



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:19 AM GMT

PDB ID : 1V0E  
Title : ENDOSIALIDASE OF BACTERIOPHAGE K1F  
Authors : Stummeyer, K.; Dickmanns, A.; Muehlenhoff, M.; Gerady-Schahn, R.; Ficner, R.  
Deposited on : 2004-03-28  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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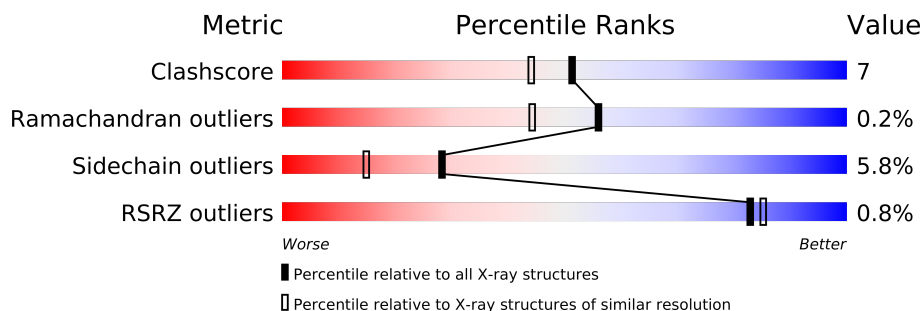
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	666	
1	B	666	
1	C	666	
1	D	666	
1	E	666	
1	F	666	

## 2 Entry composition

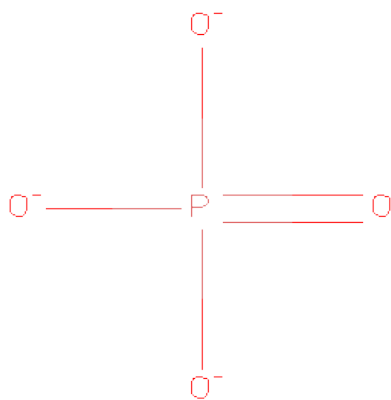
There are 3 unique types of molecules in this entry. The entry contains 34485 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ENDO-ALPHA-SIALIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	B	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	C	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	D	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	E	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	F	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is water.

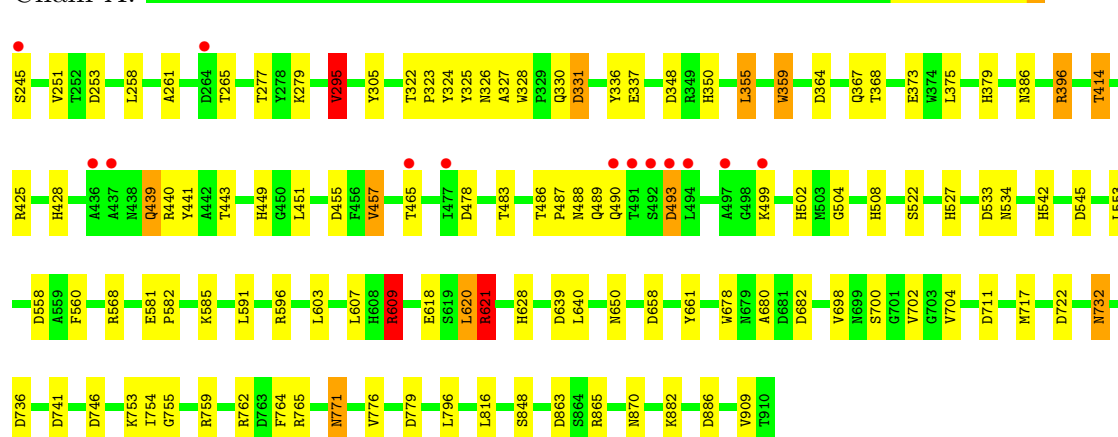
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	528	Total O 528 528	0	0
3	B	534	Total O 534 534	0	0
3	C	516	Total O 516 516	0	0
3	D	529	Total O 529 529	0	0
3	E	459	Total O 459 459	0	0
3	F	509	Total O 509 509	0	0

### 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 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 ( $RSRZ > 2$ ). 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.

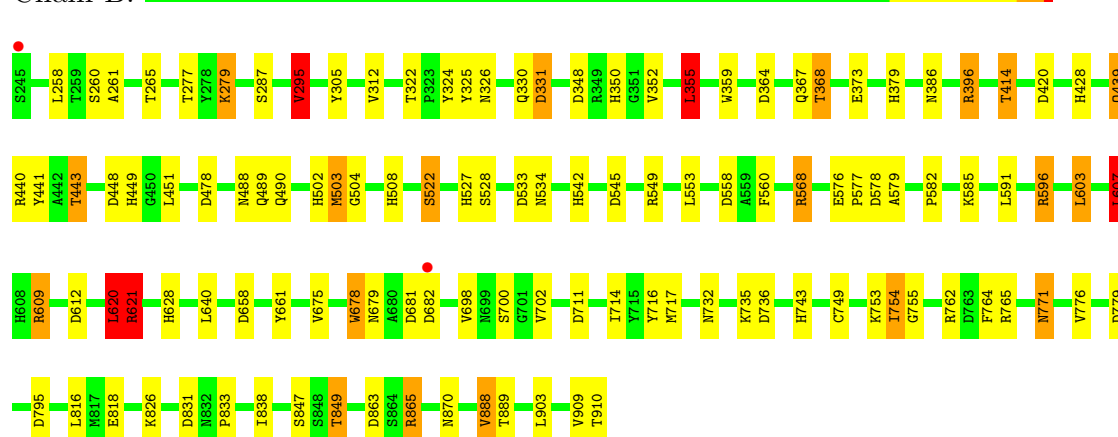
#### • Molecule 1: ENDO-ALPHA-SIALIDASE

Chain A:



