



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:02 am GMT

PDB ID : 1RBO  
Title : SPINACH RUBISCO IN COMPLEX WITH THE INHIBITOR 2-CARBOX  
YARABINITOL-1,5-DIPHOSPHATE  
Authors : Taylor, T.C.; Andersson, I.  
Deposited on : 1996-10-31  
Resolution : 2.30 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

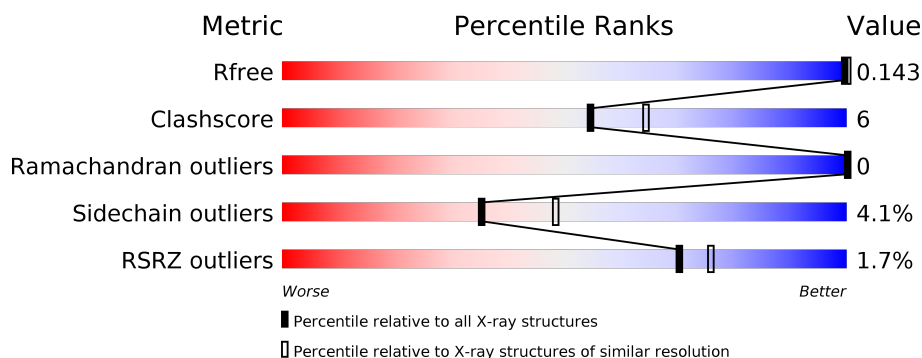
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	B	475	<div> <div>0.1%</div> <div>86%</div> <div>11%</div> <div>•</div> </div>
1	E	475	<div> <div>0.1%</div> <div>87%</div> <div>11%</div> <div>•</div> </div>
1	H	475	<div> <div>2%</div> <div>87%</div> <div>11%</div> <div>•</div> </div>
1	L	475	<div> <div>2%</div> <div>87%</div> <div>11%</div> <div>•</div> </div>
2	C	123	<div> <div>3%</div> <div>78%</div> <div>18%</div> <div>•</div> </div>
2	F	123	<div> <div>2%</div> <div>78%</div> <div>18%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	123	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>.</div> </div> </div>
2	S	123	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>.</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CAP	B	476	X	-	-	-
3	CAP	E	476	X	-	-	-
3	CAP	H	476	X	-	-	-
3	CAP	L	476	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19900 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 RIBULOSE BISPHTHOSPHATE CARBOXYLASE/OXYGEN ASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	467	Total	C	N	O	S	0	0	0
			3649	2315	640	676	18			
1	B	467	Total	C	N	O	S	0	0	0
			3649	2315	640	676	18			
1	E	467	Total	C	N	O	S	0	0	0
			3649	2315	640	676	18			
1	H	467	Total	C	N	O	S	0	0	0
			3649	2315	640	676	18			

- Molecule 2 is a protein called RIBULOSE BISPHTHOSPHATE CARBOXYLASE/OXYGEN ASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	123	Total	C	N	O	S	0	0	0
			1033	673	167	186	7			
2	C	123	Total	C	N	O	S	0	0	0
			1033	673	167	186	7			
2	F	123	Total	C	N	O	S	0	0	0
			1033	673	167	186	7			
2	I	123	Total	C	N	O	S	0	0	0
			1033	673	167	186	7			

There are 28 discrepancies between the modelled and reference sequences:

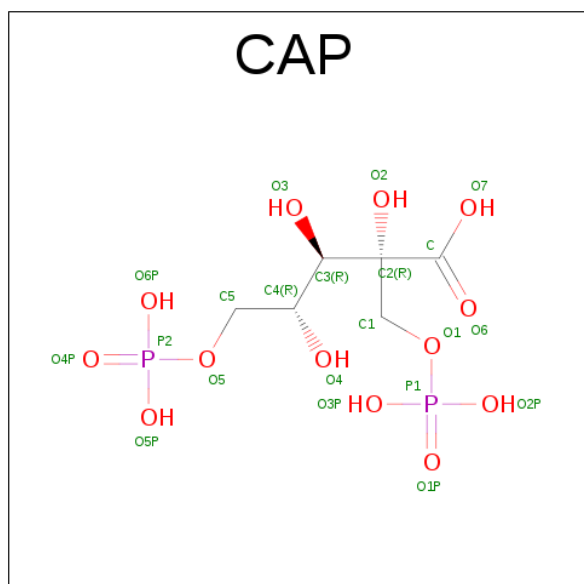
Chain	Residue	Modelled	Actual	Comment	Reference
S	2	GLN	LYS	CONFLICT	UNP P00870
S	6	ILE	THR	CONFLICT	UNP P00870
S	7	LEU	GLN	CONFLICT	UNP P00870
S	9	LEU	MET	CONFLICT	UNP P00870
S	11	LYS	ARG	CONFLICT	UNP P00870
S	109	GLU	GLN	CONFLICT	UNP P00870
S	113	ILE	VAL	CONFLICT	UNP P00870

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	GLN	LYS	CONFLICT	UNP P00870
C	6	ILE	THR	CONFLICT	UNP P00870
C	7	LEU	GLN	CONFLICT	UNP P00870
C	9	LEU	MET	CONFLICT	UNP P00870
C	11	LYS	ARG	CONFLICT	UNP P00870
C	109	GLU	GLN	CONFLICT	UNP P00870
C	113	ILE	VAL	CONFLICT	UNP P00870
F	2	GLN	LYS	CONFLICT	UNP P00870
F	6	ILE	THR	CONFLICT	UNP P00870
F	7	LEU	GLN	CONFLICT	UNP P00870
F	9	LEU	MET	CONFLICT	UNP P00870
F	11	LYS	ARG	CONFLICT	UNP P00870
F	109	GLU	GLN	CONFLICT	UNP P00870
F	113	ILE	VAL	CONFLICT	UNP P00870
I	2	GLN	LYS	CONFLICT	UNP P00870
I	6	ILE	THR	CONFLICT	UNP P00870
I	7	LEU	GLN	CONFLICT	UNP P00870
I	9	LEU	MET	CONFLICT	UNP P00870
I	11	LYS	ARG	CONFLICT	UNP P00870
I	109	GLU	GLN	CONFLICT	UNP P00870
I	113	ILE	VAL	CONFLICT	UNP P00870

