219	253	9			
1	L	158	Total	C	N	O	S	0	0	0
			1255	807	202	237	9			

There are 12 discrepancies between the modelled and reference sequences:

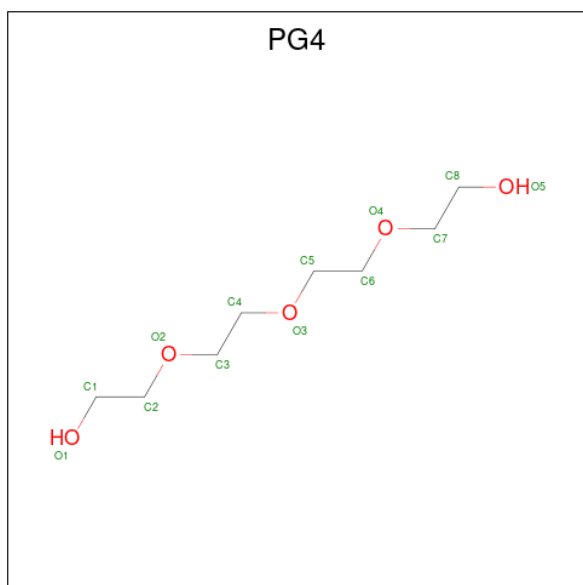
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9ZCW5
B	0	SER	-	expression tag	UNP Q9ZCW5
C	0	SER	-	expression tag	UNP Q9ZCW5
D	0	SER	-	expression tag	UNP Q9ZCW5
E	0	SER	-	expression tag	UNP Q9ZCW5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	expression tag	UNP Q9ZCW5
G	0	SER	-	expression tag	UNP Q9ZCW5
H	0	SER	-	expression tag	UNP Q9ZCW5
I	0	SER	-	expression tag	UNP Q9ZCW5
J	0	SER	-	expression tag	UNP Q9ZCW5
K	0	SER	-	expression tag	UNP Q9ZCW5
L	0	SER	-	expression tag	UNP Q9ZCW5

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			13	8	5		
2	L	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	33	Total	O	0	0
			33	33		
3	C	38	Total	O	0	0
			38	38		
3	D	30	Total	O	0	0
			30	30		

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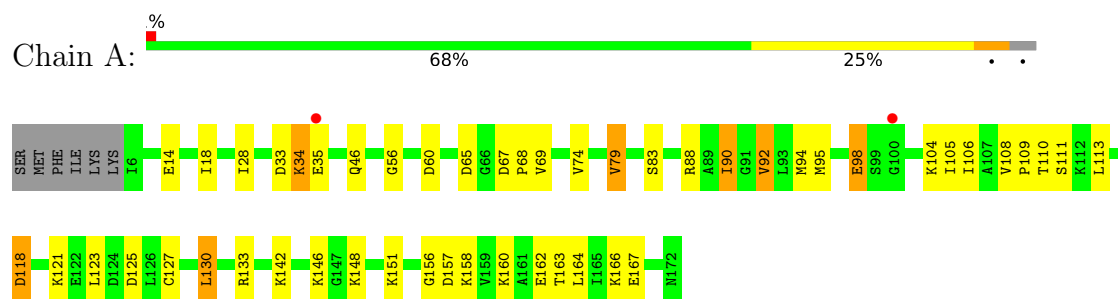
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	39	Total 39	O 39	0	0
3	F	17	Total 17	O 17	0	0
3	G	34	Total 34	O 34	0	0
3	H	29	Total 29	O 29	0	0
3	I	25	Total 25	O 25	0	0
3	J	54	Total 54	O 54	0	0
3	K	35	Total 35	O 35	0	0
3	L	39	Total 39	O 39	0	0

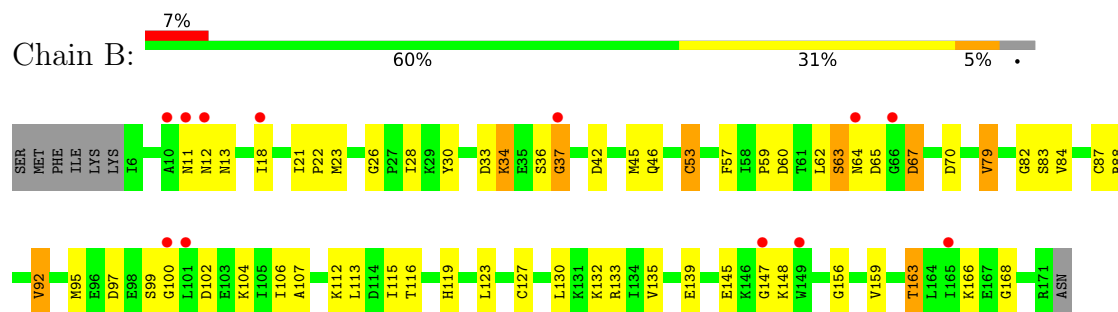
3 Residue-property plots [i](#)

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

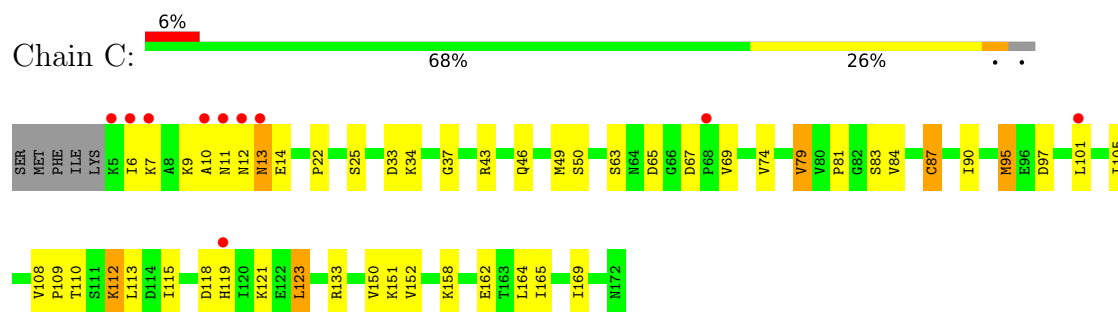
- Molecule 1: Inorganic pyrophosphatase



- Molecule 1: Inorganic pyrophosphatase



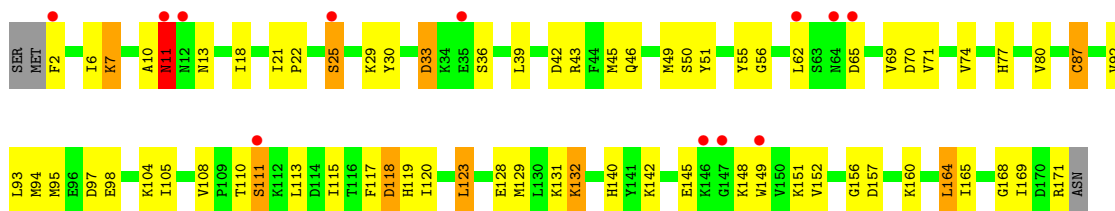
- Molecule 1: Inorganic pyrophosphatase



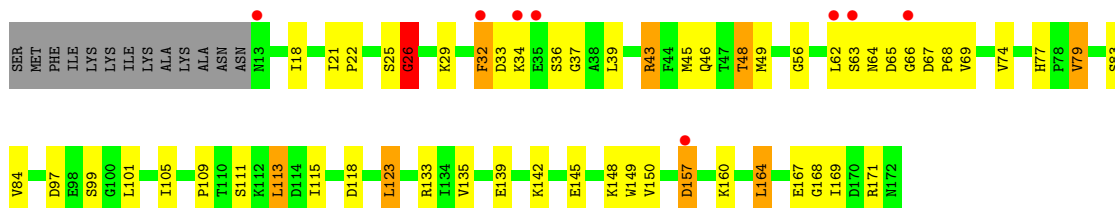
- Molecule 1: Inorganic pyrophosphatase



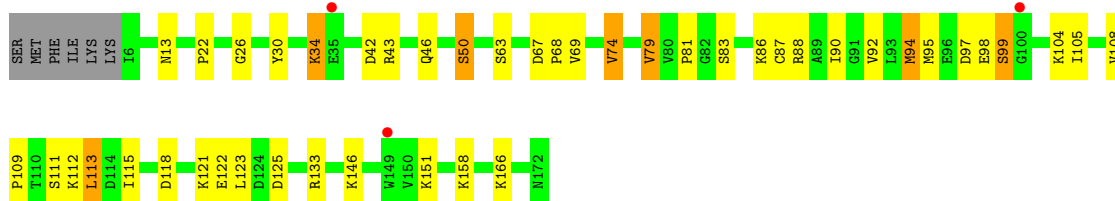




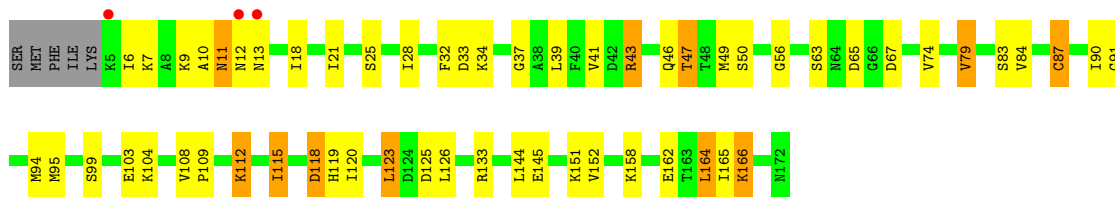
• Molecule 1: Inorganic pyrophosphatase



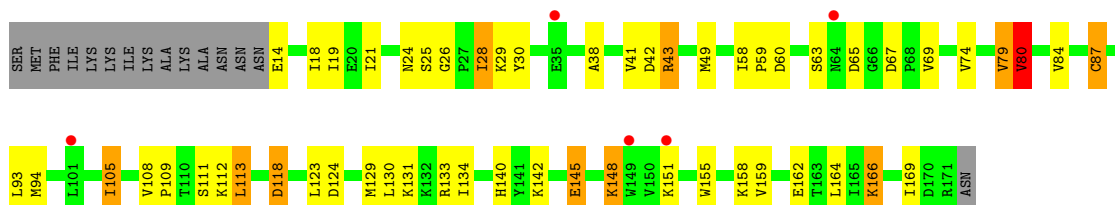
• Molecule 1: Inorganic pyrophosphatase



• Molecule 1: Inorganic pyrophosphatase



• Molecule 1: Inorganic pyrophosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.96Å 107.35Å 128.42Å 90.00° 96.05° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.7 (30.00-2.20) 93.6 (30.00-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.20Å)	Xtriage
Refinement program	REFMAC refmac_5.4.0069	Depositor
R, R_{free}	0.227 , 0.267 0.234 , 0.251	Depositor DCC
R_{free} test set	5186 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16189	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9026e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4