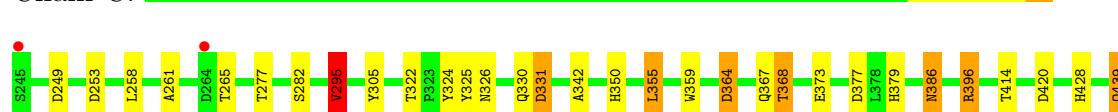
#### • Molecule 1: ENDO-ALPHA-SIALIDASE

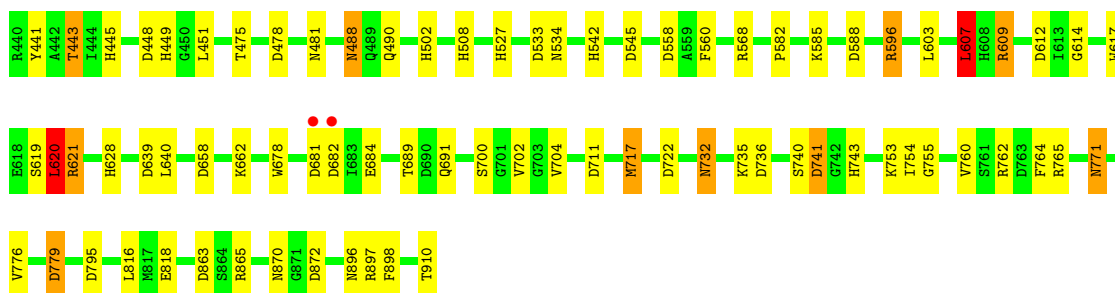
Chain B:



#### • Molecule 1: ENDO-ALPHA-SIALIDASE

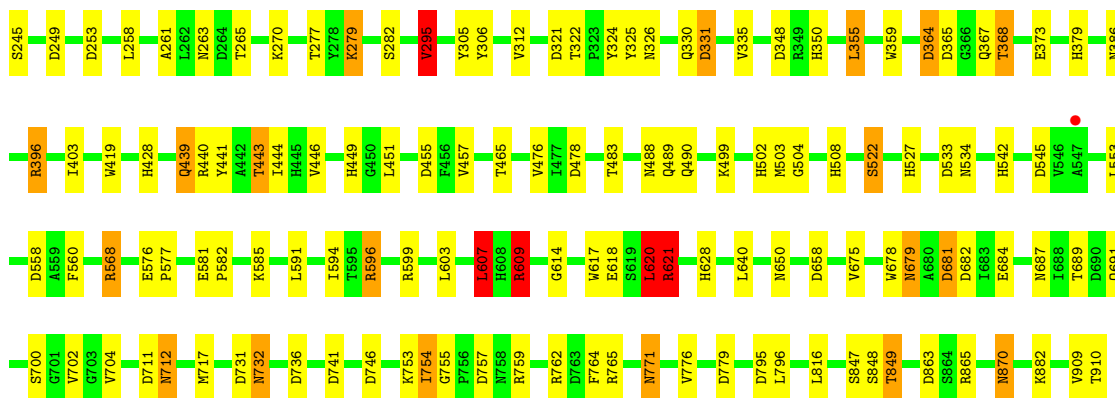
Chain C:





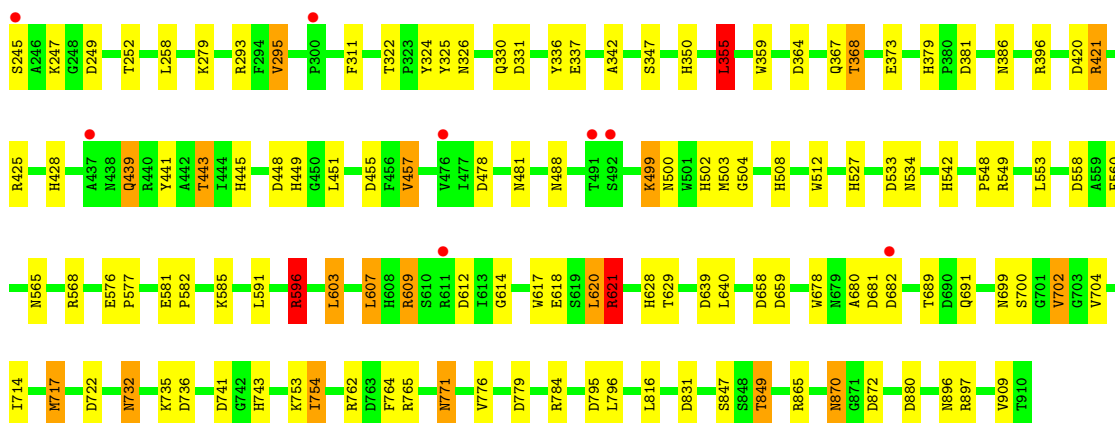
• Molecule 1: ENDO-ALPHA-SIALIDASE

Chain D:



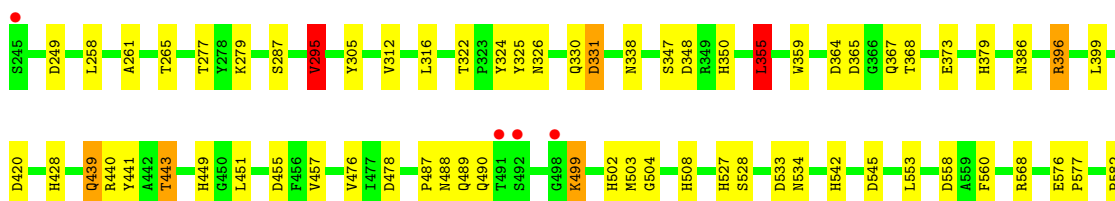
• Molecule 1: ENDO-ALPHA-SIALIDASE

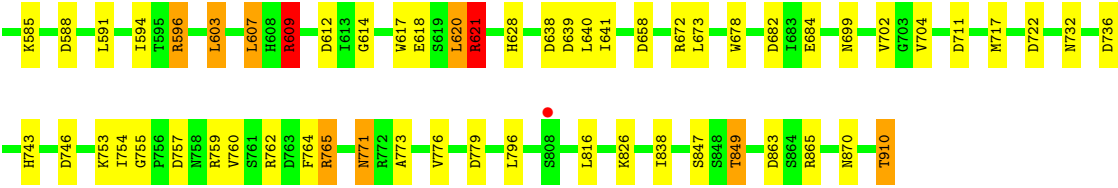
Chain E:



• Molecule 1: ENDO-ALPHA-SIALIDASE

Chain F:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.65Å 131.25Å 346.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 20.04 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.7 (30.00-1.90) 93.8 (20.04-1.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.166 , 0.202 0.183 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 31.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 335143 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	34485	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.58	0/5376	0.89	27/7325 (0.4%)
1	B	0.58	0/5376	0.90	26/7325 (0.4%)
1	C	0.55	0/5376	0.88	34/7325 (0.5%)
1	D	0.57	0/5376	0.90	32/7325 (0.4%)
1	E	0.56	0/5376	0.85	29/7325 (0.4%)
1	F	0.55	0/5376	0.89	29/7325 (0.4%)
All	All	0.57	0/32256	0.88	177/43950 (0.4%)

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	B	0	1

There are no bond length outliers.