- Molecule 3 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula:  $C_6H_{14}O_{13}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total	C	O	P	0	0
			21	6	13	2		
3	B	1	Total	C	O	P	0	0
			21	6	13	2		
3	E	1	Total	C	O	P	0	0
			21	6	13	2		
3	H	1	Total	C	O	P	0	0
			21	6	13	2		

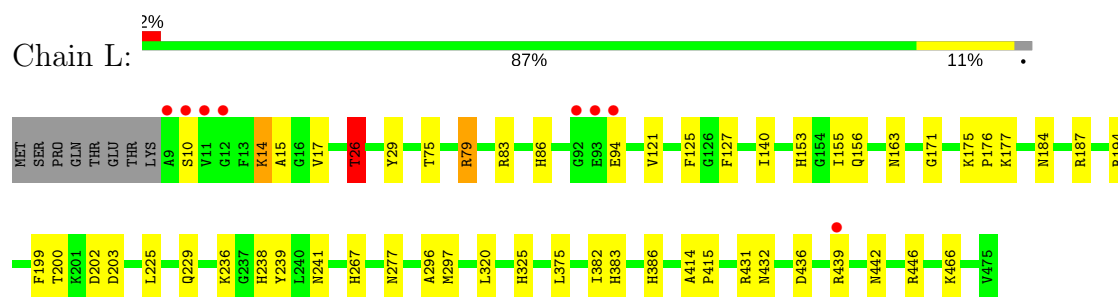
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	227	Total	O	0	0
			227	227		
4	C	43	Total	O	0	0
			43	43		
4	E	229	Total	O	0	0
			229	229		
4	F	45	Total	O	0	0
			45	45		
4	H	227	Total	O	0	0
			227	227		
4	I	44	Total	O	0	0
			44	44		
4	L	229	Total	O	0	0
			229	229		
4	S	44	Total	O	0	0
			44	44		

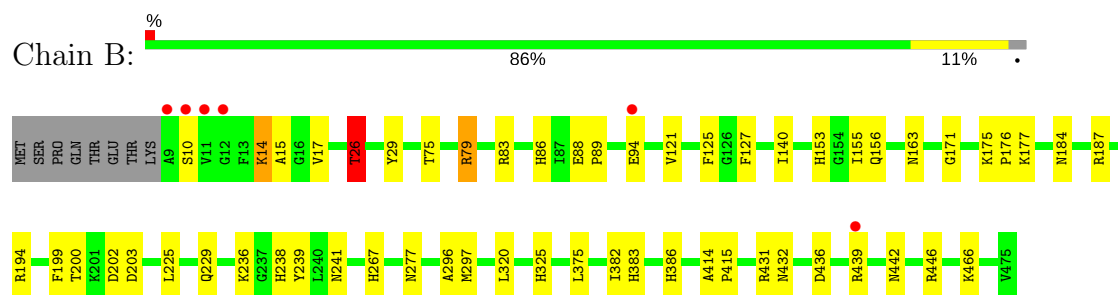
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

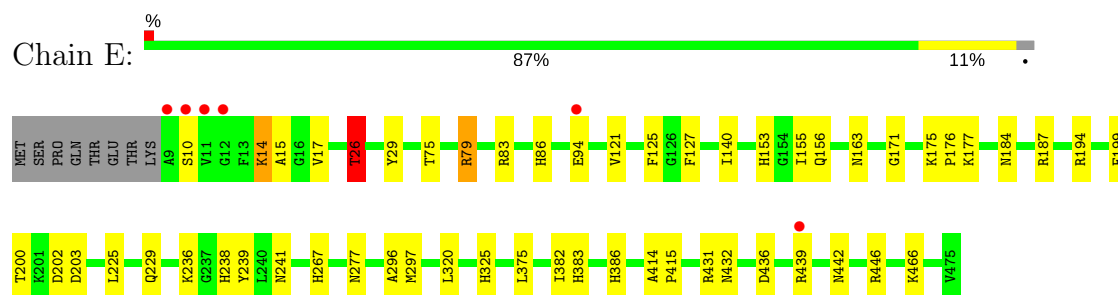
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE



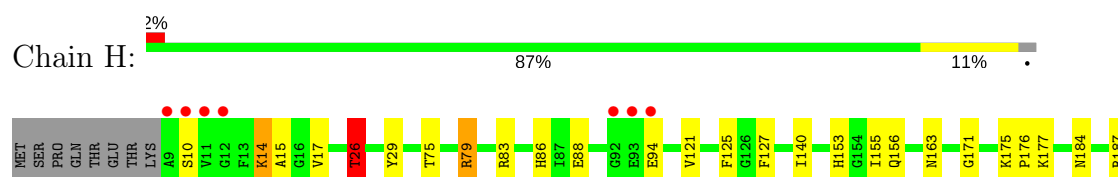
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE

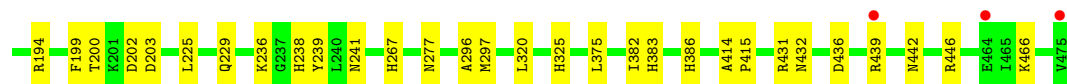


#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE

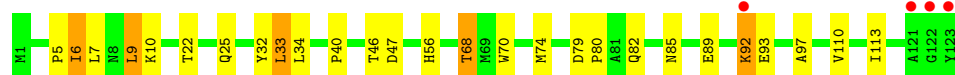
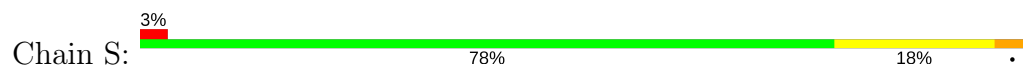


#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE

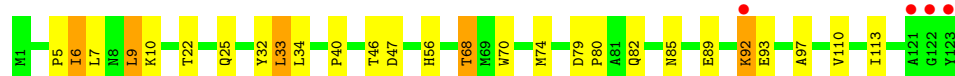
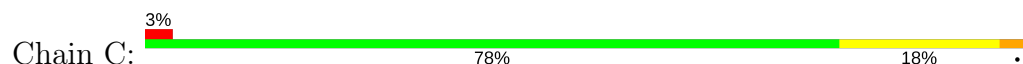