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	1.16	0/1359	1.19	4/1835 (0.2%)
1	B	1.13	0/1342	1.26	6/1812 (0.3%)
1	C	1.16	0/1379	1.25	3/1861 (0.2%)
1	D	1.10	2/1399 (0.1%)	1.29	11/1886 (0.6%)
1	E	1.25	1/1282 (0.1%)	1.27	6/1732 (0.3%)
1	F	1.10	2/1304 (0.2%)	1.20	5/1762 (0.3%)
1	G	1.17	2/1351 (0.1%)	1.20	1/1824 (0.1%)
1	H	1.15	0/1380	1.25	4/1861 (0.2%)
1	I	1.14	0/1298	1.19	4/1754 (0.2%)
1	J	1.16	1/1350 (0.1%)	1.19	0/1823
1	K	1.14	2/1368 (0.1%)	1.19	3/1846 (0.2%)
1	L	1.21	3/1282 (0.2%)	1.24	7/1732 (0.4%)
All	All	1.16	13/16094 (0.1%)	1.23	54/21728 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
1	J	0	1
All	All	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	21	ILE	CA-CB	7.37	1.59	1.54
1	K	165	ILE	CA-CB	6.34	1.61	1.54
1	L	105	ILE	CA-CB	-6.27	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	92	VAL	CA-CB	5.91	1.61	1.55
1	E	124	ASP	CB-CG	-5.85	1.37	1.52
1	K	21	ILE	CA-CB	5.50	1.58	1.54
1	D	89	ALA	CA-C	-5.44	1.45	1.52
1	D	108	VAL	C-O	-5.33	1.19	1.24
1	F	152	VAL	CA-CB	5.29	1.60	1.54
1	F	17	VAL	C-O	-5.27	1.18	1.24
1	L	124	ASP	CB-CG	-5.13	1.39	1.52
1	J	74	VAL	CA-CB	-5.12	1.47	1.53
1	G	21	ILE	CA-CB	5.02	1.58	1.54

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	GLY	CA-C-N	10.25	129.99	119.64
1	B	26	GLY	C-N-CA	10.25	129.99	119.64
1	A	108	VAL	CA-C-N	-8.57	111.55	120.03
1	A	108	VAL	C-N-CA	-8.57	111.55	120.03
1	B	67	ASP	CA-C-N	-8.04	112.37	120.98
1	B	67	ASP	C-N-CA	-8.04	112.37	120.98
1	F	156	GLY	CA-C-N	7.67	132.10	120.82
1	F	156	GLY	C-N-CA	7.67	132.10	120.82
1	I	26	GLY	CA-C-N	6.91	129.25	120.89
1	I	26	GLY	C-N-CA	6.91	129.25	120.89
1	E	28	ILE	N-CA-C	6.79	118.63	108.23
1	D	85	ILE	N-CA-C	6.74	117.60	108.17
1	I	169	ILE	CB-CA-C	-6.51	103.34	111.94
1	H	10	ALA	N-CA-C	-6.41	105.28	113.23
1	C	67	ASP	CA-C-N	-6.29	114.29	120.52
1	C	67	ASP	C-N-CA	-6.29	114.29	120.52
1	K	10	ALA	N-CA-C	-6.26	105.13	112.89
1	B	37	GLY	N-CA-C	-6.14	106.76	115.30
1	L	25	SER	N-CA-C	6.04	120.39	112.89
1	C	10	ALA	N-CA-C	-5.98	104.69	112.23
1	D	26	GLY	CA-C-N	5.95	126.83	120.47
1	D	26	GLY	C-N-CA	5.95	126.83	120.47
1	D	70	ASP	CB-CA-C	-5.93	98.55	109.46
1	E	77	HIS	CA-C-N	-5.75	114.69	120.21
1	E	77	HIS	C-N-CA	-5.75	114.69	120.21
1	E	18	ILE	CB-CA-C	-5.75	103.68	111.15
1	L	26	GLY	CA-C-N	-5.72	113.86	120.04
1	L	26	GLY	C-N-CA	-5.72	113.86	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	169	ILE	CB-CA-C	-5.70	104.36	112.22
1	K	25	SER	N-CA-C	5.64	120.16	113.16
1	A	130	LEU	N-CA-C	-5.61	105.24	111.36
1	F	26	GLY	CA-C-N	5.61	127.67	120.89
1	F	26	GLY	C-N-CA	5.61	127.67	120.89
1	L	28	ILE	N-CA-C	5.58	116.61	108.58
1	E	18	ILE	N-CA-CB	5.50	116.53	110.53
1	D	21	ILE	N-CA-C	5.49	116.38	107.71
1	G	154	GLY	N-CA-C	5.41	118.36	110.63
1	E	58	ILE	CB-CA-C	-5.39	104.94	110.71
1	A	98	GLU	N-CA-C	-5.38	106.67	113.18
1	L	80	VAL	CA-C-N	-5.37	114.22	119.76
1	L	80	VAL	C-N-CA	-5.37	114.22	119.76
1	D	28	ILE	N-CA-C	5.35	116.46	108.54
1	B	116	THR	N-CA-C	-5.30	106.65	113.01
1	H	74	VAL	CB-CA-C	-5.29	104.24	111.33
1	L	58	ILE	N-CA-C	5.27	113.09	107.76
1	H	71	VAL	N-CA-C	5.26	115.70	108.12
1	D	23	MET	CB-CA-C	-5.22	101.36	109.61
1	I	77	HIS	N-CA-C	5.19	114.81	108.11
1	D	111	SER	N-CA-C	-5.17	106.47	112.89
1	D	108	VAL	CA-C-N	-5.13	114.95	120.03
1	D	108	VAL	C-N-CA	-5.13	114.95	120.03
1	H	77	HIS	N-CA-C	5.09	114.16	108.25
1	D	10	ALA	N-CA-C	-5.09	107.07	113.28
1	K	28	ILE	N-CA-C	5.06	116.03	108.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	43	ARG	Peptide
1	D	13	ASN	Peptide
1	J	43	ARG	Peptide

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	1329	0	1335	37	0
1	B	1315	0	1323	43	0
1	C	1345	0	1355	38	0
1	D	1365	0	1393	59	0
1	E	1255	0	1258	71	0
1	F	1274	0	1275	56	0
1	G	1321	0	1329	54	0
1	H	1352	0	1369	61	0
1	I	1271	0	1270	54	0
1	J	1323	0	1329	29	0
1	K	1338	0	1348	55	0
1	L	1255	0	1258	43	0
2	E	13	0	18	2	0
2	L	13	0	18	4	0
3	A	47	0	0	1	0
3	B	33	0	0	3	0
3	C	38	0	0	0	0
3	D	30	0	0	1	0
3	E	39	0	0	3	0
3	F	17	0	0	1	0
3	G	34	0	0	0	0
3	H	29	0	0	1	0
3	I	25	0	0	1	0
3	J	54	0	0	0	0
3	K	35	0	0	4	0
3	L	39	0	0	2	0
All	All	16189	0	15878	546	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 17.