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	ARG	NE-CZ-NH2	11.90	126.25	120.30
1	B	596	ARG	NE-CZ-NH2	9.23	124.92	120.30
1	A	596	ARG	NE-CZ-NH1	-9.08	115.76	120.30
1	F	621	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	D	355	LEU	CA-CB-CG	8.68	135.26	115.30
1	A	355	LEU	CA-CB-CG	8.57	135.02	115.30
1	C	355	LEU	CA-CB-CG	8.54	134.93	115.30
1	B	533	ASP	CB-CG-OD2	8.49	125.94	118.30
1	E	355	LEU	CA-CB-CG	8.42	134.67	115.30
1	D	609	ARG	NE-CZ-NH2	8.40	124.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	620	LEU	CA-CB-CG	8.36	134.52	115.30
1	D	620	LEU	CA-CB-CG	8.34	134.49	115.30
1	F	355	LEU	CA-CB-CG	8.24	134.25	115.30
1	F	609	ARG	NE-CZ-NH2	8.22	124.41	120.30
1	D	596	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	B	596	ARG	NE-CZ-NH1	-7.43	116.59	120.30
1	F	638	ASP	CB-CG-OD2	7.23	124.81	118.30
1	F	620	LEU	CA-CB-CG	7.21	131.89	115.30
1	D	609	ARG	NE-CZ-NH1	-7.21	116.70	120.30
1	C	620	LEU	CA-CB-CG	7.15	131.74	115.30
1	B	568	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	639	ASP	CB-CG-OD2	7.08	124.67	118.30
1	D	253	ASP	CB-CG-OD2	7.06	124.66	118.30
1	E	612	ASP	CB-CG-OD2	7.06	124.65	118.30
1	C	596	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	B	355	LEU	CA-CB-CG	6.95	131.29	115.30
1	E	596	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	D	533	ASP	CB-CG-OD2	6.91	124.52	118.30
1	A	295	VAL	CB-CA-C	-6.89	98.30	111.40
1	D	455	ASP	CB-CG-OD2	6.79	124.41	118.30
1	B	396	ARG	NE-CZ-NH1	-6.78	116.91	120.30
1	C	533	ASP	CB-CG-OD2	6.73	124.35	118.30
1	D	348	ASP	CB-CG-OD2	6.69	124.32	118.30
1	C	865	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	F	609	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	A	711	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	620	LEU	CA-CB-CG	6.57	130.41	115.30
1	A	558	ASP	CB-CG-OD2	6.55	124.20	118.30
1	D	596	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	F	533	ASP	CB-CG-OD2	6.49	124.14	118.30
1	E	478	ASP	CB-CG-OD2	6.47	124.12	118.30
1	D	558	ASP	CB-CG-OD2	6.43	124.09	118.30
1	A	478	ASP	CB-CG-OD2	6.42	124.08	118.30
1	F	596	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	F	396	ARG	NE-CZ-NH1	-6.37	117.12	120.30
1	A	396	ARG	NE-CZ-NH1	-6.37	117.12	120.30
1	E	681	ASP	CB-CG-OD2	6.34	124.00	118.30
1	D	621	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	C	396	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	E	865	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	D	364	ASP	CB-CG-OD2	6.30	123.97	118.30
1	F	621	ARG	NE-CZ-NH1	6.28	123.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	741	ASP	CB-CG-OD2	6.26	123.94	118.30
1	B	711	ASP	CB-CG-OD2	6.24	123.91	118.30
1	B	478	ASP	CB-CG-OD2	6.20	123.88	118.30
1	C	558	ASP	CB-CG-OD2	6.20	123.88	118.30
1	F	249	ASP	CB-CG-OD2	6.19	123.88	118.30
1	B	420	ASP	CB-CG-OD2	6.19	123.87	118.30
1	C	364	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	545	ASP	CB-CG-OD2	6.17	123.85	118.30
1	D	331	ASP	CB-CG-OD2	6.16	123.84	118.30
1	B	621	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	F	757	ASP	CB-CG-OD2	6.11	123.80	118.30
1	D	249	ASP	CB-CG-OD2	6.10	123.79	118.30
1	E	249	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	455	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	596	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	C	722	ASP	CB-CG-OD2	6.02	123.72	118.30
1	C	682	ASP	CB-CG-OD2	6.01	123.71	118.30
1	F	612	ASP	CB-CG-OD2	5.96	123.67	118.30
1	A	348	ASP	CB-CG-OD2	5.96	123.67	118.30
1	E	558	ASP	CB-CG-OD2	5.96	123.66	118.30
1	D	757	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	872	ASP	CB-CG-OD2	5.90	123.61	118.30
1	F	746	ASP	CB-CG-OD2	5.90	123.61	118.30
1	E	355	LEU	CB-CG-CD1	5.89	121.01	111.00
1	A	253	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	364	ASP	CB-CG-OD2	5.87	123.59	118.30
1	C	779	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	609	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	F	478	ASP	CB-CG-OD2	5.83	123.55	118.30
1	C	377	ASP	CB-CG-OD2	5.83	123.55	118.30
1	C	448	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	722	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	863	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	493	ASP	CB-CG-OD2	5.75	123.47	118.30
1	D	865	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	D	396	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	C	795	ASP	CB-CG-OD2	5.72	123.45	118.30