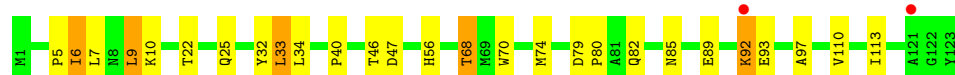
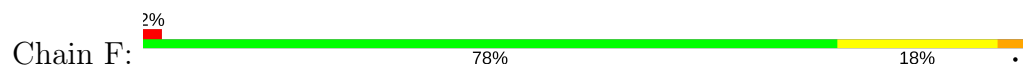
- Molecule 2: RIBULOSE BIPHOSPHATE CARBOXYLASE/OXYGENASE



- Molecule 2: RIBULOSE BIPHOSPHATE CARBOXYLASE/OXYGENASE



- Molecule 2: RIBULOSE BIPHOSPHATE CARBOXYLASE/OXYGENASE



- Molecule 2: RIBULOSE BIPHOSPHATE CARBOXYLASE/OXYGENASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.20Å 157.20Å 201.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.30 19.65 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (7.00-2.30) 98.6 (19.65-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	12.33 (at 2.30Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.154 , 0.171 0.144 , 0.143	Depositor DCC
$R_{free}$ test set	5279 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.9	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.038 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19900	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	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 31.15 % 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 1.1607e-03. 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, 0.333 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: CAP

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	B	0.52	0/3739	0.75	2/5071 (0.0%)
1	E	0.52	0/3739	0.75	2/5071 (0.0%)
1	H	0.52	0/3739	0.75	2/5071 (0.0%)
1	L	0.52	0/3739	0.75	2/5071 (0.0%)
2	C	0.52	0/1068	0.73	1/1453 (0.1%)
2	F	0.52	0/1068	0.72	1/1453 (0.1%)
2	I	0.52	0/1068	0.73	1/1453 (0.1%)
2	S	0.52	0/1068	0.72	1/1453 (0.1%)
All	All	0.52	0/19228	0.74	12/26096 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	33	LEU	CA-CB-CG	7.30	132.09	115.30
2	C	33	LEU	CA-CB-CG	7.30	132.08	115.30
2	S	33	LEU	CA-CB-CG	7.29	132.06	115.30
2	I	33	LEU	CA-CB-CG	7.28	132.05	115.30
1	B	325	HIS	CB-CA-C	-5.46	99.49	110.40
1	H	325	HIS	CB-CA-C	-5.45	99.49	110.40
1	L	325	HIS	CB-CA-C	-5.45	99.51	110.40
1	E	325	HIS	CB-CA-C	-5.44	99.51	110.40
1	H	26	THR	N-CA-CB	-5.08	100.66	110.30
1	L	26	THR	N-CA-CB	-5.07	100.67	110.30
1	E	26	THR	N-CA-CB	-5.07	100.67	110.30
1	B	26	THR	N-CA-CB	-5.06	100.69	110.30

There are no chirality outliers.

There are no planarity outliers.

## 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	B	3649	0	3565	35	1
1	E	3649	0	3565	34	1
1	H	3649	0	3565	35	2
1	L	3649	0	3565	35	1
2	C	1033	0	990	26	0
2	F	1033	0	990	27	0
2	I	1033	0	990	26	2
2	S	1033	0	990	26	0
3	B	21	0	9	0	0
3	E	21	0	9	0	0
3	H	21	0	9	0	0
3	L	21	0	9	0	0
4	B	227	0	0	3	15
4	C	43	0	0	1	1
4	E	229	0	0	3	22
4	F	45	0	0	1	1
4	H	227	0	0	3	16
4	I	44	0	0	1	1
4	L	229	0	0	3	24
4	S	44	0	0	1	1
All	All	19900	0	18256	222	57