All (546) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:LYS:HB3	1:G:146:LYS:CG	1.57	1.31
1:D:111:SER:HB2	1:D:118:ASP:OD1	1.15	1.31
1:H:111:SER:HB2	1:H:118:ASP:OD1	1.11	1.27
1:K:158:LYS:HE2	1:K:162:GLU:OE2	1.42	1.20
1:K:43:ARG:NH1	1:K:145:GLU:OE2	1.75	1.19
1:C:95:MET:HE3	1:C:152:VAL:HG22	1.19	1.16
1:D:111:SER:CB	1:D:118:ASP:OD1	2.03	1.06
1:E:146:LYS:HB3	1:G:146:LYS:CB	1.88	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:111:SER:CB	1:H:118:ASP:OD1	2.06	1.02
1:B:159:VAL:O	1:B:163:THR:HG23	1.60	1.01
1:C:95:MET:CE	1:C:152:VAL:HG22	1.90	1.01
1:J:111:SER:OG	1:J:118:ASP:OD1	1.79	0.99
1:H:129:MET:HE3	1:H:129:MET:HA	1.42	0.98
1:C:158:LYS:HE2	1:C:162:GLU:OE2	1.66	0.96
1:J:86:LYS:HZ3	1:J:112:LYS:HZ3	1.06	0.96
1:E:146:LYS:HB3	1:G:146:LYS:CD	1.95	0.95
1:L:145:GLU:HG2	1:L:148:LYS:HB2	1.46	0.95
1:D:33:ASP:OD2	1:D:36:SER:OG	1.84	0.95
1:F:157:ASP:OD1	1:F:159:VAL:HG12	1.67	0.95
1:C:87:CYS:HB3	1:C:108:VAL:O	1.68	0.94
1:E:146:LYS:HB3	1:G:146:LYS:HG2	1.49	0.93
1:B:63:SER:HB3	1:B:65:ASP:OD1	1.70	0.90
1:L:111:SER:OG	1:L:118:ASP:OD1	1.89	0.89
1:I:157:ASP:H	1:I:160:LYS:HD2	1.37	0.89
1:E:146:LYS:CB	1:G:146:LYS:CG	2.49	0.88
1:F:17:VAL:HG21	1:F:87[B]:CYS:SG	2.14	0.87
1:H:33:ASP:OD2	1:H:36:SER:OG	1.93	0.87
1:B:63:SER:CB	1:B:65:ASP:OD1	2.23	0.86
1:G:159:VAL:O	1:G:163:THR:HG23	1.75	0.86
1:E:96:GLU:HG2	1:E:100:GLY:O	1.76	0.85
1:G:85:ILE:HD12	1:G:113:LEU:HD12	1.57	0.84
1:E:96:GLU:CG	1:E:100:GLY:O	2.25	0.84
1:E:146:LYS:HB3	1:G:146:LYS:HB3	1.57	0.84
1:E:70:ASP:OD2	1:E:104:LYS:NZ	2.09	0.84
1:I:79:VAL:HG13	1:I:83:SER:OG	1.79	0.82
1:D:129:MET:HE2	1:E:144:LEU:HD13	1.61	0.82
1:D:7:LYS:HE2	1:D:7:LYS:H	1.43	0.82
1:K:79:VAL:HG13	1:K:83:SER:OG	1.79	0.82
1:G:63:SER:OG	1:G:65:ASP:OD1	1.96	0.81
1:J:86:LYS:HZ3	1:J:112:LYS:NZ	1.78	0.81
1:K:63:SER:HB2	1:K:65:ASP:OD1	1.81	0.80
1:J:87:CYS:HB3	1:J:108:VAL:O	1.81	0.80
1:H:11:ASN:HD22	1:H:13:ASN:H	1.27	0.80
1:A:69:VAL:CG1	1:A:105:ILE:HD12	2.12	0.79
1:I:25:SER:O	1:I:26:GLY:O	1.99	0.79
1:D:87:CYS:HB3	1:D:108:VAL:O	1.81	0.79
1:L:111:SER:OG	1:L:118:ASP:CG	2.25	0.79
1:F:17:VAL:CG2	1:F:87[B]:CYS:SG	2.71	0.79
1:E:146:LYS:CB	1:G:146:LYS:HB3	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:ARG:HH22	1:H:142:LYS:HD3	1.48	0.78
1:H:69:VAL:CG1	1:H:105:ILE:HD12	2.13	0.78
1:F:79:VAL:HG13	1:F:83:SER:OG	1.84	0.77
1:C:95:MET:CE	1:C:152:VAL:CG2	2.62	0.77
1:B:42:ASP:O	1:F:113:LEU:HD22	1.84	0.76
1:E:145:GLU:HG2	1:E:148:LYS:HB2	1.67	0.76
1:K:158:LYS:CE	1:K:162:GLU:OE2	2.30	0.76
1:A:69:VAL:CG1	1:A:105:ILE:CD1	2.65	0.75
1:A:79:VAL:HG13	1:A:83:SER:OG	1.86	0.75
1:E:18:ILE:N	1:E:18:ILE:HD13	2.01	0.75
1:E:98:GLU:HA	1:E:149:TRP:CZ2	2.21	0.75
1:E:146:LYS:CB	1:G:146:LYS:HG2	2.16	0.75
1:H:165:ILE:O	1:H:169:ILE:HG13	1.85	0.75
1:E:111:SER:OG	1:E:118:ASP:CG	2.30	0.74
1:K:87:CYS:CB	1:K:108:VAL:O	2.35	0.74
1:H:46:GLN:O	1:L:133:ARG:HD3	1.87	0.74
1:G:85:ILE:HD12	1:G:113:LEU:CD1	2.17	0.74
1:H:87:CYS:HB3	1:H:108:VAL:O	1.88	0.74
1:C:79:VAL:HG13	1:C:83:SER:OG	1.88	0.73
1:D:46:GLN:O	1:E:133:ARG:HD3	1.87	0.73
1:H:95:MET:HE3	1:H:104:LYS:HE2	1.69	0.73
1:J:79:VAL:HG13	1:J:83:SER:OG	1.87	0.73
1:E:14:GLU:OE1	3:E:186:HOH:O	2.07	0.73
1:E:146:LYS:CB	1:G:146:LYS:CD	2.66	0.72
1:E:166:LYS:NZ	1:E:170:ASP:OD2	2.23	0.72
1:A:69:VAL:HG11	1:A:105:ILE:CD1	2.20	0.72
1:C:7:LYS:HE2	1:C:9:LYS:O	1.89	0.72
1:D:73:VAL:HG11	1:D:85:ILE:HD13	1.70	0.72
1:I:69:VAL:CG1	1:I:105:ILE:HD13	2.20	0.71
1:J:69:VAL:CG1	1:J:105:ILE:HD13	2.20	0.71
1:K:43:ARG:HH11	1:K:145:GLU:CD	1.99	0.71
1:J:86:LYS:NZ	1:J:112:LYS:HZ3	1.85	0.71
1:L:24:ASN:OD1	3:L:211:HOH:O	2.07	0.70
1:E:111:SER:OG	1:E:118:ASP:OD1	2.09	0.70
1:D:13:ASN:HB3	1:D:14:GLU:HG3	1.73	0.69
1:G:85:ILE:CD1	1:G:113:LEU:HD12	2.22	0.69
1:C:95:MET:HE3	1:C:152:VAL:CG2	2.11	0.69
1:I:157:ASP:HB2	1:I:160:LYS:HG3	1.74	0.69
1:A:90:ILE:HD13	1:A:106:ILE:O	1.93	0.69
1:C:50:SER:H	1:F:48:THR:HG23	1.57	0.69
1:F:32:PHE:CE1	1:F:39:LEU:HD13	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:159:VAL:HG23	3:L:191:HOH:O	1.92	0.68
1:B:159:VAL:O	1:B:163:THR:CG2	2.39	0.68
1:K:43:ARG:NH1	1:K:145:GLU:CD	2.52	0.67
1:D:25:SER:O	1:D:50:SER:HB3	1.95	0.67
1:E:145:GLU:HG2	1:E:148:LYS:HD2	1.76	0.67
1:G:98:GLU:HA	1:G:149:TRP:CZ2	2.29	0.67
1:E:147:GLY:O	1:E:148:LYS:HG3	1.95	0.67
1:E:145:GLU:CG	1:E:148:LYS:HD2	2.25	0.66
1:A:46:GLN:O	1:B:133:ARG:HD3	1.94	0.66
1:H:43:ARG:NH2	1:H:142:LYS:HD3	2.11	0.66
1:E:69:VAL:CG1	1:E:105:ILE:HD12	2.26	0.66
1:D:7:LYS:H	1:D:7:LYS:CE	2.09	0.66
1:I:133:ARG:HD3	1:K:46:GLN:O	1.96	0.66
1:F:118:ASP:O	1:F:121:LYS:NZ	2.28	0.66
1:F:45:MET:HE3	3:F:178:HOH:O	1.95	0.65
1:D:2:PHE:HD2	1:D:6:ILE:HD11	1.62	0.65
1:K:87:CYS:HB3	1:K:108:VAL:O	1.96	0.65
1:G:95:MET:HE1	1:G:104:LYS:HE2	1.79	0.64
1:I:167:GLU:O	1:I:171:ARG:HB2	1.97	0.64
1:A:111:SER:HG	1:A:118:ASP:CG	2.05	0.64
1:C:63:SER:HB2	1:C:65:ASP:OD1	1.97	0.64
1:L:131:LYS:HE3	2:L:173:PG4:H51	1.78	0.64
1:C:69:VAL:CG1	1:C:105:ILE:HD12	2.28	0.64
1:H:69:VAL:HG12	1:H:105:ILE:HD12	1.79	0.64
1:C:69:VAL:CG1	1:C:105:ILE:CD1	2.76	0.63
1:D:129:MET:HA	1:D:129:MET:HE3	1.79	0.63
1:E:95:MET:HG2	1:E:152:VAL:HG22	1.80	0.63
1:K:11:ASN:ND2	1:K:13:ASN:H	1.97	0.63
1:H:69:VAL:HG11	1:H:105:ILE:CD1	2.29	0.63
1:E:146:LYS:HB3	1:G:146:LYS:HD3	1.81	0.63
1:L:169:ILE:HG22	1:L:169:ILE:O	1.99	0.63
1:J:86:LYS:NZ	1:J:112:LYS:NZ	2.43	0.62
1:B:18:ILE:HG21	1:B:57:PHE:CZ	2.34	0.62
1:B:63:SER:HB2	1:B:65:ASP:OD1	1.98	0.62
1:H:129:MET:HA	1:H:129:MET:CE	2.24	0.62
1:E:79:VAL:HG13	1:E:83:SER:OG	1.99	0.62
1:L:131:LYS:CE	2:L:173:PG4:H51	2.30	0.62
1:D:7:LYS:HE2	1:D:7:LYS:N	2.13	0.62
1:E:158:LYS:HE2	3:E:199:HOH:O	2.00	0.62
1:K:7:LYS:HE2	1:K:9:LYS:O	2.00	0.62
1:H:129:MET:HE3	1:H:129:MET:CA	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:ASP:OD1	1:E:67:ASP:HB2	2.00	0.61
1:L:155:TRP:HE1	2:L:173:PG4:C2	2.12	0.61
1:C:46:GLN:O	1:F:133:ARG:HD3	2.01	0.61
1:I:142:LYS:HE3	1:I:148:LYS:HB3	1.83	0.61
1:F:25:SER:O	1:F:26:GLY:O	2.19	0.61
1:H:2:PHE:O	1:H:6:ILE:HG13	2.01	0.60
1:K:87:CYS:HB2	1:K:108:VAL:O	2.01	0.60
