



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:28 AM GMT

PDB ID : 3EMJ  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

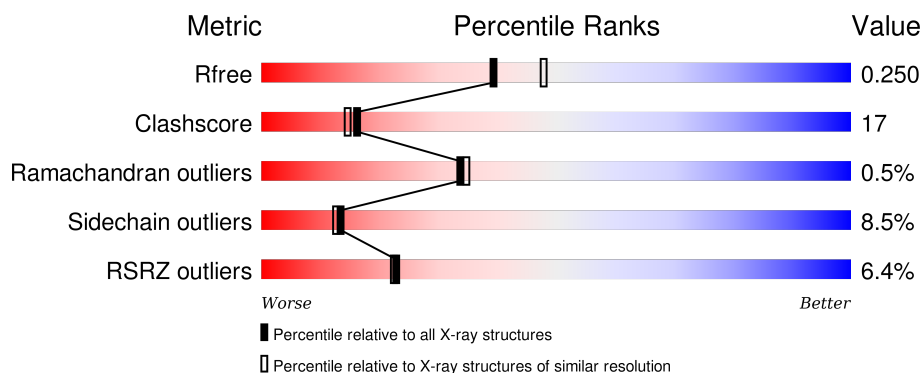
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	173	<div> <div>3%</div> <div>69% 25% ...</div> </div>
1	B	173	<div> <div>10%</div> <div>63% 28% 5% .</div> </div>
1	C	173	<div> <div>6%</div> <div>68% 25% . . .</div> </div>
1	D	173	<div> <div>6%</div> <div>60% 31% 6% . .</div> </div>
1	E	173	<div> <div>9%</div> <div>57% 28% 6% 9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	173	
1	G	173	
1	H	173	
1	I	173	
1	J	173	
1	K	173	
1	L	173	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PG4	L	173	-	-	-	X

## 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 (three-letter code: 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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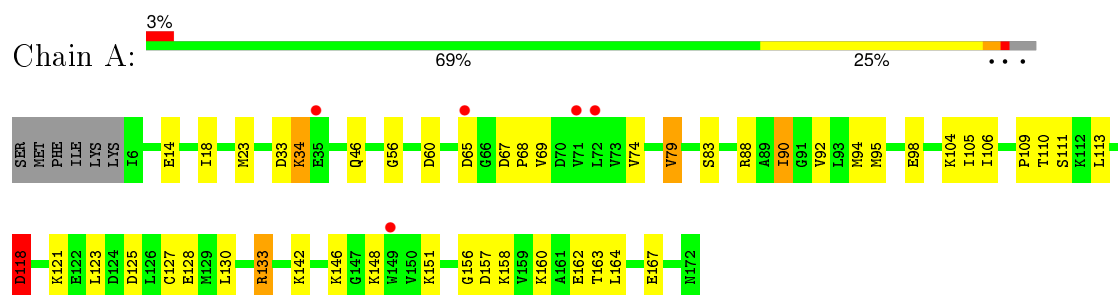
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	39	Total	O	0	0
			39	39		
3	F	17	Total	O	0	0
			17	17		
3	G	34	Total	O	0	0
			34	34		
3	H	29	Total	O	0	0
			29	29		
3	I	25	Total	O	0	0
			25	25		
3	J	54	Total	O	0	0
			54	54		
3	K	35	Total	O	0	0
			35	35		
3	L	39	Total	O	0	0
			39	39		

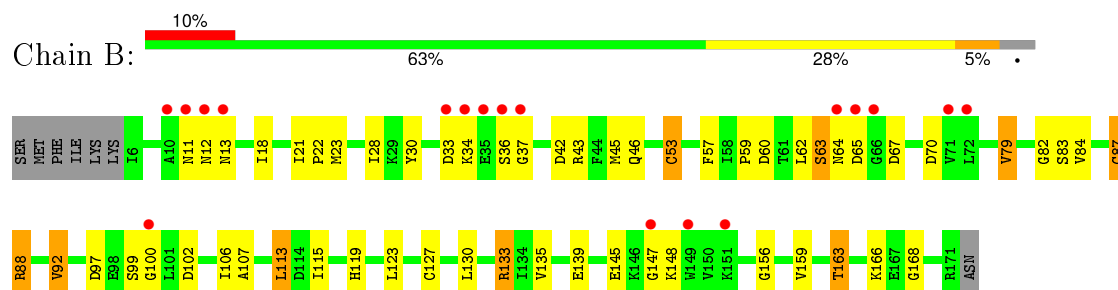
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

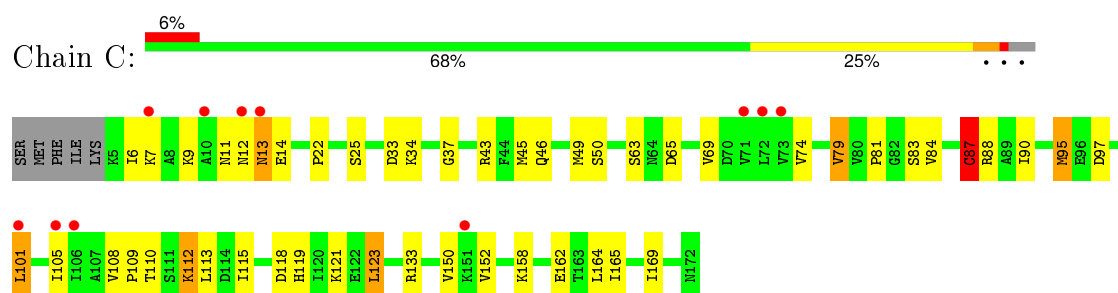
#### • Molecule 1: Inorganic pyrophosphatase



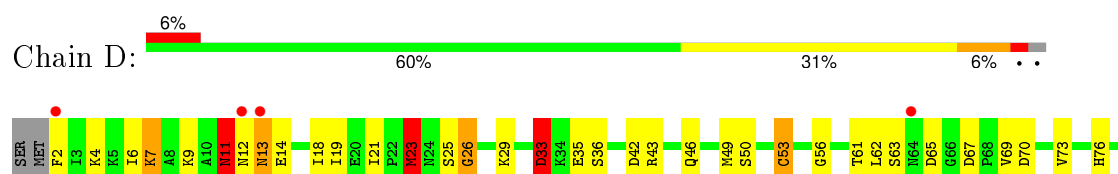
#### • Molecule 1: Inorganic pyrophosphatase