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (222) 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)
2:I:89:GLU:HG3	2:I:92:LYS:NZ	1.85	0.92
2:F:89:GLU:HG3	2:F:92:LYS:NZ	1.85	0.91
2:C:89:GLU:HG3	2:C:92:LYS:NZ	1.85	0.91
2:S:89:GLU:HG3	2:S:92:LYS:NZ	1.85	0.89
1:H:267:HIS:HD2	1:H:277:ASN:HD22	1.23	0.87
1:L:267:HIS:HD2	1:L:277:ASN:HD22	1.23	0.86
1:B:267:HIS:HD2	1:B:277:ASN:HD22	1.23	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:HIS:HD2	1:E:277:ASN:HD22	1.23	0.84
2:C:89:GLU:HG3	2:C:92:LYS:HZ3	1.41	0.82
2:S:89:GLU:HG3	2:S:92:LYS:HZ3	1.44	0.80
2:I:89:GLU:HG3	2:I:92:LYS:HZ1	1.47	0.79
1:H:26:THR:HG23	1:H:29:TYR:HB2	1.67	0.77
1:L:26:THR:HG23	1:L:29:TYR:HB2	1.67	0.77
2:F:89:GLU:HG3	2:F:92:LYS:HZ1	1.50	0.76
1:B:26:THR:HG23	1:B:29:TYR:HB2	1.67	0.74
1:E:26:THR:HG23	1:E:29:TYR:HB2	1.67	0.74
2:S:22:THR:H	2:S:25:GLN:HE21	1.38	0.72
1:B:267:HIS:CD2	1:B:277:ASN:HD22	2.07	0.72
2:F:22:THR:H	2:F:25:GLN:HE21	1.38	0.72
2:F:89:GLU:HG3	2:F:92:LYS:HZ3	1.55	0.71
2:I:22:THR:H	2:I:25:GLN:HE21	1.38	0.71
2:C:22:THR:H	2:C:25:GLN:HE21	1.38	0.71
1:E:267:HIS:CD2	1:E:277:ASN:HD22	2.07	0.71
1:H:267:HIS:CD2	1:H:277:ASN:HD22	2.07	0.71
1:L:267:HIS:CD2	1:L:277:ASN:HD22	2.07	0.68
2:I:89:GLU:HG3	2:I:92:LYS:HZ3	1.59	0.67
2:F:92:LYS:HE2	2:F:93:GLU:HB2	1.79	0.65
1:H:155:ILE:HG12	1:H:375:LEU:HD13	1.79	0.65
2:I:89:GLU:O	2:I:92:LYS:HG3	1.97	0.65
2:S:89:GLU:O	2:S:92:LYS:HG3	1.97	0.65
1:E:155:ILE:HG12	1:E:375:LEU:HD13	1.79	0.64
2:I:92:LYS:HE2	2:I:93:GLU:HB2	1.79	0.64
1:B:155:ILE:HG12	1:B:375:LEU:HD13	1.79	0.64
2:C:92:LYS:HE2	2:C:93:GLU:HB2	1.79	0.64
1:L:155:ILE:HG12	1:L:375:LEU:HD13	1.79	0.63
2:C:89:GLU:O	2:C:92:LYS:HG3	1.97	0.63
2:F:89:GLU:O	2:F:92:LYS:HG3	1.97	0.63
2:S:89:GLU:HG3	2:S:92:LYS:HZ1	1.62	0.63
1:L:194:ARG:NH1	2:S:6:ILE:HD12	2.15	0.62
2:S:92:LYS:HE2	2:S:93:GLU:HB2	1.79	0.62
4:F:985:HOH:O	1:H:187:ARG:HD3	2.00	0.62
1:B:194:ARG:NH1	2:C:6:ILE:HD12	2.14	0.62
1:L:187:ARG:HD3	4:I:130:HOH:O	2.00	0.61
2:I:32:TYR:HE2	2:I:113:ILE:HD11	1.65	0.61
2:F:32:TYR:HE2	2:F:113:ILE:HD11	1.65	0.61
1:H:194:ARG:NH1	2:I:6:ILE:HD12	2.14	0.61
1:L:383:HIS:H	1:L:386:HIS:HD2	1.49	0.61
4:S:164:HOH:O	1:B:187:ARG:HD3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:194:ARG:NH1	2:F:6:ILE:HD12	2.15	0.61
1:B:383:HIS:H	1:B:386:HIS:HD2	1.49	0.60
4:C:713:HOH:O	1:E:187:ARG:HD3	2.00	0.60
2:C:89:GLU:HG3	2:C:92:LYS:HZ1	1.65	0.60
2:S:32:TYR:HE2	2:S:113:ILE:HD11	1.65	0.60
1:E:383:HIS:H	1:E:386:HIS:HD2	1.49	0.60
1:H:383:HIS:H	1:H:386:HIS:HD2	1.49	0.60
1:H:229:GLN:HE21	1:H:236:LYS:H	1.49	0.59
1:E:229:GLN:HE21	1:E:236:LYS:H	1.49	0.59
2:C:32:TYR:HE2	2:C:113:ILE:HD11	1.65	0.59
1:L:229:GLN:HE21	1:L:236:LYS:H	1.49	0.59
2:C:32:TYR:CE2	2:C:113:ILE:HD11	2.39	0.58
1:E:140:ILE:HD13	1:E:320:LEU:HD11	1.86	0.58
2:F:32:TYR:CE2	2:F:113:ILE:HD11	2.39	0.58
1:H:140:ILE:HD13	1:H:320:LEU:HD11	1.86	0.58
1:B:229:GLN:HE21	1:B:236:LYS:H	1.49	0.58
4:H:684:HOH:O	2:I:10:LYS:HE3	2.04	0.57
2:I:32:TYR:CE2	2:I:113:ILE:HD11	2.39	0.57
1:L:200:THR:OG1	1:L:238:HIS:HD2	1.87	0.57
4:L:681:HOH:O	2:S:10:LYS:HE3	2.04	0.57
1:L:140:ILE:HD13	1:L:320:LEU:HD11	1.86	0.57
2:S:32:TYR:CE2	2:S:113:ILE:HD11	2.39	0.57
1:B:140:ILE:HD13	1:B:320:LEU:HD11	1.86	0.57
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.87	0.57
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.87	0.57
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.88	0.57
1:E:26:THR:HG21	1:E:83:ARG:HD3	1.87	0.57
1:H:202:ASP:OD1	1:H:238:HIS:HE1	1.88	0.57
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.88	0.57
4:E:684:HOH:O	2:F:10:LYS:HE3	2.04	0.57
1:H:200:THR:OG1	1:H:238:HIS:HD2	1.87	0.57
1:B:26:THR:HG21	1:B:83:ARG:HD3	1.87	0.56
4:B:683:HOH:O	2:C:10:LYS:HE3	2.04	0.56
1:H:26:THR:HG21	1:H:83:ARG:HD3	1.87	0.56
1:L:26:THR:HG21	1:L:83:ARG:HD3	1.87	0.56
1:H:26:THR:CG2	1:H:29:TYR:HB2	2.36	0.56
1:L:202:ASP:OD1	1:L:238:HIS:HE1	1.88	0.56
1:E:153:HIS:HE1	4:E:630:HOH:O	1.90	0.55
1:L:14:LYS:HE2	1:L:15:ALA:O	2.07	0.55
1:B:14:LYS:HE2	1:B:15:ALA:O	2.07	0.55
1:E:14:LYS:HE2	1:E:15:ALA:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:153:HIS:HE1	4:H:630:HOH:O	1.90	0.55
1:L:153:HIS:HE1	4:L:627:HOH:O	1.90	0.55
1:H:14:LYS:HE2	1:H:15:ALA:O	2.07	0.54
1:B:153:HIS:HE1	4:B:629:HOH:O	1.90	0.54
1:L:26:THR:CG2	1:L:29:TYR:HB2	2.36	0.54
1:H:26:THR:CG2	1:H:26:THR:O	2.56	0.54
1:H:414:ALA:HB3	1:H:415:PRO:HD3	1.90	0.54
1:B:26:THR:CG2	1:B:26:THR:O	2.56	0.53
1:E:26:THR:CG2	1:E:26:THR:O	2.56	0.53
1:E:26:THR:CG2	1:E:29:TYR:HB2	2.36	0.53
1:B:431:ARG:HH21	1:B:432:ASN:HD21	1.57	0.53
1:B:26:THR:CG2	1:B:29:TYR:HB2	2.36	0.53
1:L:26:THR:O	1:L:26:THR:CG2	2.56	0.53
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.90	0.53
1:E:431:ARG:HH21	1:E:432:ASN:HD21	1.57	0.52
1:H:431:ARG:HH21	1:H:432:ASN:HD21	1.57	0.52
1:B:414:ALA:HB3	1:B:415:PRO:HD3	1.90	0.52
1:L:414:ALA:HB3	1:L:415:PRO:HD3	1.90	0.52
1:L:431:ARG:HH21	1:L:432:ASN:HD21	1.57	0.52