1	F	396	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	A	746	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	295	VAL	CB-CA-C	-5.69	100.60	111.40
1	D	795	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	621	ARG	NE-CZ-NH2	-5.67	117.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	455	ASP	CB-CG-OD2	5.66	123.39	118.30
1	D	682	ASP	CB-CG-OD2	5.66	123.39	118.30
1	E	448	ASP	CB-CG-OD2	5.64	123.38	118.30
1	F	348	ASP	CB-CG-OD2	5.64	123.38	118.30
1	C	741	ASP	CB-CG-OD2	5.64	123.37	118.30
1	F	639	ASP	CB-CG-OD2	5.64	123.37	118.30
1	E	621	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	D	478	ASP	CB-CG-OD2	5.62	123.36	118.30
1	E	607	LEU	CA-CB-CG	5.62	128.22	115.30
1	B	568	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	F	711	ASP	CB-CG-OD2	5.61	123.35	118.30
1	D	607	LEU	CA-CB-CG	5.60	128.17	115.30
1	B	795	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	558	ASP	CB-CG-OD2	5.56	123.31	118.30
1	E	533	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	545	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	639	ASP	CB-CG-OD2	5.52	123.27	118.30
1	F	295	VAL	CB-CA-C	-5.51	100.93	111.40
1	E	872	ASP	CB-CG-OD2	5.50	123.25	118.30
1	F	545	ASP	CB-CG-OD2	5.45	123.20	118.30
1	C	607	LEU	CA-CB-CG	5.45	127.83	115.30
1	C	612	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	612	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	295	VAL	CB-CA-C	-5.41	101.11	111.40
1	F	558	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	253	ASP	CB-CG-OD2	5.38	123.14	118.30
1	E	620	LEU	CA-CB-CG	5.38	127.68	115.30
1	B	682	ASP	CB-CG-OD2	5.38	123.14	118.30
1	E	880	ASP	CB-CG-OD2	5.37	123.13	118.30
1	E	865	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	D	295	VAL	CB-CA-C	-5.34	101.25	111.40
1	E	295	VAL	CB-CA-C	-5.33	101.27	111.40
1	D	545	ASP	CB-CG-OD2	5.32	123.09	118.30
1	F	365	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	711	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	578	ASP	CB-CG-OD2	5.29	123.06	118.30
1	F	455	ASP	CB-CG-OD2	5.29	123.06	118.30
1	E	596	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	F	331	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	545	ASP	CB-CG-OD2	5.26	123.03	118.30
1	F	863	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	831	ASP	CB-CG-OD2	5.26	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	863	ASP	CB-CG-OD2	5.25	123.03	118.30
1	C	863	ASP	CB-CG-OD2	5.25	123.02	118.30
1	E	722	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	331	ASP	CB-CG-OD2	5.24	123.01	118.30
1	C	865	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	863	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	478	ASP	CB-CG-OD2	5.23	123.00	118.30
1	D	731	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	681	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	331	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	355	LEU	CB-CG-CD1	5.21	119.86	111.00
1	C	396	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	D	365	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	420	ASP	CB-CG-OD2	5.18	122.96	118.30
1	E	741	ASP	CB-CG-OD2	5.16	122.94	118.30
1	E	831	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	533	ASP	CB-CG-OD2	5.14	122.93	118.30
1	E	381	ASP	CB-CG-OD2	5.14	122.92	118.30
1	E	795	ASP	CB-CG-OD2	5.14	122.92	118.30
1	F	682	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	741	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	295	VAL	CG1-CB-CG2	5.08	119.03	110.90
1	B	607	LEU	CA-CB-CG	5.08	126.98	115.30
1	F	722	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	711	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	331	ASP	CB-CG-OD2	5.06	122.86	118.30
1	C	249	ASP	CB-CG-OD2	5.06	122.85	118.30
1	E	420	ASP	CB-CG-OD2	5.05	122.85	118.30
1	E	639	ASP	CB-CG-OD2	5.05	122.85	118.30
1	E	682	ASP	CB-CG-OD2	5.05	122.84	118.30
1	F	355	LEU	CB-CG-CD1	5.03	119.56	111.00
1	A	682	ASP	CB-CG-OD2	5.03	122.83	118.30
1	E	659	ASP	CB-CG-OD2	5.03	122.83	118.30
1	D	746	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	681	ASP	CB-CG-OD2	5.03	122.83	118.30
1	D	321	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	448	ASP	CB-CG-OD2	5.03	122.82	118.30
1	C	588	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	348	ASP	CB-CG-OD2	5.01	122.81	118.30
1	B	865	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	865	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	503	MET	Peptide