#### • Molecule 1: Inorganic pyrophosphatase

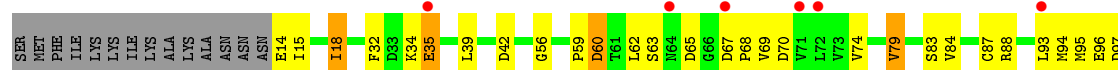


#### • Molecule 1: Inorganic pyrophosphatase

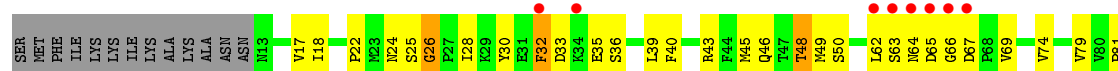




- Molecule 1: Inorganic pyrophosphatase



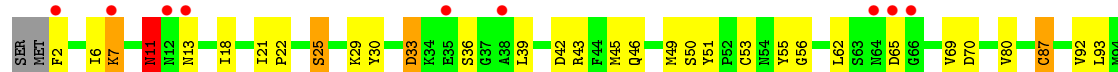
- Molecule 1: Inorganic pyrophosphatase



- Molecule 1: Inorganic pyrophosphatase



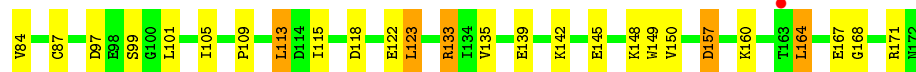
- Molecule 1: Inorganic pyrophosphatase



- Molecule 1: Inorganic pyrophosphatase



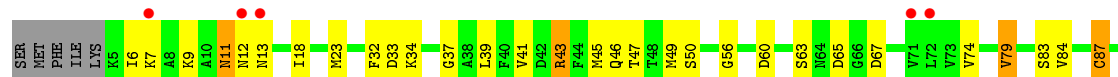




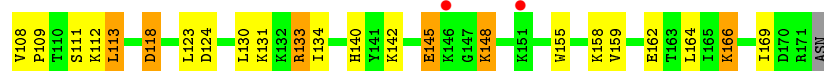
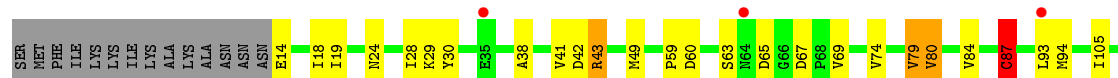
- Molecule 1: Inorganic pyrophosphatase



- 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, $\alpha$ , $\beta$ , $\gamma$	80.96Å 107.35Å 128.42Å 90.00° 96.05° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.78 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.7 (30.00-2.20) 93.7 (29.78-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, $R_{free}$	0.227 , 0.267 0.234 , 0.250	Depositor DCC
$R_{free}$ test set	5186 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	8 of 103742 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.92	1/1359 (0.1%)	0.92	4/1835 (0.2%)
1	B	0.87	1/1342 (0.1%)	0.98	4/1812 (0.2%)
1	C	0.89	1/1379 (0.1%)	0.93	2/1861 (0.1%)
1	D	0.87	0/1399	0.98	4/1886 (0.2%)
1	E	1.02	3/1282 (0.2%)	1.04	3/1732 (0.2%)
1	F	0.91	0/1304	0.94	1/1762 (0.1%)
1	G	0.91	2/1351 (0.1%)	1.00	4/1824 (0.2%)
1	H	0.90	1/1380 (0.1%)	0.95	2/1861 (0.1%)
1	I	0.94	3/1298 (0.2%)	0.94	2/1754 (0.1%)
1	J	0.91	0/1350	0.94	3/1823 (0.2%)
1	K	0.87	0/1368	0.90	0/1846
1	L	0.97	2/1282 (0.2%)	1.02	3/1732 (0.2%)
All	All	0.91	14/16094 (0.1%)	0.96	32/21728 (0.1%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	87	CYS	CB-SG	-8.17	1.68	1.82
1	E	87	CYS	CB-SG	-8.16	1.68	1.82
1	L	87	CYS	CB-SG	-7.48	1.69	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	CYS	CB-SG	-7.25	1.70	1.82
1	E	124	ASP	CB-CG	-6.82	1.37	1.51
1	I	122	GLU	CD-OE1	6.72	1.33	1.25
1	A	128	GLU	CB-CG	-6.05	1.40	1.52
1	L	124	ASP	CB-CG	-5.97	1.39	1.51
1	E	111	SER	CB-OG	5.73	1.49	1.42
1	G	53	CYS	CB-SG	-5.56	1.72	1.81
1	H	53	CYS	CB-SG	-5.54	1.72	1.81
1	G	87	CYS	CB-SG	-5.43	1.73	1.81
1	C	87	CYS	CB-SG	-5.40	1.73	1.81
1	I	122	GLU	CG-CD	5.22	1.59	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	124	ASP	CB-CG-OD1	-11.27	108.16	118.30
1	E	124	ASP	CB-CG-OD1	-10.98	108.42	118.30
1	L	133	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	B	133	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	B	133	ARG	NE-CZ-NH2	-9.37	115.62	120.30
1	E	133	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	G	133	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	J	133	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	G	143	ASP	CB-CG-OD1	7.01	124.61	118.30
1	L	133	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	I	133	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	G	133	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	F	133	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	J	133	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	C	101	LEU	CA-CB-CG	-6.00	101.50	115.30
1	J	113	LEU	CA-CB-CG	5.94	128.97	115.30
1	D	49	MET	CG-SD-CE	5.94	109.70	100.20
1	D	70	ASP	CB-CA-C	-5.93	98.55	110.40
1	B	113	LEU	CA-CB-CG	5.81	128.67	115.30
1	D	33	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	C	88	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	A	133	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	E	133	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	H	113	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	113	LEU	CA-CB-CG	5.45	127.83	115.30
1	B	88	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	G	113	LEU	CA-CB-CG	5.34	127.57	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	133	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	H	132	LYS	CD-CE-NZ	-5.23	99.67	111.70
1	D	23	MET	CG-SD-CE	-5.20	91.89	100.20
1	A	23	MET	CG-SD-CE	5.14	108.42	100.20
1	A	118	ASP	CB-CG-OD1	-5.12	113.69	118.30