1:L:121:VAL:HG22	1:L:125:PHE:CE1	2.45	0.52
1:E:121:VAL:HG22	1:E:125:PHE:CE1	2.45	0.52
1:B:121:VAL:HG22	1:B:125:PHE:CE1	2.45	0.51
1:H:121:VAL:HG22	1:H:125:PHE:CE1	2.45	0.50
1:E:296:ALA:O	1:E:297:MET:HB3	2.12	0.50
1:H:296:ALA:O	1:H:297:MET:HB3	2.12	0.50
1:B:296:ALA:O	1:B:297:MET:HB3	2.12	0.50
2:S:46:THR:HG22	2:S:97:ALA:HB2	1.94	0.49
1:L:296:ALA:O	1:L:297:MET:HB3	2.12	0.49
2:C:46:THR:HG22	2:C:97:ALA:HB2	1.94	0.49
2:F:46:THR:HG22	2:F:97:ALA:HB2	1.94	0.49
1:E:383:HIS:H	1:E:386:HIS:CD2	2.30	0.48
1:B:442:ASN:O	1:B:446:ARG:HG3	2.13	0.48
2:I:46:THR:HG22	2:I:97:ALA:HB2	1.95	0.48
1:H:442:ASN:O	1:H:446:ARG:HG3	2.13	0.48
1:L:442:ASN:O	1:L:446:ARG:HG3	2.13	0.48
1:H:383:HIS:H	1:H:386:HIS:CD2	2.30	0.48
1:E:431:ARG:HE	1:E:432:ASN:ND2	2.12	0.48
1:H:431:ARG:HE	1:H:432:ASN:ND2	2.12	0.48
1:E:442:ASN:O	1:E:446:ARG:HG3	2.13	0.47
1:L:431:ARG:HE	1:L:432:ASN:ND2	2.12	0.47
1:B:431:ARG:HE	1:B:432:ASN:ND2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:70:TRP:HZ2	2:I:89:GLU:HG2	1.80	0.47
1:B:383:HIS:H	1:B:386:HIS:CD2	2.30	0.47
1:L:382:ILE:HA	1:L:386:HIS:CD2	2.50	0.47
1:E:382:ILE:HA	1:E:386:HIS:CD2	2.50	0.46
2:I:34:LEU:HD12	2:I:80:PRO:HG3	1.97	0.46
2:S:70:TRP:HZ2	2:S:89:GLU:HG2	1.80	0.46
2:F:34:LEU:HD12	2:F:80:PRO:HG3	1.97	0.46
2:F:6:ILE:HG22	2:F:7:LEU:HG	1.98	0.46
1:L:184:ASN:ND2	1:L:187:ARG:HH21	2.14	0.46
2:C:70:TRP:HZ2	2:C:89:GLU:HG2	1.80	0.46
1:H:156:GLN:HG3	2:I:110:VAL:HG12	1.98	0.46
1:B:184:ASN:ND2	1:B:187:ARG:HH21	2.14	0.46
2:I:6:ILE:HG22	2:I:7:LEU:HG	1.98	0.46
2:F:70:TRP:HZ2	2:F:89:GLU:HG2	1.80	0.45
1:H:382:ILE:HA	1:H:386:HIS:CD2	2.50	0.45
2:C:6:ILE:HG22	2:C:7:LEU:HG	1.98	0.45
2:I:40:PRO:HG2	2:I:74:MET:HB2	1.98	0.45
1:B:382:ILE:HA	1:B:386:HIS:CD2	2.50	0.45
2:S:34:LEU:HD12	2:S:80:PRO:HG3	1.97	0.45
2:C:40:PRO:HG2	2:C:74:MET:HB2	1.98	0.45
1:E:79:ARG:HH11	1:E:79:ARG:CG	2.30	0.45
1:H:177:LYS:HG2	1:H:203:ASP:OD2	2.16	0.45
1:B:79:ARG:HH11	1:B:79:ARG:CG	2.30	0.45
1:E:184:ASN:ND2	1:E:187:ARG:HH21	2.14	0.45
1:E:156:GLN:HG3	2:F:110:VAL:HG12	1.98	0.45
1:H:184:ASN:ND2	1:H:187:ARG:HH21	2.14	0.45
1:H:79:ARG:HH11	1:H:79:ARG:CG	2.30	0.45
1:L:177:LYS:HG2	1:L:203:ASP:OD2	2.16	0.45
1:B:177:LYS:HG2	1:B:203:ASP:OD2	2.17	0.45
2:S:40:PRO:HG2	2:S:74:MET:HB2	1.98	0.45
2:S:6:ILE:CD1	2:I:68:THR:HG21	2.47	0.44
1:L:383:HIS:H	1:L:386:HIS:CD2	2.30	0.44
1:L:79:ARG:CG	1:L:79:ARG:HH11	2.30	0.44
1:B:156:GLN:HG3	2:C:110:VAL:HG12	1.98	0.44
2:C:34:LEU:HD12	2:C:80:PRO:HG3	1.97	0.44
2:S:6:ILE:HG22	2:S:7:LEU:HG	1.98	0.44
2:S:6:ILE:HG12	2:I:68:THR:HG21	2.00	0.44
1:L:156:GLN:HG3	2:S:110:VAL:HG12	1.98	0.44
2:F:40:PRO:HG2	2:F:74:MET:HB2	1.98	0.44
2:S:6:ILE:HD11	2:I:68:THR:HG21	2.00	0.44
2:S:68:THR:HG21	2:C:6:ILE:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:68:THR:HG21	2:C:6:ILE:HD11	2.00	0.44
1:E:177:LYS:HG2	1:E:203:ASP:OD2	2.16	0.43
2:C:68:THR:HG21	2:F:6:ILE:HG12	2.00	0.43
2:C:68:THR:HG21	2:F:6:ILE:CD1	2.48	0.43
2:I:89:GLU:CG	2:I:92:LYS:HZ1	2.24	0.43
1:L:171:GLY:HA2	1:L:199:PHE:O	2.19	0.43
1:B:79:ARG:HH11	1:B:79:ARG:HG3	1.84	0.43
1:L:79:ARG:HG3	1:L:79:ARG:HH11	1.84	0.43
2:S:79:ASP:HB3	2:S:82:GLN:OE1	2.19	0.43
1:B:171:GLY:HA2	1:B:199:PHE:O	2.19	0.43
1:E:171:GLY:HA2	1:E:199:PHE:O	2.19	0.42
1:H:171:GLY:HA2	1:H:199:PHE:O	2.19	0.42
2:F:68:THR:HG21	2:I:6:ILE:CD1	2.48	0.42
2:F:68:THR:HG21	2:I:6:ILE:HD11	2.01	0.42
1:B:86:HIS:HD2	4:B:674:HOH:O	2.03	0.42
2:F:79:ASP:HB3	2:F:82:GLN:OE1	2.19	0.42
1:B:382:ILE:HA	1:B:386:HIS:HD2	1.85	0.42
1:E:436:ASP:OD2	1:E:439:ARG:HG3	2.20	0.42
1:H:382:ILE:HA	1:H:386:HIS:HD2	1.85	0.42
1:L:436:ASP:OD2	1:L:439:ARG:HG3	2.20	0.42
1:L:86:HIS:HD2	4:L:672:HOH:O	2.02	0.42
2:C:79:ASP:HB3	2:C:82:GLN:OE1	2.19	0.42
1:H:79:ARG:HH11	1:H:79:ARG:HG3	1.84	0.42
1:E:86:HIS:HD2	4:E:675:HOH:O	2.02	0.42
1:H:229:GLN:NE2	1:H:236:LYS:H	2.17	0.42
1:H:436:ASP:OD2	1:H:439:ARG:HG3	2.20	0.42
1:B:88:GLU:HA	1:B:89:PRO:HD3	1.96	0.41
1:E:79:ARG:HH11	1:E:79:ARG:HG3	1.84	0.41
2:I:79:ASP:HB3	2:I:82:GLN:OE1	2.19	0.41
2:C:68:THR:HG21	2:F:6:ILE:HD11	2.01	0.41
1:B:436:ASP:OD2	1:B:439:ARG:HG3	2.20	0.41
2:F:22:THR:H	2:F:25:GLN:NE2	2.13	0.41
2:C:79:ASP:HA	2:C:80:PRO:HD3	1.91	0.41
1:E:382:ILE:HA	1:E:386:HIS:HD2	1.85	0.41
2:F:68:THR:HG21	2:I:6:ILE:HG12	2.02	0.41
2:F:89:GLU:CG	2:F:92:LYS:HZ1	2.27	0.41
1:H:86:HIS:HD2	4:H:675:HOH:O	2.02	0.41
1:L:382:ILE:HA	1:L:386:HIS:HD2	1.85	0.41
2:S:68:THR:HG21	2:C:6:ILE:HG12	2.02	0.41
2:F:5:PRO:HB2	2:F:9:LEU:HG	2.03	0.41
2:S:5:PRO:HB2	2:S:9:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:5:PRO:HB2	2:C:9:LEU:HG	2.03	0.41
1:H:175:LYS:HA	1:H:176:PRO:C	2.41	0.41
2:I:5:PRO:HB2	2:I:9:LEU:HG	2.03	0.41
1:L:229:GLN:NE2	1:L:236:LYS:H	2.17	0.41
1:E:175:LYS:HA	1:E:176:PRO:C	2.42	0.41
2:S:7:LEU:HD21	2:I:46:THR:OG1	2.20	0.41
1:B:175:LYS:HA	1:B:176:PRO:C	2.42	0.40
2:C:46:THR:OG1	2:F:7:LEU:HD21	2.21	0.40
1:L:175:LYS:HA	1:L:176:PRO:C	2.42	0.40
2:S:22:THR:H	2:S:25:GLN:NE2	2.13	0.40