1:D:129:MET:HE3	1:D:132:LYS:HB2	1.82	0.60
1:I:157:ASP:HB3	1:I:160:LYS:H	1.66	0.60
1:B:79:VAL:HG13	1:B:83:SER:OG	2.00	0.60
1:G:133:ARG:HD3	1:J:46:GLN:O	2.02	0.60
1:C:133:ARG:HD3	1:F:46:GLN:O	2.02	0.60
1:D:129:MET:CE	1:E:144:LEU:HD13	2.30	0.60
1:I:97:ASP:C	1:I:99:SER:H	2.09	0.60
1:I:157:ASP:CB	1:I:160:LYS:HG3	2.31	0.60
1:L:65:ASP:OD1	1:L:67:ASP:HB2	2.02	0.60
1:G:111:SER:HB3	1:G:115:ILE:HD12	1.84	0.60
1:B:95:MET:HE1	1:B:104:LYS:HE2	1.84	0.60
1:H:45:MET:HE3	3:H:184:HOH:O	2.01	0.59
1:H:95:MET:HB3	1:H:152:VAL:HA	1.83	0.59
1:F:97:ASP:C	1:F:99:SER:H	2.10	0.59
1:A:34:LYS:HD2	1:A:34:LYS:N	2.17	0.59
1:K:115:ILE:O	1:K:118:ASP:HB2	2.03	0.59
1:L:111:SER:CB	1:L:118:ASP:OD1	2.50	0.59
1:L:19:ILE:HG13	1:L:79:VAL:HG11	1.85	0.59
1:A:90:ILE:HD11	1:A:106:ILE:HG22	1.85	0.58
1:K:120:ILE:HD11	3:K:195:HOH:O	2.03	0.58
1:K:11:ASN:HD22	1:K:13:ASN:H	1.51	0.58
1:D:23:MET:HG3	1:D:53:CYS:HA	1.83	0.58
1:D:76:HIS:HD2	3:D:198:HOH:O	1.87	0.58
1:E:135:VAL:HG21	2:E:173:PG4:H12	1.84	0.58
1:L:155:TRP:HE1	2:L:173:PG4:H21	1.69	0.58
1:F:126:LEU:HB2	1:F:131:LYS:HE2	1.86	0.58
1:J:34:LYS:HE2	1:J:68:PRO:HG2	1.84	0.58
1:F:63:SER:OG	1:F:65:ASP:OD1	2.22	0.58
1:E:146:LYS:CB	1:G:146:LYS:HD3	2.34	0.57
1:K:34:LYS:HD2	1:K:34:LYS:N	2.18	0.57
1:F:157:ASP:H	1:F:160:LYS:HZ2	1.51	0.57
1:G:11:ASN:CG	1:G:12:ASN:H	2.12	0.57
1:G:41:VAL:HG12	1:I:113:LEU:HD13	1.86	0.57
1:C:69:VAL:HG11	1:C:105:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:112:LYS:HZ3	1:K:112:LYS:H	1.51	0.57
1:L:111:SER:HG	1:L:118:ASP:CG	2.07	0.57
1:I:79:VAL:CG1	1:I:83:SER:OG	2.53	0.57
1:F:79:VAL:CG1	1:F:83:SER:OG	2.51	0.57
1:D:156:GLY:CA	1:D:160:LYS:HD3	2.35	0.56
1:C:69:VAL:HG11	1:C:105:ILE:CD1	2.35	0.56
1:F:94:MET:HE2	1:F:155:TRP:C	2.29	0.56
1:C:11:ASN:HD22	1:C:12:ASN:N	2.03	0.56
1:F:135:VAL:O	1:F:139:GLU:HG3	2.05	0.56
1:G:95:MET:HG2	1:G:152:VAL:HG22	1.87	0.56
1:F:17:VAL:HG23	1:F:87[B]:CYS:SG	2.46	0.56
1:I:157:ASP:N	1:I:160:LYS:HD2	2.16	0.56
1:F:95:MET:HE1	1:F:104:LYS:HG3	1.88	0.56
1:G:18:ILE:HG21	1:G:57:PHE:CZ	2.41	0.56
1:H:95:MET:CE	1:H:104:LYS:HE2	2.35	0.56
1:H:98:GLU:HB3	1:H:149:TRP:NE1	2.21	0.56
1:I:64:ASN:C	1:I:66:GLY:H	2.12	0.56
1:K:11:ASN:HD22	1:K:13:ASN:N	2.03	0.56
1:E:145:GLU:CD	1:E:148:LYS:HD2	2.31	0.56
1:D:119:HIS:CD2	1:D:119:HIS:H	2.24	0.56
1:E:18:ILE:HD12	1:E:84:VAL:HG22	1.87	0.56
1:K:95:MET:HG2	1:K:152:VAL:HG22	1.88	0.55
1:D:76:HIS:HE1	1:D:116:THR:OG1	1.88	0.55
1:D:43[A]:ARG:NE	1:D:145:GLU:OE2	2.39	0.55
1:E:146:LYS:HD2	1:G:146:LYS:CB	2.37	0.55
1:E:147:GLY:O	1:E:148:LYS:HE2	2.06	0.55
1:C:14:GLU:OE1	1:C:112:LYS:HE2	2.06	0.55
1:F:111:SER:OG	1:F:118:ASP:OD1	2.08	0.55
1:D:19[B]:ILE:HG21	1:D:79:VAL:HG21	1.88	0.55
1:F:74:VAL:O	1:F:109:PRO:HD3	2.06	0.55
1:G:159:VAL:O	1:G:163:THR:CG2	2.51	0.55
1:D:19[B]:ILE:HG21	1:D:79:VAL:CG2	2.37	0.55
1:A:133:ARG:HD3	1:B:46:GLN:O	2.07	0.55
1:J:63:SER:HB2	1:J:67:ASP:O	2.07	0.55
1:A:34:LYS:HE2	1:A:68:PRO:HG2	1.89	0.54
1:C:34:LYS:HD2	1:C:34:LYS:N	2.21	0.54
1:H:2:PHE:CE2	1:H:18:ILE:HD13	2.41	0.54
1:K:11:ASN:HD22	1:K:11:ASN:C	2.16	0.54
1:D:11:ASN:HD22	1:D:13:ASN:H	1.56	0.54
1:G:42:ASP:O	1:I:113:LEU:HD22	2.07	0.54
1:G:46:GLN:O	1:J:133:ARG:HD3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:47:THR:OG1	1:K:49:MET:HG3	2.07	0.54
1:H:7:LYS:H	1:H:7:LYS:CE	2.21	0.54
1:I:48:THR:HG23	1:K:50:SER:H	1.73	0.54
1:E:115:ILE:O	1:E:118:ASP:HB2	2.06	0.54
1:I:32:PHE:CE1	1:I:39:LEU:HD13	2.43	0.54
1:F:69:VAL:CG1	1:F:105:ILE:HD13	2.38	0.54
1:I:160:LYS:O	1:I:164:LEU:HD22	2.08	0.54
1:C:115:ILE:O	1:C:118:ASP:HB2	2.07	0.54
1:J:113:LEU:HD13	1:K:41:VAL:HG12	1.89	0.54
1:B:127:CYS:HB3	1:B:130:LEU:HB3	1.89	0.53
1:D:2:PHE:HD2	1:D:6:ILE:CD1	2.20	0.53
1:F:142:LYS:HE2	1:F:150:VAL:HG23	1.89	0.53
1:D:19[B]:ILE:HG23	1:D:83:SER:O	2.08	0.53
1:D:43[A]:ARG:HG3	1:D:43[A]:ARG:HH11	1.73	0.53
1:H:69:VAL:HG11	1:H:105:ILE:HD12	1.85	0.53
1:K:95:MET:HE1	1:K:104:LYS:HG3	1.91	0.53
1:K:103:GLU:OE2	1:K:164:LEU:HD21	2.08	0.53
1:A:127:CYS:HB3	1:A:130:LEU:HB3	1.89	0.53
1:F:22:PRO:HB3	1:F:79:VAL:O	2.08	0.53
1:A:95:MET:HE1	1:A:104:LYS:HE2	1.90	0.53
1:E:146:LYS:HD2	1:G:146:LYS:HB3	1.89	0.53
1:H:11:ASN:ND2	1:H:13:ASN:H	2.02	0.53
1:E:96:GLU:HG3	1:E:100:GLY:O	2.05	0.53
1:L:14:GLU:OE2	1:L:14:GLU:HA	2.09	0.53
1:D:69:VAL:CG1	1:D:105:ILE:HD12	2.38	0.53
1:E:146:LYS:CD	1:G:146:LYS:HB3	2.39	0.53
1:E:69:VAL:CG1	1:E:105:ILE:CD1	2.87	0.53
1:F:33:ASP:OD2	1:F:36:SER:OG	2.17	0.53
1:I:18:ILE:HG12	1:I:84:VAL:HG22	1.91	0.53
1:C:50:SER:N	1:F:48:THR:HG23	2.24	0.52
1:A:163:THR:O	1:A:167:GLU:HG3	2.09	0.52
1:D:19[B]:ILE:HD11	1:D:21:ILE:C	2.34	0.52
1:D:25:SER:O	1:D:50:SER:CB	2.57	0.52
1:J:92:VAL:HG11	1:J:94:MET:HE3	1.90	0.52
1:L:87:CYS:HB3	1:L:108:VAL:O	2.09	0.52
1:E:96:GLU:HA	1:E:100:GLY:O	2.09	0.52
1:H:55:TYR:OH	1:H:70:ASP:OD2	2.28	0.52
1:K:11:ASN:HD22	1:K:12:ASN:N	2.08	0.52
1:C:9:LYS:NZ	1:C:13:ASN:HA	2.25	0.52
1:D:62:LEU:O	1:D:171:ARG:NH1	2.43	0.52
1:L:169:ILE:O	1:L:169:ILE:CG2	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:VAL:HG21	1:I:79:VAL:HG21	1.92	0.52
1:H:22:PRO:O	1:H:25:SER:HB2	2.10	0.52
1:I:48:THR:CG2	1:K:49:MET:HB3	2.40	0.52
1:K:6:ILE:HD11	1:L:38:ALA:CB	2.40	0.52
1:C:9:LYS:HZ1	1:C:13:ASN:HA	1.74	0.51
1:D:25:SER:O	1:D:26:GLY:O	2.27	0.51
1:F:167:GLU:HB3	1:F:171:ARG:HH22	1.75	0.51
1:L:142:LYS:HD3	1:L:148:LYS:HB3	1.92	0.51
1:B:63:SER:HB2	1:B:67:ASP:O	2.10	0.51
1:G:145:GLU:CD	1:G:148:LYS:HD2	2.36	0.51
1:E:69:VAL:HG12	1:E:105:ILE:HD12	1.91	0.51
1:H:156:GLY:CA	1:H:160:LYS:HD3	2.40	0.51
1:K:119:HIS:CE1	3:K:195:HOH:O	2.63	0.51
1:L:29:LYS:O	1:L:42:ASP:HB3	2.11	0.51
1:F:64:ASN:C	1:F:66:GLY:H	2.17	0.51
1:I:63:SER:OG	1:I:65:ASP:OD1	2.26	0.51
1:C:97:ASP:HB3	1:C:150:VAL:HG22	1.93	0.51
1:C:110:THR:OG1	1:C:112:LYS:HD2	2.11	0.51
1:I:48:THR:HG23	1:I:48:THR:O	2.10	0.51
1:B:28:ILE:HG21	1:B:30:TYR:CZ	2.47	0.50
1:E:93:LEU:HD13	1:E:155:TRP:CH2	2.46	0.50
1:F:167:GLU:HB3	1:F:171:ARG:NH2	2.26	0.50
1:F:119:HIS:CE1	1:F:120:ILE:HD11	2.46	0.50
1:A:14:GLU:CD	1:A:110:THR:HG21	2.36	0.50