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1329	0	1335	35	0
1	B	1315	0	1323	40	0
1	C	1345	0	1355	39	0
1	D	1365	0	1393	59	0
1	E	1255	0	1258	73	0
1	F	1274	0	1275	49	0
1	G	1321	0	1329	51	0
1	H	1352	0	1369	60	0
1	I	1271	0	1270	52	0
1	J	1323	0	1329	27	0
1	K	1338	0	1348	57	0
1	L	1255	0	1258	42	0
2	E	13	0	18	3	0
2	L	13	0	18	4	0
3	A	47	0	0	1	0
3	B	33	0	0	2	0
3	C	38	0	0	1	0
3	D	30	0	0	1	0
3	E	39	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	5	0
3	L	39	0	0	2	0
All	All	16189	0	15878	530	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 (530) 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	1.22	1.12
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
1:H:111:SER:CB	1:H:118:ASP:OD1	2.06	1.02
1:C:95:MET:CE	1:C:152:VAL:HG22	1.90	1.01
1:B:159:VAL:O	1:B:163:THR:HG23	1.60	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	1.43	0.99
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:146:LYS:HB3	1:G:146:LYS:HB3	1.57	0.84
1:E:96:GLU:CG	1:E:100:GLY:O	2.25	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:7:LYS:H	1:D:7:LYS:HE2	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: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
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:I:79:VAL:HG13	1:I:83:SER:HG	1.51	0.76
1:E:111:SER:HG	1:E:118:ASP:CG	1.89	0.76
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:E:18:ILE:HD13	1:E:18:ILE:N	2.01	0.75
1:A:79:VAL:HG13	1:A:83:SER:OG	1.86	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: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:L:111:SER:OG	1:L:118:ASP:CG	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:GLN:O	1:E:133:ARG:HD3	1.87	0.73
1:C:79:VAL:HG13	1:C:83:SER:OG	1.88	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: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:E:111:SER:OG	1:E:118:ASP:CG	2.30	0.69
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:I:157:ASP:HB2	1:I:160:LYS:HG3	1.74	0.69
1:C:50:SER:H	1:F:48:THR:HG23	1.57	0.69
1:A:90:ILE:HD13	1:A:106:ILE:O	1.93	0.69
1:F:32:PHE:CE1	1:F:39:LEU:HD13	2.28	0.68
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: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:K:43:ARG:HH11	1:K:145:GLU:CD	1.99	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	0.65
1:K:87:CYS:HB3	1:K:108:VAL:O	1.96	0.65
1:D:2:PHE:HD2	1:D:6:ILE:HD11	1.62	0.65
1:F:45:MET:HE3	3:F:178:HOH:O	1.96	0.64
1:I:167:GLU:O	1:I:171:ARG:HB2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:95:MET:HG2	1:E:152:VAL:HG22	1.80	0.63
1:C:69:VAL:CG1	1:C:105:ILE:CD1	2.76	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:O	1:L:169:ILE:HG22	1.99	0.63
1:K:43:ARG:NH1	1:K:145:GLU:CD	2.52	0.62
1:J:86:LYS:NZ	1:J:112:LYS:NZ	2.43	0.62
1:H:45:MET:HE3	3:H:184:HOH:O	1.98	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:CE	1:H:129:MET:HA	2.24	0.62
1:D:129:MET:HE2	1:E:144:LEU:HD13	1.82	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:N	1:D:7:LYS:HE2	2.13	0.62
1:K:7:LYS:HE2	1:K:9:LYS:O	2.00	0.62
1:E:158:LYS:HE2	3:E:199:HOH:O	2.00	0.62
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:I:157:ASP:HB3	1:I:160:LYS:H	1.66	0.60
1:G:133:ARG:HD3	1:J:46:GLN:O	2.02	0.60
1:B:79:VAL:HG13	1:B:83:SER:OG	2.00	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:H:129:MET:HE3	1:H:129:MET:CA	2.27	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:A:111:SER:HG	1:A:118:ASP:CG	2.05	0.59
1:H:95:MET:HB3	1:H:152:VAL:HA	1.83	0.59
1:A:34:LYS:HD2	1:A:34:LYS:N	2.17	0.59
1:L:111:SER:CB	1:L:118:ASP:OD1	2.50	0.59
1:K:115:ILE:O	1:K:118:ASP:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:19:ILE:HG13	1:L:79:VAL:HG11	1.85	0.59
1:F:111:SER:OG	1:F:118:ASP:OD1	2.08	0.59
1:A:95:MET:HE1	1:A:104:LYS:HG3	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:J:79:VAL:HG13	1:J:83:SER:HG	1.67	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:G:41:VAL:HG12	1:I:113:LEU:HD13	1.86	0.57
1:D:129:MET:HE3	1:D:132:LYS:HB2	1.87	0.57
1:C:69:VAL:HG11	1:C:105:ILE:HD11	1.87	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: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:E:131:LYS:HZ2	2:E:173:PG4:H51	1.70	0.56
1:I:157:ASP:N	1:I:160:LYS:HD2	2.16	0.56
1:F:17:VAL:HG23	1:F:87[B]:CYS:SG	2.46	0.56
1:H:95:MET:CE	1:H:104:LYS:HE2	2.35	0.56
1:G:18:ILE:HG21	1:G:57:PHE:CZ	2.41	0.56
1:C:45:MET:HE3	3:C:174:HOH:O	2.05	0.56
1:K:11:ASN:HD22	1:K:13:ASN:N	2.03	0.56
1:H:98:GLU:HB3	1:H:149:TRP:NE1	2.21	0.56
1:E:18:ILE:HD12	1:E:84:VAL:HG22	1.87	0.56