All (57) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:645:HOH:O	4:H:646:HOH:O[3_555]	0.69	1.51
4:L:642:HOH:O	4:E:646:HOH:O[3_555]	0.71	1.49
4:L:643:HOH:O	4:E:645:HOH:O[3_555]	0.72	1.48
4:B:644:HOH:O	4:B:645:HOH:O[3_555]	0.75	1.45
4:B:523:HOH:O	4:B:523:HOH:O[3_555]	0.75	1.45
4:L:520:HOH:O	4:E:523:HOH:O[3_555]	0.76	1.44
4:H:524:HOH:O	4:H:524:HOH:O[3_555]	0.76	1.44
4:H:650:HOH:O	4:H:662:HOH:O[3_555]	0.92	1.28
4:L:659:HOH:O	4:E:650:HOH:O[3_555]	0.93	1.27
4:H:519:HOH:O	4:H:529:HOH:O[3_555]	0.93	1.27
4:L:515:HOH:O	4:E:528:HOH:O[3_555]	0.94	1.26
4:L:525:HOH:O	4:E:518:HOH:O[3_555]	0.95	1.25
4:B:518:HOH:O	4:B:528:HOH:O[3_555]	0.96	1.24
4:L:647:HOH:O	4:E:662:HOH:O[3_555]	0.97	1.23
4:B:649:HOH:O	4:B:661:HOH:O[3_555]	0.97	1.23
4:L:651:HOH:O	4:E:649:HOH:O[3_555]	0.99	1.21
4:H:649:HOH:O	4:H:654:HOH:O[3_555]	1.00	1.20
4:B:648:HOH:O	4:B:653:HOH:O[3_555]	1.00	1.20
4:L:646:HOH:O	4:E:654:HOH:O[3_555]	1.01	1.19
4:B:651:HOH:O	4:B:652:HOH:O[3_555]	1.12	1.08
4:H:527:HOH:O	4:H:527:HOH:O[3_555]	1.13	1.07
4:H:651:HOH:O	4:H:651:HOH:O[3_555]	1.13	1.07
4:B:526:HOH:O	4:B:526:HOH:O[3_555]	1.14	1.06
4:L:523:HOH:O	4:E:526:HOH:O[3_555]	1.14	1.06
4:L:648:HOH:O	4:E:651:HOH:O[3_555]	1.14	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:649:HOH:O	4:E:653:HOH:O[3_555]	1.14	1.06
4:L:650:HOH:O	4:E:652:HOH:O[3_555]	1.15	1.05
4:H:652:HOH:O	4:H:653:HOH:O[3_555]	1.17	1.03
4:B:650:HOH:O	4:B:650:HOH:O[3_555]	1.17	1.03
4:H:486:HOH:O	4:H:486:HOH:O[3_555]	1.18	1.02
4:L:482:HOH:O	4:E:485:HOH:O[3_555]	1.19	1.01
4:E:532:HOH:O	4:H:477:HOH:O[3_555]	1.20	1.00
4:E:704:HOH:O	4:H:533:HOH:O[3_555]	1.21	0.99
4:B:485:HOH:O	4:B:485:HOH:O[3_555]	1.21	0.99
4:L:529:HOH:O	4:B:703:HOH:O[3_555]	1.25	0.95
4:L:701:HOH:O	4:B:532:HOH:O[3_555]	1.25	0.95
4:E:615:HOH:O	4:H:615:HOH:O[3_555]	1.26	0.94
4:L:612:HOH:O	4:B:614:HOH:O[3_555]	1.31	0.89
4:L:671:HOH:O	4:E:661:HOH:O[3_555]	1.41	0.79
4:H:661:HOH:O	4:H:674:HOH:O[3_555]	1.42	0.78
4:B:660:HOH:O	4:B:673:HOH:O[3_555]	1.42	0.78
4:L:658:HOH:O	4:E:674:HOH:O[3_555]	1.44	0.76
4:L:654:HOH:O	4:H:657:HOH:O[7_455]	1.67	0.53
4:B:655:HOH:O	4:B:679:HOH:O[3_555]	1.92	0.28
4:L:677:HOH:O	4:E:656:HOH:O[3_555]	1.92	0.28
1:H:10:SER:CB	4:F:814:HOH:O[3_555]	1.93	0.27
4:L:653:HOH:O	4:E:680:HOH:O[3_555]	1.94	0.26
4:H:656:HOH:O	4:H:680:HOH:O[3_555]	1.94	0.26
1:E:10:SER:CB	4:I:166:HOH:O[3_555]	1.94	0.26
1:L:10:SER:CB	4:C:542:HOH:O[3_555]	1.98	0.22
1:B:10:SER:CB	4:S:156:HOH:O[3_555]	2.00	0.20
4:H:673:HOH:O	4:H:673:HOH:O[3_555]	2.10	0.10
4:L:670:HOH:O	4:E:673:HOH:O[3_555]	2.11	0.09
4:B:672:HOH:O	4:B:672:HOH:O[3_555]	2.11	0.09
2:I:24:ASP:OD1	2:I:28:ARG:NH2[4_555]	2.16	0.04
2:I:24:ASP:OD2	2:I:28:ARG:NE[4_555]	2.18	0.02
1:H:88:GLU:OE1	4:L:654:HOH:O[7_445]	2.18	0.02