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5230	0	4942	72	0
1	B	5230	0	4942	78	0
1	C	5230	0	4942	70	0
1	D	5230	0	4942	84	0
1	E	5230	0	4942	91	0
1	F	5230	0	4942	80	0
2	B	5	0	0	1	0
2	C	10	0	0	1	0
2	D	5	0	0	0	0
2	F	10	0	0	0	0
3	A	528	0	0	13	0
3	B	534	0	0	14	0
3	C	516	0	0	11	0
3	D	529	0	0	12	0
3	E	459	0	0	18	0
3	F	509	0	0	19	0
All	All	34485	0	29652	447	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (447) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:263:ASN:HB3	3:D:2012:HOH:O	1.36	1.19
1:A:449:HIS:HD2	1:A:451:LEU:H	1.03	1.00
1:B:490:GLN:HG3	3:B:2170:HOH:O	1.61	0.99
1:E:499:LYS:HE3	1:E:500:ASN:H	1.27	0.98
3:A:2050:HOH:O	1:B:368:THR:HG21	1.65	0.96
1:B:261:ALA:O	1:B:265:THR:HG23	1.71	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:475:THR:HB	3:C:2195:HOH:O	1.69	0.90
1:F:449:HIS:HD2	1:F:451:LEU:H	1.14	0.90
1:E:565:ASN:HB3	3:E:2222:HOH:O	1.73	0.89
1:C:449:HIS:HD2	1:C:451:LEU:H	1.20	0.89
1:B:449:HIS:HD2	1:B:451:LEU:H	1.18	0.86
1:A:765:ARG:HH12	1:C:367:GLN:HE21	1.24	0.86
1:D:765:ARG:HH12	1:E:367:GLN:HE21	1.21	0.85
1:D:449:HIS:HD2	1:D:451:LEU:H	1.22	0.85
1:D:367:GLN:HE22	1:D:764:PHE:H	1.25	0.84
1:F:609:ARG:HG2	1:F:678:TRP:CH2	2.12	0.84
1:A:449:HIS:CD2	1:A:451:LEU:H	1.93	0.83
1:A:368:THR:HG21	3:C:2043:HOH:O	1.78	0.83
1:C:295:VAL:HG13	1:C:305:TYR:CE2	2.15	0.82
1:B:367:GLN:HE21	1:C:765:ARG:HH12	1.28	0.82
1:E:449:HIS:HD2	1:E:451:LEU:H	1.24	0.81
1:E:367:GLN:HE22	1:E:764:PHE:H	1.27	0.81
1:B:295:VAL:HG13	1:B:305:TYR:CE2	2.16	0.80
1:D:295:VAL:HG13	1:D:305:TYR:CE2	2.16	0.80
1:F:621:ARG:HD2	3:F:2297:HOH:O	1.81	0.80
1:A:620:LEU:HD21	1:A:680:ALA:HB2	1.63	0.79
1:A:367:GLN:HE21	1:B:765:ARG:HH12	1.27	0.79
1:A:295:VAL:HG13	1:A:305:TYR:CE2	2.18	0.78
1:B:440:ARG:HE	1:B:489:GLN:HE21	1.29	0.78
1:E:765:ARG:HH12	1:F:367:GLN:HE21	1.29	0.78
1:D:553:LEU:HD22	1:D:591:LEU:HD21	1.66	0.78
1:B:322:THR:HG21	3:B:2054:HOH:O	1.83	0.78
1:A:261:ALA:O	1:A:265:THR:HG23	1.83	0.77
1:C:367:GLN:HE22	1:C:764:PHE:H	1.31	0.77
1:A:367:GLN:HE22	1:A:764:PHE:H	1.32	0.77
1:F:367:GLN:HE22	1:F:764:PHE:H	1.33	0.76
1:C:609:ARG:HG2	1:C:678:TRP:CH2	2.19	0.76
1:F:443:THR:HG21	3:F:2118:HOH:O	1.86	0.75
1:E:503:MET:HG2	1:E:504:GLY:HA3	1.69	0.75
1:B:367:GLN:HE22	1:B:764:PHE:H	1.35	0.74
1:E:609:ARG:HG2	1:E:678:TRP:CH2	2.21	0.74
1:C:443:THR:HG22	3:C:2161:HOH:O	1.87	0.74
1:B:847:SER:OG	1:B:849:THR:HB	1.88	0.73
1:B:449:HIS:CD2	1:B:451:LEU:H	2.04	0.73
1:E:245:SER:HB3	3:E:2001:HOH:O	1.88	0.73
1:E:322:THR:HG22	1:E:324:TYR:H	1.52	0.72
1:F:449:HIS:CD2	1:F:451:LEU:H	2.03	0.72
1:F:364:ASP:OD1	1:F:368:THR:HG22	1.90	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:499:LYS:CE	1:E:500:ASN:H	2.02	0.71
1:B:443:THR:HG21	3:B:2183:HOH:O	1.91	0.71
1:D:449:HIS:CD2	1:D:451:LEU:H	2.08	0.71
1:F:322:THR:HG22	1:F:324:TYR:H	1.56	0.70
3:B:2047:HOH:O	1:C:368:THR:HG21	1.92	0.70
1:D:609:ARG:HG2	1:D:678:TRP:CZ2	2.25	0.70
1:B:364:ASP:OD1	1:B:368:THR:HB	1.92	0.70
1:C:373:GLU:OE2	1:C:508:HIS:HE1	1.75	0.70
1:C:322:THR:HG22	1:C:324:TYR:H	1.56	0.70
1:D:440:ARG:HE	1:D:489:GLN:HE21	1.37	0.70
1:F:295:VAL:HG13	1:F:305:TYR:CE2	2.26	0.69
1:F:322:THR:HG21	3:F:2048:HOH:O	1.90	0.69