1:D:119:HIS:H	1:D:119:HIS:CD2	2.24	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: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:D:43[A]:ARG:NE	1:D:145:GLU:OE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:97:ASP:C	1:I:99:SER:H	2.09	0.55
1:C:14:GLU:OE1	1:C:112:LYS:HE2	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:HG21	1.88	0.55
1:F:74:VAL:O	1:F:109:PRO:HD3	2.06	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:H:2:PHE:CE2	1:H:18:ILE:HD13	2.41	0.54
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:D:11:ASN:HD22	1:D:13:ASN:H	1.56	0.54
1:F:97:ASP:C	1:F:99:SER:H	2.10	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
1:K:47:THR:OG1	1:K:49:MET:HG3	2.07	0.54
1:K:79:VAL:HG13	1:K:83:SER:HG	1.70	0.54
1:I:48:THR:HG23	1:K:50:SER:H	1.73	0.54
1:H:7:LYS:H	1:H:7:LYS:CE	2.21	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:D:129:MET:HE3	1:D:129:MET:HA	1.90	0.54
1:B:45:MET:HE3	3:B:173:HOH:O	2.07	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:D:2:PHE:HD2	1:D:6:ILE:CD1	2.20	0.53
1:B:127:CYS:HB3	1:B:130:LEU:HB3	1.89	0.53
1:F:142:LYS:HE2	1:F:150:VAL:HG23	1.89	0.53
1:H:69:VAL:HG11	1:H:105:ILE:HD12	1.85	0.53
1:D:43[A]:ARG:HH11	1:D:43[A]:ARG:HG3	1.73	0.53
1:D:19[B]:ILE:HG23	1:D:83:SER:O	2.08	0.53
1:K:103:GLU:OE2	1:K:164:LEU:HD21	2.08	0.53
1:F:22:PRO:HB3	1:F:79:VAL:O	2.08	0.53
1:A:127:CYS:HB3	1:A:130:LEU:HB3	1.89	0.53
1:L:111:SER:HG	1:L:118:ASP:CG	2.07	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:I:63:SER:OG	1:I:65:ASP:OD1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14:GLU:HA	1:L:14:GLU:OE2	2.09	0.53
1:E:146:LYS:CD	1:G:146:LYS:HB3	2.39	0.53
1:D:69:VAL:CG1	1:D:105:ILE:HD12	2.38	0.53
1:G:11:ASN:CG	1:G:12:ASN:H	2.12	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:25:SER:O	1:D:50:SER:CB	2.57	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:L:169:ILE:O	1:L:169:ILE:CG2	2.58	0.52
1:D:62:LEU:O	1:D:171:ARG:NH1	2.43	0.52
1:G:41:VAL:HG21	1:I:79:VAL:HG21	1.92	0.52
1:I:48:THR:CG2	1:K:49:MET:HB3	2.40	0.52
1:H:22:PRO:O	1:H:25:SER:HB2	2.10	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:I:64:ASN:C	1:I:66:GLY:H	2.12	0.51
1:B:63:SER:HB2	1:B:67:ASP:O	2.10	0.51
1:E:69:VAL:HG12	1:E:105:ILE:HD12	1.91	0.51
1:K:45:MET:HE3	3:K:175:HOH:O	2.10	0.51
1:E:145:GLU:CD	1:E:148:LYS:HD2	2.31	0.51
1:K:119:HIS:CE1	3:K:195:HOH:O	2.63	0.51
1:H:156:GLY:CA	1:H:160:LYS:HD3	2.40	0.51
1:L:29:LYS:O	1:L:42:ASP:HB3	2.11	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:C:97:ASP:HB3	1:C:150:VAL:HG22	1.93	0.51
1:B:28:ILE:HG21	1:B:30:TYR:CZ	2.47	0.50
1:F:167:GLU:HB3	1:F:171:ARG:NH2	2.26	0.50
1:E:93:LEU:HD13	1:E:155:TRP:CH2	2.46	0.50
1:F:119:HIS:CE1	1:F:120:ILE:HD11	2.46	0.50
1:K:112:LYS:HZ3	1:K:112:LYS:H	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:45:MET:HE3	3:I:197:HOH:O	2.09	0.50
1:L:63:SER:N	1:L:67:ASP:O	2.38	0.50
1:E:112:LYS:H	1:E:112:LYS:HD2	1.77	0.50
1:K:11:ASN:HD22	1:K:11:ASN:C	2.16	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:E:146:LYS:CA	1:G:146:LYS:HB3	2.41	0.49
1:C:119[A]:HIS:CD2	1:C:119[A]:HIS:H	2.30	0.49
1:F:157:ASP:HB2	1:F:160:LYS:CE	2.42	0.49
1:E:97:ASP:N	1:E:100:GLY:O	2.45	0.49
1:K:119:HIS:CD2	1:K:119:HIS:H	2.30	0.49
1:F:48:THR:O	1:F:48:THR:HG23	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:G:95:MET:HE1	1:G:104:LYS:HE2	1.94	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:I:32:PHE:CD1	1:I:39:LEU:HD13	2.48	0.49
1:E:34:LYS:HE2	1:E:68:PRO:HG2	1.95	0.49
1:D:95:MET:HB3	1:D:152:VAL:HA	1.95	0.49
1:D:43[A]:ARG:NH1	1:D:43[A]:ARG:HG3	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:J:111:SER:CB	1:J:118:ASP:OD1	2.61	0.48
1:F:160:LYS:O	1:F:164:LEU:HD22	2.13	0.48
1:H:95:MET:HE1	1:H:104:LYS:HE2	1.94	0.48
1:B:33:ASP:O	1:B:37:GLY:N	2.37	0.48
1:K:79:VAL:HG21	1:L:41:VAL:HG21	1.96	0.48
1:F:157:ASP:HB3	1:F:160:LYS:H	1.79	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:E:18:ILE:O	1:E:56:GLY:HA3	2.13	0.48
1:D:11:ASN:ND2	1:D:13:ASN:H	2.10	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:K:65:ASP:OD2	1:K:67:ASP:HB2	2.12	0.48
1:D:19[B]:ILE:HD11	1:D:21:ILE:C	2.34	0.48
1:G:28:ILE:HG21	1:G:30:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:LYS:CG	1:G:146:LYS:HD3	2.45	0.47
1:C:49:MET:HG2	1:F:49:MET:HG2	1.96	0.47
1:C:22:PRO:HB2	1:C:25:SER:HB3	1.96	0.47
1:E:88:ARG:NH2	1:E:117:PHE:O	2.47	0.47
1:D:63:SER:OG	1:D:67:ASP:O	2.32	0.47
1:H:69:VAL:CG1	1:H:105:ILE:CD1	2.84	0.47