1:E:112:LYS:H	1:E:112:LYS:HD2	1.77	0.50
1:L:63:SER:N	1:L:67:ASP:O	2.38	0.50
1:D:85:ILE:HG12	1:D:87:CYS:SG	2.52	0.49
1:H:21:ILE:HD12	1:H:51:TYR:CZ	2.47	0.49
1:C:119[A]:HIS:H	1:C:119[A]:HIS:CD2	2.30	0.49
1:E:146:LYS:CA	1:G:146:LYS:HB3	2.41	0.49
1:E:97:ASP:N	1:E:100:GLY:O	2.45	0.49
1:F:157:ASP:HB2	1:F:160:LYS:CE	2.42	0.49
1:K:119:HIS:H	1:K:119:HIS:CD2	2.30	0.49
1:F:48:THR:HG23	1:F:48:THR:O	2.11	0.49
1:C:69:VAL:HG12	1:C:105:ILE:HD12	1.94	0.49
1:F:65:ASP:OD1	1:F:67:ASP:HB2	2.12	0.49
1:D:2:PHE:O	1:D:6:ILE:HD12	2.12	0.49
1:F:24:ASN:HA	1:F:50:SER:HB3	1.95	0.49
1:E:34:LYS:HE2	1:E:68:PRO:HG2	1.95	0.49
1:I:32:PHE:CD1	1:I:39:LEU:HD13	2.48	0.49
1:D:95:MET:HB3	1:D:152:VAL:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43[A]:ARG:HG3	1:D:43[A]:ARG:NH1	2.28	0.48
1:J:95:MET:CE	1:J:104:LYS:HG2	2.42	0.48
1:L:18:ILE:HD12	1:L:84:VAL:HG22	1.95	0.48
1:E:111:SER:CB	1:E:118:ASP:OD1	2.61	0.48
1:I:49:MET:HG2	1:K:49:MET:HG2	1.95	0.48
1:C:90:ILE:HG13	1:C:123:LEU:HD13	1.96	0.48
1:B:33:ASP:O	1:B:37:GLY:N	2.37	0.48
1:D:11:ASN:HD22	1:D:11:ASN:C	2.21	0.48
1:F:160:LYS:O	1:F:164:LEU:HD22	2.13	0.48
1:J:111:SER:CB	1:J:118:ASP:OD1	2.61	0.48
1:K:79:VAL:HG21	1:L:41:VAL:HG21	1.96	0.48
1:A:33:ASP:OD2	1:A:33:ASP:C	2.57	0.48
1:B:18:ILE:CG2	1:B:57:PHE:CZ	2.97	0.48
1:C:22:PRO:HG3	1:C:81:PRO:HD3	1.95	0.48
1:F:157:ASP:HB3	1:F:160:LYS:H	1.79	0.48
1:I:45:MET:HE3	3:I:197:HOH:O	2.13	0.48
1:D:11:ASN:ND2	1:D:13:ASN:H	2.10	0.48
1:E:18:ILE:O	1:E:56:GLY:HA3	2.13	0.48
1:L:74:VAL:O	1:L:109:PRO:HD3	2.14	0.48
1:K:95:MET:CE	1:K:104:LYS:HG3	2.44	0.48
1:G:28:ILE:HG21	1:G:30:TYR:CZ	2.49	0.48
1:K:65:ASP:OD2	1:K:67:ASP:HB2	2.12	0.48
1:C:22:PRO:HB2	1:C:25:SER:HB3	1.96	0.47
1:C:49:MET:HG2	1:F:49:MET:HG2	1.96	0.47
1:D:63:SER:OG	1:D:67:ASP:O	2.32	0.47
1:E:88:ARG:NH2	1:E:117:PHE:O	2.47	0.47
1:E:146:LYS:CG	1:G:146:LYS:HD3	2.45	0.47
1:A:111:SER:OG	1:A:118:ASP:OD1	2.25	0.47
1:H:69:VAL:CG1	1:H:105:ILE:CD1	2.84	0.47
1:H:70:ASP:HB3	1:H:104:LYS:HG2	1.96	0.47
1:I:63:SER:HA	1:I:171:ARG:NH1	2.29	0.47
1:L:166:LYS:HB2	1:L:166:LYS:HE2	1.44	0.47
1:D:156:GLY:HA2	1:D:160:LYS:HD3	1.96	0.47
1:C:165:ILE:O	1:C:169:ILE:HG13	2.15	0.47
1:I:79:VAL:HG13	1:I:83:SER:HG	1.78	0.47
1:I:135:VAL:O	1:I:139:GLU:HG3	2.14	0.47
1:J:74:VAL:O	1:J:109:PRO:HD3	2.15	0.47
1:J:98:GLU:HG2	1:J:99:SER:N	2.30	0.47
1:B:145:GLU:O	1:B:148:LYS:HB2	2.15	0.47
1:C:6:ILE:HD13	1:C:84:VAL:HG21	1.97	0.47
1:I:97:ASP:C	1:I:99:SER:N	2.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:ASN:HD22	1:D:12:ASN:N	2.13	0.47
1:E:74:VAL:O	1:E:109:PRO:HD3	2.15	0.47
1:F:157:ASP:OD1	1:F:159:VAL:CG1	2.52	0.47
1:H:62:LEU:O	1:H:171:ARG:NH1	2.48	0.47
1:H:128:GLU:O	1:H:132:LYS:HD3	2.15	0.47
1:D:18:ILE:O	1:D:56:GLY:HA3	2.16	0.46
1:E:145:GLU:HG2	1:E:148:LYS:CB	2.42	0.46
1:I:63:SER:OG	1:I:67:ASP:O	2.33	0.46
1:H:129:MET:CE	1:H:132:LYS:HB2	2.45	0.46
1:B:11:ASN:ND2	1:B:12:ASN:H	2.12	0.46
1:G:74:VAL:O	1:G:109:PRO:HD3	2.16	0.46
1:H:157:ASP:H	1:H:160:LYS:HD3	1.80	0.46
1:K:6:ILE:HD13	1:K:84:VAL:HG21	1.97	0.46
1:K:112:LYS:O	1:L:43:ARG:NH2	2.49	0.46
1:B:18:ILE:HD12	1:B:84:VAL:HG22	1.97	0.46
1:B:18:ILE:HD11	1:B:82:GLY:O	2.15	0.46
1:K:11:ASN:ND2	1:K:13:ASN:N	2.62	0.46
1:K:91:GLY:HA3	1:K:123:LEU:CD2	2.44	0.46
1:C:79:VAL:CG1	1:C:83:SER:OG	2.62	0.46
1:I:115:ILE:O	1:I:118:ASP:HB2	2.15	0.46
1:G:97:ASP:OD1	1:G:97:ASP:C	2.57	0.46
1:A:69:VAL:HG12	1:A:105:ILE:HD12	1.94	0.46
1:B:135:VAL:O	1:B:139:GLU:HG3	2.16	0.46
1:F:157:ASP:HB2	1:F:160:LYS:HZ2	1.81	0.46
1:L:69:VAL:HG11	1:L:105:ILE:HD11	1.97	0.46
1:B:88:ARG:NH1	1:B:88:ARG:HG3	2.31	0.46
1:H:29:LYS:O	1:H:42:ASP:HB3	2.15	0.46
1:E:95:MET:CE	1:E:104:LYS:HG3	2.46	0.45
1:K:74:VAL:O	1:K:109:PRO:HD3	2.17	0.45
1:I:64:ASN:C	1:I:66:GLY:N	2.74	0.45
1:A:60:ASP:OD2	3:A:179:HOH:O	2.21	0.45
1:G:18:ILE:CG2	1:G:57:PHE:CZ	2.99	0.45
1:H:93:LEU:HD11	1:H:152:VAL:CG1	2.47	0.45
1:D:145:GLU:O	1:D:148:LYS:HB2	2.17	0.45
1:H:140:HIS:CE1	1:L:140:HIS:CE1	3.04	0.45
1:I:157:ASP:HB2	1:I:160:LYS:CG	2.43	0.45
1:B:88:ARG:HG3	1:B:88:ARG:HH11	1.81	0.45
1:D:65:ASP:OD1	1:D:65:ASP:C	2.59	0.45
1:I:22:PRO:HB3	1:I:79:VAL:O	2.16	0.45
1:A:18:ILE:O	1:A:56:GLY:HA3	2.17	0.45
1:H:129:MET:HE3	1:H:132:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:VAL:HG13	1:A:83:SER:HG	1.81	0.45
1:G:119:HIS:CD2	1:G:119:HIS:H	2.35	0.45
1:G:147:GLY:C	1:G:148:LYS:HG2	2.42	0.45
1:H:7:LYS:HE2	1:H:7:LYS:HB2	1.52	0.45
1:H:123:LEU:O	1:H:131:LYS:NZ	2.42	0.45
1:I:97:ASP:HB2	1:I:149:TRP:O	2.17	0.45
1:J:30:TYR:CZ	1:L:80:VAL:HG22	2.52	0.45
1:K:6:ILE:HD11	1:L:38:ALA:HB2	1.97	0.45
1:C:49:MET:HB3	1:F:48:THR:CG2	2.47	0.45
1:F:97:ASP:C	1:F:99:SER:N	2.73	0.45
1:F:157:ASP:H	1:F:160:LYS:NZ	2.15	0.45
1:G:92:VAL:HG13	1:G:156:GLY:HA3	1.98	0.45
1:L:18:ILE:HG12	1:L:59:PRO:HD3	1.98	0.45
1:B:57:PHE:HA	1:B:70:ASP:HA	1.99	0.44
1:B:23:MET:CB	1:B:53:CYS:HA	2.46	0.44
1:B:33:ASP:HB3	1:B:36:SER:OG	2.17	0.44
1:L:18:ILE:CD1	1:L:84:VAL:HG22	2.47	0.44
1:B:97:ASP:OD1	1:B:100:GLY:O	2.35	0.44
1:G:11:ASN:CG	1:G:12:ASN:N	2.74	0.44
1:G:72:LEU:HD12	1:G:106:ILE:CD1	2.47	0.44
1:K:166:LYS:HE2	1:K:166:LYS:HB2	1.56	0.44
1:D:98:GLU:HA	1:D:149:TRP:CE2	2.53	0.44
1:F:162:GLU:O	1:F:163:THR:C	2.61	0.44
1:I:33:ASP:O	1:I:37:GLY:N	2.48	0.44
1:J:122:GLU:O	1:J:125:ASP:HB2	2.18	0.44
1:D:76:HIS:CE1	1:D:116:THR:OG1	2.69	0.44
1:G:7:LYS:O	1:G:16:ASN:ND2	2.45	0.44
1:I:33:ASP:OD2	1:I:36:SER:OG	2.20	0.44
1:D:63:SER:OG	1:D:65:ASP:OD1	2.23	0.44
1:G:145:GLU:HG2	1:G:148:LYS:HG3	1.99	0.44
1:H:98:GLU:HB3	1:H:149:TRP:CD1	2.53	0.44
1:B:23:MET:HB3	1:B:53:CYS:HA	2.00	0.44
1:B:102:ASP:OD1	3:B:176:HOH:O	2.21	0.44
1:I:21:ILE:HA	1:I:22:PRO:HD3	1.82	0.44
1:I:97:ASP:O	1:I:99:SER:N	2.51	0.44
1:A:98:GLU:OE2	1:A:98:GLU:N	2.43	0.44
1:A:111:SER:OG	1:A:118:ASP:CG	2.61	0.44
1:E:15:ILE:HG21	1:E:165:ILE:HD13	1.99	0.44
1:F:33:ASP:HB2	1:F:40:PHE:CD1	2.52	0.44
1:J:22:PRO:HG3	1:J:81:PRO:HD3	2.00	0.44
1:L:158:LYS:HG2	1:L:162:GLU:OE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ASP:O	1:A:121:LYS:HE3	2.18	0.43
1:E:96:GLU:CA	1:E:100:GLY:O	2.65	0.43