1:C:277:THR:HG22	1:C:295:VAL:HG22	1.75	0.69
1:F:588:ASP:HB3	3:F:2278:HOH:O	1.92	0.69
1:A:771:ASN:HD21	1:A:776:VAL:H	1.40	0.69
1:A:322:THR:HG21	3:A:2056:HOH:O	1.91	0.69
3:D:2051:HOH:O	1:F:368:THR:HG21	1.91	0.69
1:D:553:LEU:CD2	1:D:591:LEU:HD21	2.23	0.68
1:F:732:ASN:HD21	1:F:736:ASP:H	1.41	0.68
1:A:553:LEU:HD22	1:A:591:LEU:HD21	1.74	0.68
1:D:322:THR:HG21	3:D:2056:HOH:O	1.93	0.68
1:F:553:LEU:CD2	1:F:591:LEU:HD21	2.24	0.68
1:A:621:ARG:HD3	3:A:2307:HOH:O	1.93	0.67
1:A:620:LEU:HD21	1:A:680:ALA:CB	2.24	0.67
1:B:443:THR:HG22	3:B:2182:HOH:O	1.93	0.67
1:A:621:ARG:CD	3:A:2307:HOH:O	2.41	0.67
1:F:396:ARG:HD3	1:F:534:ASN:O	1.93	0.67
1:E:771:ASN:HD21	1:E:776:VAL:H	1.42	0.67
1:E:449:HIS:CD2	1:E:451:LEU:H	2.10	0.66
1:F:847:SER:OG	1:F:849:THR:HB	1.95	0.66
1:A:414:THR:HG21	3:A:2141:HOH:O	1.96	0.66
1:E:499:LYS:HG3	3:E:2149:HOH:O	1.96	0.66
1:E:603:LEU:HG	1:E:621:ARG:HD3	1.77	0.66
1:D:771:ASN:HD21	1:D:776:VAL:H	1.43	0.66
1:D:732:ASN:HD21	1:D:736:ASP:H	1.43	0.65
1:E:439:GLN:HE22	1:E:441:TYR:HB2	1.62	0.65
1:B:771:ASN:HD21	1:B:776:VAL:H	1.45	0.65
1:F:542:HIS:HD2	3:F:2235:HOH:O	1.81	0.64
1:E:897:ARG:CZ	3:E:2451:HOH:O	2.46	0.64
1:D:609:ARG:HG2	1:D:678:TRP:CH2	2.32	0.64
1:D:882:LYS:HD2	1:E:896:ASN:HB2	1.80	0.64
1:A:325:TYR:OH	1:A:350:HIS:HE1	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:439:GLN:HE22	1:F:441:TYR:HB2	1.63	0.63
1:C:330:GLN:HB2	1:C:527:HIS:HE1	1.63	0.63
1:D:367:GLN:HE21	1:F:765:ARG:HH12	1.46	0.63
1:D:396:ARG:HD3	1:D:534:ASN:O	1.99	0.63
1:A:367:GLN:HE21	1:B:765:ARG:NH1	1.96	0.63
1:D:628:HIS:HE1	1:D:658:ASP:OD1	1.82	0.63
1:A:765:ARG:NH1	1:C:367:GLN:HE21	1.95	0.63
1:A:553:LEU:CD2	1:A:591:LEU:HD21	2.29	0.63
1:E:620:LEU:HD21	1:E:680:ALA:HB2	1.80	0.63
1:E:549:ARG:HG3	3:E:2207:HOH:O	1.99	0.62
1:A:443:THR:HG22	1:A:483:THR:HG22	1.81	0.62
1:B:428:HIS:ND1	1:B:502:HIS:HD2	1.96	0.62
1:E:330:GLN:HB2	1:E:527:HIS:HE1	1.64	0.62
1:A:396:ARG:HD3	1:A:534:ASN:O	1.99	0.62
1:D:364:ASP:OD1	1:D:368:THR:HG22	2.00	0.62
1:C:428:HIS:ND1	1:C:502:HIS:HD2	1.97	0.62
1:F:771:ASN:HD21	1:F:776:VAL:H	1.48	0.62
1:B:396:ARG:HD3	1:B:534:ASN:O	2.00	0.61
1:A:367:GLN:NE2	1:B:765:ARG:HH12	1.97	0.61
1:F:347:SER:HB3	1:F:355:LEU:HB2	1.82	0.61
1:F:428:HIS:ND1	1:F:502:HIS:HD2	1.98	0.61
1:C:449:HIS:CD2	1:C:451:LEU:H	2.09	0.61
1:C:439:GLN:NE2	1:C:441:TYR:H	1.98	0.61
1:B:373:GLU:OE2	1:B:508:HIS:HE1	1.82	0.61
1:C:277:THR:CG2	1:C:295:VAL:HG22	2.31	0.60
1:D:712:ASN:HD22	1:D:712:ASN:H	1.49	0.60
1:C:322:THR:HG21	3:C:2049:HOH:O	2.00	0.60
1:C:325:TYR:OH	1:C:350:HIS:HE1	1.84	0.60
1:D:443:THR:HG22	3:D:2158:HOH:O	2.01	0.60
1:D:765:ARG:NH1	1:E:367:GLN:HE21	1.95	0.59
1:B:527:HIS:HD2	1:B:582:PRO:O	1.84	0.59
1:A:732:ASN:HD21	1:A:736:ASP:H	1.49	0.59
1:D:350:HIS:HD2	3:D:2192:HOH:O	1.85	0.59
1:A:527:HIS:HD2	1:A:582:PRO:O	1.84	0.59
1:C:771:ASN:HD21	1:C:776:VAL:H	1.50	0.59
1:F:553:LEU:HD22	1:F:591:LEU:HD21	1.83	0.59
1:C:609:ARG:HG2	1:C:678:TRP:CZ2	2.38	0.59
1:C:527:HIS:HD2	1:C:582:PRO:O	1.85	0.59
1:B:396:ARG:HB3	1:B:560:PHE:CZ	2.37	0.59
1:E:439:GLN:NE2	1:E:441:TYR:H	2.00	0.59
1:B:771:ASN:ND2	1:B:776:VAL:H	2.00	0.59
1:D:847:SER:OG	1:D:849:THR:HB	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:527:HIS:HD2	1:D:582:PRO:O	1.84	0.59