1:A:111:SER:OG	1:A:118:ASP:OD1	2.25	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:135:VAL:O	1:I:139:GLU:HG3	2.14	0.47
1:J:98:GLU:HG2	1:J:99:SER:N	2.30	0.47
1:J:74:VAL:O	1:J:109:PRO:HD3	2.15	0.47
1:C:6:ILE:HD13	1:C:84:VAL:HG21	1.97	0.47
1:G:145:GLU:CD	1:G:148:LYS:HD2	2.36	0.47
1:B:145:GLU:O	1:B:148:LYS:HB2	2.15	0.47
1:H:128:GLU:O	1:H:132:LYS:HD3	2.15	0.47
1:F:157:ASP:OD1	1:F:159:VAL:CG1	2.52	0.47
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:H:62:LEU:O	1:H:171:ARG:NH1	2.48	0.47
1:E:145:GLU:HG2	1:E:148:LYS:CB	2.42	0.46
1:D:18:ILE:O	1:D:56:GLY:HA3	2.16	0.46
1:H:129:MET:CE	1:H:132:LYS:HB2	2.45	0.46
1:A:79:VAL:HG13	1:A:83:SER:HG	1.80	0.46
1:K:6:ILE:HD13	1:K:84:VAL:HG21	1.97	0.46
1:H:157:ASP:H	1:H:160:LYS:HD3	1.80	0.46
1:K:112:LYS:O	1:L:43:ARG:NH2	2.49	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: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:F:64:ASN:C	1:F:66:GLY:H	2.17	0.46
1:H:129:MET:HE3	1:H:132:LYS:HD3	1.96	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:A:69:VAL:HG12	1:A:105:ILE:HD12	1.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:69:VAL:HG11	1:L:105:ILE:HD11	1.97	0.46
1:B:135:VAL:O	1:B:139:GLU:HG3	2.16	0.46
1:H:29:LYS:O	1:H:42:ASP:HB3	2.15	0.46
1:B:88:ARG:HG3	1:B:88:ARG:NH1	2.31	0.46
1:A:14:GLU:CD	1:A:110:THR:HG21	2.36	0.45
1:C:95:MET:HE3	1:C:152:VAL:CG2	2.14	0.45
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:H:93:LEU:HD11	1:H:152:VAL:CG1	2.47	0.45
1:G:18:ILE:CG2	1:G:57:PHE:CZ	2.99	0.45
1:A:60:ASP:OD2	3:A:179:HOH:O	2.21	0.45
1:D:145:GLU:O	1:D:148:LYS:HB2	2.17	0.45
1:I:157:ASP:HB2	1:I:160:LYS:CG	2.43	0.45
1:H:140:HIS:CE1	1:L:140:HIS:CE1	3.04	0.45
1:I:22:PRO:HB3	1:I:79:VAL:O	2.16	0.45
1:H:95:MET:HE3	1:H:104:LYS:HE2	1.97	0.45
1:B:88:ARG:HG3	1:B:88:ARG:HH11	1.81	0.45
1:F:157:ASP:HB2	1:F:160:LYS:HZ2	1.81	0.45
1:A:18:ILE:O	1:A:56:GLY:HA3	2.17	0.45
1:I:97:ASP:HB2	1:I:149:TRP:O	2.17	0.45
1:H:7:LYS:HB2	1:H:7:LYS:HE2	1.52	0.45
1:K:6:ILE:HD11	1:L:38:ALA:HB2	1.97	0.45
1:J:30:TYR:CZ	1:L:80:VAL:HG22	2.52	0.45
1:G:119:HIS:CD2	1:G:119:HIS:H	2.35	0.45
1:H:123:LEU:O	1:H:131:LYS:NZ	2.42	0.45
1:F:157:ASP:H	1:F:160:LYS:NZ	2.15	0.45
1:C:49:MET:HB3	1:F:48:THR:CG2	2.47	0.45
1:L:18:ILE:HG12	1:L:59:PRO:HD3	1.98	0.45
1:G:92:VAL:HG13	1:G:156:GLY:HA3	1.98	0.45
1:B:57:PHE:HA	1:B:70:ASP:HA	1.99	0.44
1:B:33:ASP:HB3	1:B:36:SER:OG	2.17	0.44
1:B:23:MET:CB	1:B:53:CYS:HA	2.46	0.44
1:L:18:ILE:CD1	1:L:84:VAL:HG22	2.47	0.44
1:G:95:MET:CE	1:G:104:LYS:HE2	2.47	0.44
1:I:97:ASP:C	1:I:99:SER:N	2.71	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:B:97:ASP:OD1	1:B:100:GLY:O	2.35	0.44
1:J:122:GLU:O	1:J:125:ASP:HB2	2.18	0.44
1:D:98:GLU:HA	1:D:149:TRP:CE2	2.53	0.44
1:I:33:ASP:O	1:I:37:GLY:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:HIS:CE1	1:D:116:THR:OG1	2.69	0.44
1:I:33:ASP:OD2	1:I:36:SER:OG	2.20	0.44
1:G:7:LYS:O	1:G:16:ASN:ND2	2.45	0.44
1:H:98:GLU:HB3	1:H:149:TRP:CD1	2.53	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: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: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:F:33:ASP:HB2	1:F:40:PHE:CD1	2.52	0.44
1:A:98:GLU:N	1:A:98:GLU:OE2	2.43	0.44
1:E:15:ILE:HG21	1:E:165:ILE:HD13	1.99	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
1:E:96:GLU:CA	1:E:100:GLY:O	2.65	0.43
1:A:118:ASP:O	1:A:121:LYS:HE3	2.18	0.43
1:I:67:ASP:HB3	1:I:68:PRO:HD2	2.00	0.43
1:D:11:ASN:C	1:D:11:ASN:HD22	2.21	0.43
1:G:18:ILE:HD11	1:G:82:GLY:HA2	1.99	0.43
1:K:87:CYS:HB3	1:K:109:PRO:HA	2.00	0.43
1:E:14:GLU:CG	3:E:186:HOH:O	2.65	0.43
1:K:13:ASN:HA	3:K:192:HOH:O	2.18	0.43
1:L:19:ILE:HG21	1:L:79:VAL:HG12	1.99	0.43
1:F:128:GLU:OE2	1:F:131:LYS:NZ	2.41	0.43
1:I:48:THR:HG23	1:K:50:SER:N	2.32	0.43
1:A:157:ASP:O	1:A:160:LYS:HB3	2.18	0.43
1:A:156:GLY:HA3	1:A:160:LYS:HG2	2.00	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:A:33:ASP:OD2	1:A:33:ASP:C	2.57	0.43
1:F:156:GLY:CA	1:F:160:LYS:HD2	2.49	0.43
1:C:113:LEU:HD22	1:E:42:ASP:O	2.19	0.43
1:H:129:MET:HE3	1:H:132:LYS:HB2	2.01	0.43
1:H:129:MET:HA	1:H:132:LYS:HD3	2.00	0.43
1:H:97:ASP:CB	1:H:149:TRP:O	2.67	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:46:GLN:O	1:K:133:ARG:HD3	2.19	0.43
1:I:74:VAL:O	1:I:109:PRO:HD3	2.19	0.43
1:I:43:ARG:CZ	1:I:145:GLU:OE1	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:ASP:O	1:G:37:GLY:N	2.48	0.43
1:E:32:PHE:CE2	1:E:39:LEU:HD13	2.54	0.43
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:I:21:ILE:HD11	1:I:29:LYS:HG3	2.01	0.42
1:D:61:THR:HB	1:D:69:VAL:HG23	2.01	0.42