1:I:67:ASP:HB3	1:I:68:PRO:HD2	2.00	0.43
1:G:18:ILE:HD11	1:G:82:GLY:HA2	1.99	0.43
1:A:156:GLY:HA3	1:A:160:LYS:HG2	2.00	0.43
1:A:157:ASP:O	1:A:160:LYS:HB3	2.18	0.43
1:E:14:GLU:CG	3:E:186:HOH:O	2.65	0.43
1:F:128:GLU:OE2	1:F:131:LYS:NZ	2.41	0.43
1:H:46:GLN:HG3	1:L:129:MET:HE3	2.00	0.43
1:I:48:THR:HG23	1:K:50:SER:N	2.32	0.43
1:K:13:ASN:HA	3:K:192:HOH:O	2.18	0.43
1:K:87:CYS:HB3	1:K:109:PRO:HA	2.00	0.43
1:L:19:ILE:HG21	1:L:79:VAL:HG12	1.99	0.43
1:B:12:ASN:HB3	1:B:13:ASN:HD22	1.83	0.43
1:E:59:PRO:O	1:E:60:ASP:HB2	2.18	0.43
1:C:113:LEU:HD22	1:E:42:ASP:O	2.19	0.43
1:F:156:GLY:CA	1:F:160:LYS:HD2	2.49	0.43
1:I:111:SER:OG	1:I:118:ASP:OD1	2.20	0.43
1:F:64:ASN:C	1:F:66:GLY:N	2.76	0.43
1:H:129:MET:HE3	1:H:132:LYS:HB2	2.01	0.43
1:B:132:LYS:NZ	3:B:193:HOH:O	2.52	0.43
1:H:97:ASP:CB	1:H:149:TRP:O	2.67	0.43
1:H:129:MET:HA	1:H:132:LYS:HD3	2.00	0.43
1:I:46:GLN:O	1:K:133:ARG:HD3	2.19	0.43
1:I:62:LEU:O	1:I:168:GLY:HA2	2.19	0.43
1:I:62:LEU:N	1:I:168:GLY:O	2.52	0.43
1:I:74:VAL:O	1:I:109:PRO:HD3	2.19	0.43
1:E:32:PHE:CE2	1:E:39:LEU:HD13	2.54	0.43
1:G:33:ASP:O	1:G:37:GLY:N	2.48	0.43
1:I:43:ARG:CZ	1:I:145:GLU:OE1	2.67	0.43
1:G:95:MET:CE	1:G:104:LYS:HE2	2.47	0.42
1:H:43:ARG:NH2	1:H:145:GLU:OE1	2.52	0.42
1:H:117:PHE:HA	1:H:120:ILE:HD12	2.00	0.42
1:K:32:PHE:CZ	1:K:39:LEU:HD13	2.54	0.42
1:K:33:ASP:O	1:K:37:GLY:N	2.48	0.42
1:H:149:TRP:HZ3	1:H:151:LYS:HG3	1.83	0.42
1:K:123:LEU:HD12	1:K:126:LEU:HD12	2.00	0.42
1:B:28:ILE:HG21	1:B:30:TYR:CE1	2.54	0.42
1:D:61:THR:HB	1:D:69:VAL:HG23	2.01	0.42
1:I:21:ILE:HD11	1:I:29:LYS:HG3	2.01	0.42
1:J:42:ASP:O	1:L:113:LEU:HD22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:130:LEU:O	1:L:134:ILE:HG13	2.19	0.42
1:A:74:VAL:O	1:A:109:PRO:HD3	2.20	0.42
1:E:146:LYS:HA	1:G:146:LYS:HB3	2.01	0.42
1:E:166:LYS:NZ	1:E:170:ASP:CG	2.77	0.42
1:K:47:THR:HG22	1:K:144:LEU:HG	2.00	0.42
1:A:34:LYS:N	1:A:34:LYS:CD	2.81	0.42
1:B:62:LEU:O	1:B:168:GLY:HA2	2.20	0.42
1:F:22:PRO:HG3	1:F:81:PRO:HD3	2.01	0.42
1:D:2:PHE:CE2	1:D:18:ILE:HD13	2.54	0.42
1:D:98:GLU:HA	1:D:149:TRP:CZ2	2.54	0.42
1:H:62:LEU:O	1:H:168:GLY:HA2	2.20	0.42
1:A:34:LYS:HD2	1:A:34:LYS:HA	1.78	0.42
1:B:33:ASP:O	1:B:34:LYS:C	2.61	0.42
1:C:33:ASP:O	1:C:37:GLY:N	2.49	0.42
1:D:164:LEU:HA	1:D:164:LEU:HD12	1.61	0.42
1:A:90:ILE:CD1	1:A:106:ILE:HG22	2.50	0.42
1:D:142:LYS:HB3	1:D:148:LYS:HB3	2.02	0.42
1:H:69:VAL:HG11	1:H:105:ILE:HD11	2.00	0.42
1:L:69:VAL:CG1	1:L:105:ILE:HD11	2.49	0.42
1:B:92:VAL:HG13	1:B:156:GLY:CA	2.50	0.41
1:B:147:GLY:O	1:B:148:LYS:HG2	2.20	0.41
1:E:112:LYS:H	1:E:112:LYS:CD	2.33	0.41
1:L:93:LEU:HD13	1:L:155:TRP:CH2	2.55	0.41
1:E:131:LYS:NZ	2:E:173:PG4:H51	2.34	0.41
1:F:170:ASP:C	1:F:172:ASN:N	2.77	0.41
1:I:18:ILE:O	1:I:56:GLY:HA3	2.21	0.41
1:J:26:GLY:H	1:J:50:SER:HB3	1.85	0.41
1:J:121:LYS:O	1:J:158:LYS:CE	2.69	0.41
1:K:18:ILE:O	1:K:56:GLY:HA3	2.20	0.41
1:K:47:THR:HG23	3:K:175:HOH:O	2.20	0.41
1:A:98:GLU:H	1:A:98:GLU:CD	2.25	0.41
1:G:11:ASN:O	1:G:12:ASN:C	2.62	0.41
1:A:92:VAL:HG21	1:A:160:LYS:HG3	2.02	0.41
1:F:18:ILE:HG12	1:F:84:VAL:HG22	2.02	0.41
1:H:42:ASP:O	1:H:43:ARG:HB3	2.21	0.41
1:H:49:MET:HG2	1:L:49:MET:HG2	2.02	0.41
1:A:65:ASP:OD1	1:A:67:ASP:HB2	2.20	0.41
1:D:36:SER:H	1:D:36:SER:HG	1.59	0.41
1:D:93:LEU:HA	1:D:93:LEU:HD12	1.77	0.41
1:J:151:LYS:HD2	1:J:151:LYS:HA	1.74	0.41
1:A:142:LYS:HD3	1:A:148:LYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:THR:HG22	1:A:167:GLU:OE2	2.19	0.41
1:B:119:HIS:CD2	1:B:119:HIS:H	2.39	0.41
1:C:74:VAL:O	1:C:109:PRO:HD3	2.21	0.41
1:D:29:LYS:O	1:D:42:ASP:HB3	2.21	0.41
1:D:157:ASP:OD1	1:D:159:VAL:N	2.54	0.41
1:F:28:ILE:HG21	1:F:30:TYR:CZ	2.56	0.41
1:F:157:ASP:H	1:F:160:LYS:HD2	1.85	0.41
1:H:94:MET:HB2	1:H:94:MET:HE2	1.79	0.41
1:E:63:SER:N	1:E:67:ASP:O	2.39	0.41
1:E:166:LYS:HZ1	1:E:170:ASP:CG	2.28	0.41
1:F:142:LYS:HE2	1:F:150:VAL:CG2	2.51	0.41
1:G:18:ILE:O	1:G:56:GLY:HA3	2.21	0.41
1:G:63:SER:OG	1:G:67:ASP:O	2.39	0.41
1:H:164:LEU:HD12	1:H:164:LEU:HA	1.79	0.41
1:B:59:PRO:O	1:B:60:ASP:CB	2.69	0.41
1:B:92:VAL:HG13	1:B:156:GLY:HA3	2.03	0.41
1:E:62:LEU:O	1:E:171:ARG:HD2	2.20	0.41
1:H:55:TYR:HE1	1:H:104:LYS:HD3	1.86	0.41
1:J:34:LYS:HD2	1:J:34:LYS:N	2.36	0.41
1:J:97:ASP:C	1:J:97:ASP:OD1	2.64	0.41
1:K:11:ASN:ND2	1:K:11:ASN:C	2.78	0.41
1:B:45:MET:HE3	3:B:173:HOH:O	2.21	0.40
1:H:119:HIS:H	1:H:119:HIS:CD2	2.39	0.40
1:J:79:VAL:HG13	1:J:83:SER:HG	1.83	0.40
1:F:157:ASP:HB2	1:F:160:LYS:HE3	2.03	0.40
1:H:18:ILE:O	1:H:56:GLY:HA3	2.21	0.40
1:H:110:THR:O	1:H:113:LEU:N	2.52	0.40
1:I:123:LEU:HD12	1:I:123:LEU:HA	1.85	0.40
1:D:70:ASP:OD2	1:D:104:LYS:NZ	2.55	0.40
1:D:98:GLU:H	1:D:98:GLU:CD	2.29	0.40
1:H:30:TYR:HB3	1:H:39:LEU:HD11	2.04	0.40
1:L:28:ILE:HG21	1:L:30:TYR:CZ	2.56	0.40
1:L:63:SER:C	1:L:65:ASP:N	2.80	0.40
1:A:158:LYS:O	1:A:162:GLU:HG3	2.21	0.40
1:E:146:LYS:CB	1:G:146:LYS:CB	2.70	0.40
1:G:41:VAL:CG1	1:I:113:LEU:HD13	2.50	0.40
1:I:142:LYS:HE2	1:I:150:VAL:HG23	2.03	0.40
1:J:115:ILE:O	1:J:118:ASP:HB2	2.22	0.40
1:B:21:ILE:HA	1:B:22:PRO:HD3	1.92	0.40
1:B:87:CYS:HB3	1:B:107:ALA:HB1	2.04	0.40
1:B:92:VAL:HA	1:B:106:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:PHE:CZ	1:E:39:LEU:HD13	2.56	0.40
1:H:93:LEU:HD11	1:H:152:VAL:HG11	2.02	0.40
1:K:9:LYS:HB3	1:K:11:ASN:O	2.22	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	166/173 (96%)	162 (98%)	4 (2%)	0	100	100
1	B	164/173 (95%)	157 (96%)	7 (4%)	0	100	100
1	C	168/173 (97%)	165 (98%)	3 (2%)	0	100	100
1	D	170/173 (98%)	161 (95%)	7 (4%)	2 (1%)	10	8
1	E	156/173 (90%)	151 (97%)	4 (3%)	1 (1%)	21	23
1	F	159/173 (92%)	147 (92%)	10 (6%)	2 (1%)	9	8
1	G	165/173 (95%)	158 (96%)	6 (4%)	1 (1%)	21	23
1	H	168/173 (97%)	161 (96%)	5 (3%)	2 (1%)	10	8
1	I	158/173 (91%)	152 (96%)	5 (3%)	1 (1%)	21	23
1	J	165/173 (95%)	157 (95%)	8 (5%)	0	100	100
1	K	167/173 (96%)	163 (98%)	3 (2%)	1 (1%)	21	23
1	L	156/173 (90%)	153 (98%)	3 (2%)	0	100	100
All	All	1962/2076 (94%)	1887 (96%)	65 (3%)	10 (0%)	24	27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	11	ASN