## 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	B	465/475 (98%)	452 (97%)	13 (3%)	0	100	100
1	E	465/475 (98%)	452 (97%)	13 (3%)	0	100	100
1	H	465/475 (98%)	452 (97%)	13 (3%)	0	100	100
1	L	465/475 (98%)	452 (97%)	13 (3%)	0	100	100
2	C	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
2	F	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
2	I	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
2	S	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
All	All	2344/2392 (98%)	2276 (97%)	68 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	B	378/386 (98%)	366 (97%)	12 (3%)	44	60
1	E	378/386 (98%)	366 (97%)	12 (3%)	44	60
1	H	378/386 (98%)	366 (97%)	12 (3%)	44	60
1	L	378/386 (98%)	366 (97%)	12 (3%)	44	60
2	C	112/112 (100%)	104 (93%)	8 (7%)	17	22
2	F	112/112 (100%)	104 (93%)	8 (7%)	17	22
2	I	112/112 (100%)	104 (93%)	8 (7%)	17	22
2	S	112/112 (100%)	104 (93%)	8 (7%)	17	22
All	All	1960/1992 (98%)	1880 (96%)	80 (4%)	35	48

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	14	LYS
1	L	17	VAL
1	L	26	THR
1	L	75	THR
1	L	79	ARG
1	L	94	GLU
1	L	127	PHE
1	L	163	ASN
1	L	225	LEU
1	L	239	TYR
1	L	241	ASN
1	L	466	LYS
2	S	6	ILE
2	S	9	LEU
2	S	33	LEU
2	S	47	ASP
2	S	56	HIS
2	S	68	THR
2	S	85	ASN
2	S	92	LYS
1	B	14	LYS
1	B	17	VAL
1	B	26	THR
1	B	75	THR
1	B	79	ARG
1	B	94	GLU
1	B	127	PHE
1	B	163	ASN
1	B	225	LEU
1	B	239	TYR
1	B	241	ASN
1	B	466	LYS
2	C	6	ILE
2	C	9	LEU
2	C	33	LEU
2	C	47	ASP
2	C	56	HIS
2	C	68	THR
2	C	85	ASN
2	C	92	LYS
1	E	14	LYS
1	E	17	VAL
1	E	26	THR

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Mol	Chain	Res	Type
1	E	75	THR
1	E	79	ARG
1	E	94	GLU
1	E	127	PHE
1	E	163	ASN
1	E	225	LEU
1	E	239	TYR
1	E	241	ASN
1	E	466	LYS
2	F	6	ILE
2	F	9	LEU
2	F	33	LEU
2	F	47	ASP
2	F	56	HIS
2	F	68	THR
2	F	85	ASN
2	F	92	LYS
1	H	14	LYS
1	H	17	VAL
1	H	26	THR
1	H	75	THR
1	H	79	ARG
1	H	94	GLU
1	H	127	PHE
1	H	163	ASN
1	H	225	LEU
1	H	239	TYR
1	H	241	ASN
1	H	466	LYS
2	I	6	ILE
2	I	9	LEU
2	I	33	LEU
2	I	47	ASP
2	I	56	HIS
2	I	68	THR
2	I	85	ASN
2	I	92	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	86	HIS

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Mol	Chain	Res	Type
1	L	153	HIS
1	L	156	GLN
1	L	163	ASN
1	L	184	ASN
1	L	229	GLN
1	L	238	HIS
1	L	241	ASN
1	L	267	HIS
1	L	277	ASN
1	L	304	GLN
1	L	386	HIS
1	L	401	GLN
1	L	420	ASN
1	L	432	ASN
2	S	25	GLN
2	S	29	GLN
1	B	86	HIS
1	B	153	HIS
1	B	156	GLN
1	B	163	ASN
1	B	184	ASN
1	B	229	GLN
1	B	238	HIS
1	B	241	ASN
1	B	267	HIS
1	B	277	ASN
1	B	304	GLN
1	B	386	HIS
1	B	401	GLN
1	B	420	ASN
1	B	432	ASN
2	C	25	GLN
2	C	29	GLN
1	E	86	HIS
1	E	153	HIS
1	E	156	GLN
1	E	163	ASN
1	E	184	ASN
1	E	229	GLN
1	E	238	HIS
1	E	241	ASN
1	E	267	HIS