1:B:28:ILE:HG21	1:B:30:TYR:CE1	2.54	0.42
1:J:42:ASP:O	1:L:113:LEU:HD22	2.19	0.42
1:L:130:LEU:O	1:L:134:ILE:HG13	2.19	0.42
1:E:146:LYS:HA	1:G:146:LYS:HB3	2.01	0.42
1:D:129:MET:CE	1:D:132:LYS:HB2	2.49	0.42
1:A:74:VAL:O	1:A:109:PRO:HD3	2.20	0.42
1:K:47:THR:HG22	1:K:144:LEU:HG	2.00	0.42
1:F:22:PRO:HG3	1:F:81:PRO:HD3	2.01	0.42
1:A:34:LYS:CD	1:A:34:LYS:N	2.81	0.42
1:B:62:LEU:O	1:B:168:GLY:HA2	2.20	0.42
1:D:2:PHE:CE2	1:D:18:ILE:HD13	2.54	0.42
1:H:62:LEU:O	1:H:168:GLY:HA2	2.20	0.42
1:D:98:GLU:HA	1:D:149:TRP:CZ2	2.54	0.42
1:A:34:LYS:HA	1:A:34:LYS:HD2	1.78	0.42
1:C:33:ASP:O	1:C:37:GLY:N	2.49	0.42
1:K:23:MET:HE2	1:K:23:MET:HB2	1.91	0.42
1:D:164:LEU:HA	1:D:164:LEU:HD12	1.61	0.42
1:H:69:VAL:HG11	1:H:105:ILE:HD11	2.00	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:L:69:VAL:CG1	1:L:105:ILE:HD11	2.49	0.42
1:B:147:GLY:O	1:B:148:LYS:HG2	2.20	0.41
1:B:92:VAL:HG13	1:B:156:GLY:CA	2.50	0.41
1:L:93:LEU:HD13	1:L:155:TRP:CH2	2.55	0.41
1:I:64:ASN:C	1:I:66:GLY:N	2.74	0.41
1:E:112:LYS:CD	1:E:112:LYS:H	2.33	0.41
1:E:131:LYS:NZ	2:E:173:PG4:H51	2.34	0.41
1:I:18:ILE:O	1:I:56:GLY:HA3	2.21	0.41
1:K:18:ILE:O	1:K:56:GLY:HA3	2.20	0.41
1:J:121:LYS:O	1:J:158:LYS:CE	2.69	0.41
1:J:26:GLY:H	1:J:50:SER:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:47:THR:HG23	3:K:175:HOH:O	2.20	0.41
1:G:97:ASP:C	1:G:97:ASP:OD1	2.57	0.41
1:H:42:ASP:O	1:H:43:ARG:HB3	2.21	0.41
1:A:92:VAL:HG21	1:A:160:LYS:HG3	2.02	0.41
1:H:49:MET:HG2	1:L:49:MET:HG2	2.02	0.41
1:F:18:ILE:HG12	1:F:84:VAL:HG22	2.02	0.41
1:D:36:SER:HG	1:D:36:SER:H	1.59	0.41
1:A:65:ASP:OD1	1:A:67:ASP:HB2	2.20	0.41
1:D:93:LEU:HD12	1:D:93:LEU:HA	1.77	0.41
1:J:151:LYS:HA	1:J:151:LYS:HD2	1.74	0.41
1:F:157:ASP:H	1:F:160:LYS:HD2	1.85	0.41
1:A:163:THR:HG22	1:A:167:GLU:OE2	2.19	0.41
1:D:65:ASP:OD1	1:D:65:ASP:C	2.59	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:B:119:HIS:H	1:B:119:HIS:CD2	2.39	0.41
1:C:74:VAL:O	1:C:109:PRO:HD3	2.21	0.41
1:A:142:LYS:HD3	1:A:148:LYS:HB3	2.03	0.41
1:F:28:ILE:HG21	1:F:30:TYR:CZ	2.56	0.41
1:G:63:SER:OG	1:G:67:ASP:O	2.39	0.41
1:E:63:SER:N	1:E:67:ASP:O	2.39	0.41
1:G:18:ILE:O	1:G:56:GLY:HA3	2.21	0.41
1:F:142:LYS:HE2	1:F:150:VAL:CG2	2.51	0.41
1:H:164:LEU:HD12	1:H:164:LEU:HA	1.79	0.41
1:E:35:GLU:O	1:E:35:GLU:HG2	2.20	0.41
1:H:55:TYR:HE1	1:H:104:LYS:HD3	1.86	0.41
1:J:34:LYS:N	1:J:34:LYS:HD2	2.36	0.41
1:B:92:VAL:HG13	1:B:156:GLY:HA3	2.03	0.41
1:B:59:PRO:O	1:B:60:ASP:CB	2.69	0.41
1:E:62:LEU:O	1:E:171:ARG:HD2	2.20	0.41
1:D:129:MET:HE1	1:E:144:LEU:HD13	2.02	0.40
1:H:119:HIS:CD2	1:H:119:HIS:H	2.39	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:L:14:GLU:OE2	1:L:14:GLU:CA	2.66	0.40
1:I:123:LEU:HD12	1:I:123:LEU:HA	1.85	0.40
1:H:110:THR:O	1:H:113:LEU:N	2.52	0.40
1:K:95:MET:HE1	1:K:104:LYS:HG3	2.04	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:E:146:LYS:CB	1:G:146:LYS:CB	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:115:ILE:O	1:J:118:ASP:HB2	2.22	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:A:158:LYS:O	1:A:162:GLU:HG3	2.21	0.40
1:K:9:LYS:HB3	1:K:11:ASN:O	2.22	0.40
1:H:93:LEU:HD11	1:H:152:VAL:HG11	2.02	0.40
1:E:32:PHE:CZ	1:E:39:LEU:HD13	2.56	0.40
1:B:92:VAL:HA	1:B:106:ILE:HD12	2.03	0.40
1:B:87:CYS:HB3	1:B:107:ALA:HB1	2.04	0.40
1:B:21:ILE:HA	1:B:22:PRO:HD3	1.92	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%)	16	12
1	E	156/173 (90%)	151 (97%)	4 (3%)	1 (1%)	30	29
1	F	159/173 (92%)	147 (92%)	10 (6%)	2 (1%)	15	11
1	G	165/173 (95%)	158 (96%)	6 (4%)	1 (1%)	30	29
1	H	168/173 (97%)	161 (96%)	5 (3%)	2 (1%)	16	12
1	I	158/173 (91%)	152 (96%)	5 (3%)	1 (1%)	30	29
1	J	165/173 (95%)	157 (95%)	8 (5%)	0	100	100
1	K	167/173 (96%)	163 (98%)	3 (2%)	1 (1%)	30	29
1	L	156/173 (90%)	153 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1962/2076 (94%)	1887 (96%)	65 (3%)	10 (0%)	34	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	11	ASN
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%)	140 (93%)	10 (7%)	20	21
1	B	148/155 (96%)	135 (91%)	13 (9%)	12	12
1	C	152/155 (98%)	143 (94%)	9 (6%)	24	27
1	D	154/155 (99%)	135 (88%)	19 (12%)	6	5
1	E	142/155 (92%)	130 (92%)	12 (8%)	13	13
1	F	145/155 (94%)	138 (95%)	7 (5%)	31	37
1	G	149/155 (96%)	133 (89%)	16 (11%)	8	7
1	H	152/155 (98%)	137 (90%)	15 (10%)	10	9
1	I	144/155 (93%)	134 (93%)	10 (7%)	19	20
1	J	149/155 (96%)	137 (92%)	12 (8%)	15	14
1	K	151/155 (97%)	137 (91%)	14 (9%)	11	10
1	L	142/155 (92%)	128 (90%)	14 (10%)	10	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1778/1860 (96%)	1627 (92%)	151 (8%)	13	13