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Mol	Chain	Res	Type
1	F	26	GLY
1	H	11	ASN
1	I	26	GLY
1	D	26	GLY
1	G	11	ASN
1	H	65	ASP
1	F	35	GLU
1	E	146	LYS
1	K	118	ASP

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	150/155 (97%)	135 (90%)	15 (10%)	7	7
1	B	148/155 (96%)	135 (91%)	13 (9%)	9	10
1	C	152/155 (98%)	142 (93%)	10 (7%)	15	18
1	D	154/155 (99%)	132 (86%)	22 (14%)	3	3
1	E	142/155 (92%)	129 (91%)	13 (9%)	8	9
1	F	145/155 (94%)	134 (92%)	11 (8%)	12	14
1	G	149/155 (96%)	133 (89%)	16 (11%)	6	6
1	H	152/155 (98%)	137 (90%)	15 (10%)	7	8
1	I	144/155 (93%)	134 (93%)	10 (7%)	14	16
1	J	149/155 (96%)	137 (92%)	12 (8%)	11	12
1	K	151/155 (97%)	137 (91%)	14 (9%)	8	9
1	L	142/155 (92%)	127 (89%)	15 (11%)	6	6
All	All	1778/1860 (96%)	1612 (91%)	166 (9%)	8	9

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ILE

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Mol	Chain	Res	Type
1	A	34	LYS
1	A	35	GLU
1	A	79	VAL
1	A	88	ARG
1	A	90	ILE
1	A	92	VAL
1	A	94	MET
1	A	113	LEU
1	A	118	ASP
1	A	123	LEU
1	A	146	LYS
1	A	151	LYS
1	A	164	LEU
1	A	166	LYS
1	B	34	LYS
1	B	53	CYS
1	B	63	SER
1	B	64	ASN
1	B	79	VAL
1	B	92	VAL
1	B	99	SER
1	B	112	LYS
1	B	113	LEU
1	B	115	ILE
1	B	123	LEU
1	B	163	THR
1	B	166	LYS
1	C	13	ASN
1	C	79	VAL
1	C	87	CYS
1	C	95	MET
1	C	101	LEU
1	C	112	LYS
1	C	121	LYS
1	C	123	LEU
1	C	151	LYS
1	C	164	LEU
1	D	4	LYS
1	D	7	LYS
1	D	9	LYS
1	D	11	ASN
1	D	23	MET