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Mol	Chain	Res	Type
1	E	277	ASN
1	E	304	GLN
1	E	386	HIS
1	E	401	GLN
1	E	420	ASN
1	E	432	ASN
2	F	25	GLN
2	F	29	GLN
1	H	86	HIS
1	H	153	HIS
1	H	156	GLN
1	H	163	ASN
1	H	184	ASN
1	H	229	GLN
1	H	238	HIS
1	H	241	ASN
1	H	267	HIS
1	H	277	ASN
1	H	304	GLN
1	H	386	HIS
1	H	401	GLN
1	H	420	ASN
1	H	432	ASN
2	I	25	GLN
2	I	29	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

4 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$
3	CAP	B	476	-	14,20,20	1.14	1 (7%)	17,31,31	1.52	4 (23%)
3	CAP	E	476	-	14,20,20	1.14	1 (7%)	17,31,31	1.51	4 (23%)
3	CAP	H	476	-	14,20,20	1.14	1 (7%)	17,31,31	1.51	4 (23%)
3	CAP	L	476	-	14,20,20	1.14	1 (7%)	17,31,31	1.51	4 (23%)

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
3	CAP	B	476	-	1/1/6/6	0/23/29/29	0/0/0/0
3	CAP	E	476	-	1/1/6/6	0/23/29/29	0/0/0/0
3	CAP	H	476	-	1/1/6/6	0/23/29/29	0/0/0/0
3	CAP	L	476	-	1/1/6/6	0/23/29/29	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	476	CAP	O2-C2	-2.09	1.39	1.43
3	B	476	CAP	O2-C2	-2.08	1.39	1.43
3	E	476	CAP	O2-C2	-2.08	1.39	1.43
3	L	476	CAP	O2-C2	-2.06	1.39	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	476	CAP	O6P-P2-O5P	2.52	117.78	107.61
3	E	476	CAP	O6P-P2-O5P	2.53	117.81	107.61
3	L	476	CAP	O6P-P2-O5P	2.53	117.81	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	476	CAP	O6P-P2-O5P	2.54	117.87	107.61
3	H	476	CAP	P2-O5-C5	2.57	125.39	118.30
3	L	476	CAP	P2-O5-C5	2.59	125.42	118.30
3	B	476	CAP	P2-O5-C5	2.59	125.44	118.30
3	E	476	CAP	P2-O5-C5	2.59	125.44	118.30
3	E	476	CAP	P1-O1-C1	2.83	126.08	118.30
3	L	476	CAP	P1-O1-C1	2.84	126.11	118.30
3	H	476	CAP	P1-O1-C1	2.85	126.13	118.30
3	B	476	CAP	P1-O1-C1	2.85	126.14	118.30
3	E	476	CAP	O3P-P1-O2P	2.85	119.12	107.61
3	H	476	CAP	O3P-P1-O2P	2.86	119.14	107.61
3	L	476	CAP	O3P-P1-O2P	2.86	119.17	107.61
3	B	476	CAP	O3P-P1-O2P	2.87	119.19	107.61

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	L	476	CAP	C3
3	B	476	CAP	C3
3	H	476	CAP	C3
3	E	476	CAP	C3

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	B	467/475 (98%)	-0.81	6 (1%) 77 81	2, 6, 24, 52	0
1	E	467/475 (98%)	-0.82	6 (1%) 77 81	2, 6, 24, 52	0
1	H	467/475 (98%)	-0.78	10 (2%) 64 70	2, 6, 24, 52	0
1	L	467/475 (98%)	-0.81	8 (1%) 70 76	2, 6, 24, 52	0
2	C	123/123 (100%)	-0.44	4 (3%) 47 54	3, 15, 30, 38	0
2	F	123/123 (100%)	-0.49	2 (1%) 72 77	3, 15, 30, 38	0
2	I	123/123 (100%)	-0.44	1 (0%) 86 89	3, 15, 30, 38	0
2	S	123/123 (100%)	-0.49	4 (3%) 47 54	3, 15, 30, 38	0
All	All	2360/2392 (98%)	-0.74	41 (1%) 70 76	2, 7, 28, 52	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	9	ALA	11.8
1	E	9	ALA	10.6
1	E	10	SER	10.0
1	H	9	ALA	9.5
1	L	9	ALA	8.7
1	H	10	SER	8.2
1	L	10	SER	7.2
1	B	10	SER	6.8
1	E	11	VAL	6.7
1	B	11	VAL	5.4
1	L	11	VAL	5.0
1	H	11	VAL	4.8
1	L	92	GLY	4.3
1	E	12	GLY	4.2
1	L	94	GLU	4.1
1	H	92	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	94	GLU	4.1
1	B	94	GLU	3.5
1	L	439	ARG	3.4
1	L	12	GLY	3.2
2	S	122	GLY	3.1
1	B	439	ARG	3.1
2	C	123	TYR	2.9
1	B	12	GLY	2.8
1	E	94	GLU	2.8
1	H	439	ARG	2.8
1	H	12	GLY	2.7
1	E	439	ARG	2.7
2	I	122	GLY	2.5
1	H	93	GLU	2.5
2	F	121	ALA	2.4
1	H	464	GLU	2.4
2	C	122	GLY	2.2
1	H	475	VAL	2.2
2	C	121	ALA	2.2
2	S	92	LYS	2.2
1	L	93	GLU	2.1
2	S	121	ALA	2.1
2	C	92	LYS	2.1
2	S	123	TYR	2.1
2	F	92	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
3	CAP	E	476	21/21	0.98	0.09	1.28	3,9,15,20	0
3	CAP	B	476	21/21	0.98	0.09	0.83	3,9,15,20	0
3	CAP	H	476	21/21	0.99	0.07	-0.33	3,9,15,20	0
3	CAP	L	476	21/21	0.99	0.07	-0.64	3,9,15,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.