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	79	VAL
1	A	88	ARG
1	A	90	ILE
1	A	94	MET
1	A	118	ASP
1	A	123	LEU
1	A	146	LYS
1	A	151	LYS
1	A	164	LEU
1	B	34	LYS
1	B	43	ARG
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	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	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	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	118	ASP
1	D	123	LEU
1	D	148	LYS
1	D	164	LEU
1	E	18	ILE
1	E	35	GLU
1	E	60	ASP
1	E	79	VAL
1	E	94	MET
1	E	101	LEU
1	E	112	LYS
1	E	118	ASP
1	E	123	LEU
1	E	148	LYS
1	E	164	LEU
1	E	166	LYS
1	F	32	PHE
1	F	43	ARG
1	F	48	THR
1	F	62	LEU
1	F	113	LEU
1	F	123	LEU
1	F	164	LEU
1	G	7	LYS
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

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Mol	Chain	Res	Type
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	9	LYS
1	J	13	ASN
1	J	34	LYS
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	123	LEU

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Mol	Chain	Res	Type
1	J	146	LYS
1	J	166	LYS
1	K	11	ASN
1	K	43	ARG
1	K	60	ASP
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	164	LEU
1	L	166	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	B	11	ASN
1	B	13	ASN
1	B	24	ASN
1	B	119	HIS
1	C	11	ASN
1	C	12	ASN
1	D	11	ASN