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Mol	Chain	Res	Type
1	D	33	ASP
1	D	35	GLU
1	D	53	CYS
1	D	62	LEU
1	D	80	VAL
1	D	85	ILE
1	D	87	CYS
1	D	92	VAL
1	D	111	SER
1	D	112	LYS
1	D	113	LEU
1	D	115	ILE
1	D	118	ASP
1	D	123	LEU
1	D	148	LYS
1	D	159	VAL
1	D	164	LEU
1	E	18	ILE
1	E	35	GLU
1	E	60	ASP
1	E	79	VAL
1	E	87	CYS
1	E	94	MET
1	E	101	LEU
1	E	112	LYS
1	E	123	LEU
1	E	146	LYS
1	E	148	LYS
1	E	164	LEU
1	E	166	LYS
1	F	31	GLU
1	F	32	PHE
1	F	34	LYS
1	F	43	ARG
1	F	48	THR
1	F	62	LEU
1	F	79	VAL
1	F	113	LEU
1	F	123	LEU
1	F	158	LYS
1	F	164	LEU
1	G	7	LYS

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Mol	Chain	Res	Type
1	G	11	ASN
1	G	18	ILE
1	G	34	LYS
1	G	35	GLU
1	G	53	CYS
1	G	64	ASN
1	G	79	VAL
1	G	85	ILE
1	G	92	VAL
1	G	94	MET
1	G	99	SER
1	G	101	LEU
1	G	123	LEU
1	G	160	LYS
1	G	163	THR
1	H	7	LYS
1	H	11	ASN
1	H	25	SER
1	H	33	ASP
1	H	50	SER
1	H	80	VAL
1	H	87	CYS
1	H	92	VAL
1	H	111	SER
1	H	115	ILE
1	H	118	ASP
1	H	123	LEU
1	H	132	LYS
1	H	148	LYS
1	H	164	LEU
1	I	32	PHE
1	I	34	LYS
1	I	43	ARG
1	I	48	THR
1	I	79	VAL
1	I	101	LEU
1	I	113	LEU
1	I	123	LEU
1	I	157	ASP
1	I	164	LEU
1	J	13	ASN
1	J	34	LYS

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Mol	Chain	Res	Type
1	J	50	SER
1	J	79	VAL
1	J	88	ARG
1	J	90	ILE
1	J	94	MET
1	J	99	SER
1	J	113	LEU
1	J	123	LEU
1	J	146	LYS
1	J	166	LYS
1	K	11	ASN
1	K	43	ARG
1	K	47	THR
1	K	79	VAL
1	K	87	CYS
1	K	90	ILE
1	K	94	MET
1	K	99	SER
1	K	112	LYS
1	K	115	ILE
1	K	123	LEU
1	K	151	LYS
1	K	164	LEU
1	K	166	LYS
1	L	43	ARG
1	L	60	ASP
1	L	79	VAL
1	L	80	VAL
1	L	87	CYS
1	L	94	MET
1	L	112	LYS
1	L	113	LEU
1	L	118	ASP
1	L	123	LEU
1	L	145	GLU
1	L	148	LYS
1	L	151	LYS
1	L	164	LEU
1	L	166	LYS

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

Mol	Chain	Res	Type
1	A	11	ASN
1	A	64	ASN
1	A	76	HIS
1	A	119	HIS
1	B	11	ASN
1	B	13	ASN
1	B	24	ASN
1	B	119	HIS
1	C	11	ASN
1	D	11	ASN
1	D	76	HIS
1	D	119	HIS
1	E	119	HIS
1	F	76	HIS
1	F	119	HIS
1	G	24	ASN
1	G	119	HIS
1	H	11	ASN
1	H	16	ASN
1	H	76	HIS
1	H	77	HIS
1	H	119	HIS
1	I	76	HIS
1	I	119	HIS
1	J	11	ASN
1	J	13	ASN
1	J	76	HIS
1	J	119	HIS
1	K	11	ASN
1	K	13	ASN
1	K	76	HIS
1	K	119	HIS
1	L	77	HIS
1	L	119	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PG4	L	173	-	12,12,12	0.87	0	11,11,11	1.26	2 (18%)
2	PG4	E	173	-	12,12,12	0.71	0	11,11,11	1.00	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PG4	L	173	-	-	7/10/10/10	-
2	PG4	E	173	-	-	5/10/10/10	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	173	PG4	O3-C5-C6	2.38	121.22	110.35
2	L	173	PG4	O2-C2-C1	2.08	119.30	110.11
2	E	173	PG4	O3-C5-C6	2.01	119.53	110.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	173	PG4	O3-C5-C6-O4
2	L	173	PG4	O3-C5-C6-O4
2	E	173	PG4	O1-C1-C2-O2
2	E	173	PG4	C5-C6-O4-C7
2	E	173	PG4	C8-C7-O4-C6
2	L	173	PG4	C8-C7-O4-C6
2	L	173	PG4	O1-C1-C2-O2
2	L	173	PG4	C6-C5-O3-C4
2	E	173	PG4	C4-C3-O2-C2
2	L	173	PG4	C5-C6-O4-C7
2	L	173	PG4	C1-C2-O2-C3
2	L	173	PG4	O4-C7-C8-O5

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	173	PG4	4	0
2	E	173	PG4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	167/173 (96%)	0.35	2 (1%) 76 74	26, 45, 62, 68	1 (0%)
1	B	166/173 (95%)	0.70	12 (7%) 21 18	38, 46, 64, 68	0
1	C	168/173 (97%)	0.50	10 (5%) 27 24	26, 45, 64, 69	2 (1%)
1	D	170/173 (98%)	0.64	12 (7%) 22 19	25, 47, 65, 70	2 (1%)
1	E	158/173 (91%)	0.61	14 (8%) 15 13	35, 44, 62, 68	0
1	F	160/173 (92%)	0.58	6 (3%) 44 41	31, 47, 64, 69	1 (0%)
1	G	166/173 (95%)	0.65	11 (6%) 24 21	27, 46, 63, 68	1 (0%)
1	H	170/173 (98%)	0.70	12 (7%) 22 19	39, 47, 65, 69	0
1	I	160/173 (92%)	0.60	8 (5%) 34 31	39, 46, 64, 69	0
1	J	167/173 (96%)	0.40	3 (1%) 67 64	36, 44, 62, 68	0
1	K	168/173 (97%)	0.43	3 (1%) 67 64	28, 46, 65, 68	1 (0%)
1	L	158/173 (91%)	0.48	5 (3%) 50 47	36, 44, 62, 68	0
All	All	1978/2076 (95%)	0.55	98 (4%) 34 31	25, 46, 64, 70	8 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	100	GLY	5.0
1	E	149	TRP	4.6
1	K	13	ASN	4.1
1	G	149	TRP	3.9
1	E	146	LYS	3.8
1	B	10	ALA	3.8
1	C	13	ASN	3.8
1	C	101	LEU	3.7
1	B	66	GLY	3.5
1	D	100	GLY	3.5
1	C	12	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	J	100	GLY	3.4
1	A	35	GLU	3.3
1	C	5	LYS	3.3
1	E	145	GLU	3.3
1	D	13	ASN	3.2
1	E	147	GLY	3.1
1	I	35	GLU	3.1
1	G	10	ALA	3.0
1	E	43	ARG	3.0
1	B	11	ASN	2.9
1	L	35	GLU	2.9
1	F	34	LYS	2.9
1	I	157	ASP	2.9
1	I	32	PHE	2.8
1	G	146	LYS	2.8
1	E	63	SER	2.8
1	J	35	GLU	2.8
1	D	35	GLU	2.8
1	E	148	LYS	2.8
1	L	151	LYS	2.7
1	I	62	LEU	2.7
1	C	10	ALA	2.7
1	E	64	ASN	2.7
1	D	101	LEU	2.7
1	F	94	MET	2.7
1	F	32	PHE	2.7
1	G	6	ILE	2.6
1	G	101	LEU	2.6
1	D	149	TRP	2.6
1	B	12	ASN	2.6
1	D	2	PHE	2.6
1	A	100	GLY	2.6
1	B	18	ILE	2.6
1	D	25	SER	2.6
1	E	96	GLU	2.6
1	H	149	TRP	2.6
1	L	149	TRP	2.5
1	B	147	GLY	2.5
1	G	100	GLY	2.5
1	C	11	ASN	2.5
1	G	11	ASN	2.5
1	E	99	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	12	ASN	2.5
1	B	37	GLY	2.4
1	H	62	LEU	2.4
1	L	101	LEU	2.4
1	D	99	SER	2.3
1	H	2	PHE	2.3
1	F	62	LEU	2.3
1	H	35	GLU	2.3
1	B	100	GLY	2.3
1	F	157	ASP	2.3
1	L	64	ASN	2.3
1	H	25	SER	2.3
1	H	111	SER	2.3
1	E	32	PHE	2.3
1	I	34	LYS	2.3
1	C	119[A]	HIS	2.3
1	H	146	LYS	2.3
1	H	147	GLY	2.2
1	K	5	LYS	2.2
1	I	13	ASN	2.2
1	I	66	GLY	2.2
1	E	151	LYS	2.2
1	B	149	TRP	2.2
1	J	149	TRP	2.2
1	B	165	ILE	2.2
1	D	11	ASN	2.2
1	D	62	LEU	2.1
1	F	13	ASN	2.1
1	C	68	PRO	2.1
1	G	147	GLY	2.1
1	C	6	ILE	2.1
1	C	7	LYS	2.1
1	B	64	ASN	2.1
1	K	12	ASN	2.1
1	I	63	SER	2.1
1	G	151	LYS	2.1
1	H	11	ASN	2.1
1	H	64	ASN	2.1
1	H	65	ASP	2.1
1	G	99	SER	2.1
1	D	10	ALA	2.1
1	B	101	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	66	GLY	2.1
1	G	60	ASP	2.0
1	E	65	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PG4	L	173	13/13	0.85	0.14	44,50,59,59	0
2	PG4	E	173	13/13	0.92	0.11	43,48,50,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.