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	E	173	-	12,12,12	0.71	0	11,11,11	1.00	1 (9%)
2	PG4	L	173	-	12,12,12	0.88	0	11,11,11	1.24	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	E	173	-	-	0/10/10/10	0/0/0/0
2	PG4	L	173	-	-	0/10/10/10	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	173	PG4	O3-C5-C6	2.06	119.53	110.36
2	L	173	PG4	O3-C5-C6	2.44	121.22	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	173	PG4	3	0
2	L	173	PG4	4	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	167/173 (96%)	0.18	5 (2%) 54 53	36, 45, 62, 68	0
1	B	166/173 (95%)	0.57	18 (10%) 8 7	38, 46, 64, 69	0
1	C	168/173 (97%)	0.36	11 (6%) 22 22	37, 45, 64, 69	0
1	D	170/173 (98%)	0.41	11 (6%) 22 22	39, 47, 65, 70	0
1	E	158/173 (91%)	0.52	15 (9%) 10 9	35, 44, 62, 68	0
1	F	160/173 (92%)	0.33	12 (7%) 17 17	38, 47, 64, 69	0
1	G	166/173 (95%)	0.56	15 (9%) 12 11	37, 46, 63, 68	0
1	H	170/173 (98%)	0.47	14 (8%) 14 14	39, 47, 65, 69	0
1	I	160/173 (92%)	0.38	10 (6%) 23 23	39, 46, 64, 69	0
1	J	167/173 (96%)	0.24	2 (1%) 81 80	36, 44, 62, 68	0
1	K	168/173 (97%)	0.37	9 (5%) 29 29	37, 46, 65, 68	0
1	L	158/173 (91%)	0.22	5 (3%) 51 50	36, 44, 62, 68	0
All	All	1978/2076 (95%)	0.38	127 (6%) 23 22	35, 46, 64, 70	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	35	GLU	5.7
1	E	100	GLY	5.6
1	I	66	GLY	5.6
1	L	35	GLU	5.6
1	E	64	ASN	5.4
1	B	12	ASN	5.3
1	B	66	GLY	5.0
1	D	100	GLY	4.9
1	H	12	ASN	4.9
1	E	146	LYS	4.7
1	H	64	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	147	GLY	4.7
1	K	12	ASN	4.6
1	A	35	GLU	4.5
1	I	64	ASN	4.4
1	G	35	GLU	4.3
1	B	64	ASN	4.3
1	D	149	TRP	4.2
1	F	34	LYS	4.2
1	B	36	SER	4.2
1	K	13	ASN	4.1
1	D	2	PHE	4.0
1	A	71	VAL	4.0
1	G	149	TRP	4.0
1	I	62	LEU	4.0
1	G	100	GLY	3.8
1	C	12	ASN	3.8
1	G	64	ASN	3.7
1	F	62	LEU	3.7
1	F	65	ASP	3.7
1	G	13	ASN	3.6
1	E	149	TRP	3.5
1	G	146	LYS	3.5
1	H	35	GLU	3.5
1	E	35	GLU	3.4
1	F	66	GLY	3.4
1	I	35	GLU	3.4
1	K	71	VAL	3.3
1	L	64	ASN	3.3
1	F	63	SER	3.3
1	J	35	GLU	3.3
1	F	64	ASN	3.3
1	B	100	GLY	3.3
1	D	12	ASN	3.2
1	B	71	VAL	3.2
1	I	65	ASP	3.1
1	I	63	SER	3.1
1	G	6	ILE	3.1
1	H	146	LYS	3.1
1	H	7	LYS	3.0
1	F	172	ASN	3.0
1	B	11	ASN	3.0
1	C	105	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	99	SER	3.0
1	E	101	LEU	2.9
1	I	34	LYS	2.9
1	G	101	LEU	2.9
1	B	149	TRP	2.8
1	K	105	ILE	2.8
1	C	72	LEU	2.8
1	D	159	VAL	2.8
1	C	71	VAL	2.8
1	F	170	ASP	2.8
1	C	7	LYS	2.7
1	D	147	GLY	2.7
1	E	105	ILE	2.7
1	L	151	LYS	2.7
1	I	32	PHE	2.7
1	D	169	ILE	2.7
1	H	100	GLY	2.6
1	K	72	LEU	2.6
1	C	101	LEU	2.5
1	B	72	LEU	2.5
1	H	149	TRP	2.5
1	J	71	VAL	2.5
1	B	13	ASN	2.5
1	E	151	LYS	2.5
1	C	73	VAL	2.5
1	E	71	VAL	2.5
1	C	10	ALA	2.5
1	H	101	LEU	2.5
1	E	72	LEU	2.4
1	C	13	ASN	2.4
1	D	64	ASN	2.4
1	B	65	ASP	2.4
1	F	67	ASP	2.4
1	H	96	GLU	2.4
1	G	66	GLY	2.4
1	F	32	PHE	2.4
1	E	98	GLU	2.3
1	K	106	ILE	2.3
1	B	37	GLY	2.3
1	D	99	SER	2.3
1	E	93	LEU	2.3
1	G	71	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	163	THR	2.3
1	B	33	ASP	2.3
1	B	34	LYS	2.2
1	L	146	LYS	2.2
1	F	159	VAL	2.2
1	K	7	LYS	2.2
1	F	125	ASP	2.2
1	I	60	ASP	2.2
1	H	38	ALA	2.2
1	C	106	ILE	2.2
1	H	2	PHE	2.2
1	G	151	LYS	2.2
1	H	13	ASN	2.2
1	B	10	ALA	2.2
1	D	146	LYS	2.2
1	D	13	ASN	2.2
1	E	67	ASP	2.1
1	H	66	GLY	2.1
1	B	151	LYS	2.1
1	A	72	LEU	2.1
1	E	145	GLU	2.1
1	A	65	ASP	2.1
1	K	166	LYS	2.1
1	G	72	LEU	2.0
1	A	149	TRP	2.0
1	G	99	SER	2.0
1	H	65	ASP	2.0
1	G	12	ASN	2.0
1	C	151	LYS	2.0
1	G	33	ASP	2.0
1	K	107	ALA	2.0
1	L	93	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PG4	L	173	13/13	0.83	0.21	2.57	44,50,59,59	0
2	PG4	E	173	13/13	0.90	0.15	0.51	43,48,50,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.