1:F:261:ALA:O	1:F:265:THR:HG23	2.03	0.58
1:A:771:ASN:ND2	1:A:776:VAL:H	2.00	0.58
1:F:373:GLU:OE2	1:F:508:HIS:HE1	1.86	0.58
1:A:609:ARG:HG2	1:A:678:TRP:CH2	2.38	0.58
1:F:443:THR:HG22	3:F:2156:HOH:O	2.03	0.58
1:B:330:GLN:HB2	1:B:527:HIS:HE1	1.69	0.58
1:E:847:SER:OG	1:E:849:THR:HB	2.04	0.58
1:E:445:HIS:HD2	1:E:481:ASN:HD21	1.51	0.58
1:D:295:VAL:HG13	1:D:305:TYR:CD2	2.39	0.58
1:E:527:HIS:HD2	1:E:582:PRO:O	1.87	0.58
1:F:457:VAL:HA	1:F:504:GLY:O	2.04	0.58
1:E:379:HIS:H	1:E:386:ASN:ND2	2.00	0.58
1:D:322:THR:HG22	1:D:324:TYR:H	1.69	0.58
1:A:428:HIS:ND1	1:A:502:HIS:HD2	2.01	0.58
1:F:277:THR:HG22	1:F:295:VAL:HG22	1.84	0.57
1:E:771:ASN:ND2	1:E:776:VAL:H	2.02	0.57
1:E:322:THR:HB	1:E:326:ASN:OD1	2.03	0.57
1:F:490:GLN:HG2	3:F:2196:HOH:O	2.04	0.57
1:A:449:HIS:HD2	1:A:451:LEU:N	1.87	0.57
1:E:396:ARG:HD3	1:E:534:ASN:O	2.04	0.57
1:E:368:THR:HG21	3:F:2041:HOH:O	2.04	0.57
1:C:628:HIS:HE1	1:C:658:ASP:OD1	1.88	0.57
1:F:779:ASP:HB2	3:F:2423:HOH:O	2.04	0.57
1:C:330:GLN:HE21	1:C:527:HIS:CE1	2.23	0.56
1:F:330:GLN:HE21	1:F:527:HIS:CE1	2.23	0.56
1:B:322:THR:HG22	1:B:324:TYR:H	1.70	0.56
1:F:527:HIS:HD2	1:F:582:PRO:O	1.88	0.56
1:B:609:ARG:HG2	1:B:678:TRP:CZ2	2.41	0.56
1:C:364:ASP:OD1	1:C:368:THR:HB	2.05	0.56
1:D:771:ASN:ND2	1:D:776:VAL:H	2.03	0.56
1:F:779:ASP:HB2	3:F:2426:HOH:O	2.05	0.56
1:C:621:ARG:HD2	3:C:2307:HOH:O	2.04	0.56
1:E:553:LEU:CD2	1:E:591:LEU:HD21	2.36	0.56
1:D:279:LYS:HA	1:D:295:VAL:HG23	1.87	0.56
1:A:279:LYS:HA	1:A:295:VAL:HG23	1.88	0.56
1:E:621:ARG:HD2	3:E:2254:HOH:O	2.07	0.55
1:E:373:GLU:OE2	1:E:508:HIS:HE1	1.89	0.55
1:F:338:ASN:ND2	3:F:2059:HOH:O	2.40	0.55
1:A:609:ARG:HG2	1:A:678:TRP:CZ2	2.41	0.55
3:B:2103:HOH:O	1:C:779:ASP:HB2	2.05	0.55
1:B:277:THR:HG22	1:B:295:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:364:ASP:OD1	1:E:368:THR:HB	2.06	0.55
1:B:542:HIS:HD2	3:B:2263:HOH:O	1.89	0.55
1:A:322:THR:HG22	1:A:324:TYR:H	1.71	0.55
1:A:765:ARG:HH12	1:C:367:GLN:NE2	2.00	0.55
1:E:457:VAL:HA	1:E:504:GLY:O	2.07	0.55
1:B:621:ARG:CD	3:B:2325:HOH:O	2.54	0.55
1:B:826:LYS:HB2	1:B:838:ILE:HG13	1.89	0.55
1:B:732:ASN:HD21	1:B:736:ASP:H	1.54	0.55
1:C:261:ALA:O	1:C:265:THR:HG23	2.07	0.55
1:F:594:ILE:HG12	1:F:607:LEU:HD23	1.88	0.55
1:C:700:SER:OG	1:C:702:VAL:HG13	2.07	0.55
1:D:368:THR:HG21	3:E:2041:HOH:O	2.07	0.55
1:B:753:LYS:HE2	1:B:755:GLY:O	2.07	0.55
1:C:330:GLN:HE21	1:C:527:HIS:HE1	1.54	0.54
1:E:342:ALA:HB2	1:E:717:MET:HE2	1.89	0.54
1:F:534:ASN:HB2	3:F:2242:HOH:O	2.07	0.54
1:B:628:HIS:HE1	1:B:658:ASP:OD1	1.90	0.54
1:E:439:GLN:NE2	3:E:2131:HOH:O	2.40	0.54
3:D:2359:HOH:O	1:F:759:ARG:HD3	2.06	0.54
1:D:373:GLU:OE2	1:D:508:HIS:HE1	1.89	0.54
1:C:396:ARG:HD3	1:C:534:ASN:O	2.07	0.54
1:F:603:LEU:HG	1:F:621:ARG:HD3	1.90	0.54
1:B:609:ARG:NH1	1:B:675:VAL:O	2.40	0.54
1:B:621:ARG:HD2	3:B:2325:HOH:O	2.07	0.54
1:C:439:GLN:HE22	1:C:441:TYR:H	1.56	0.53
1:B:503:MET:HG2	1:B:504:GLY:HA2	1.90	0.53
1:F:322:THR:HB	1:F:326:ASN:OD1	2.08	0.53
1:E:396:ARG:HB3	1:E:560:PHE:CZ	2.44	0.53
1:F:379:HIS:H	1:F:386:ASN:ND2	2.06	0.53
1:A:396:ARG:HB3	1:A:560:PHE:CZ	2.44	0.53
1:D:305:TYR:CZ	1:D:684:GLU:HG2	2.43	0.53
1:E:765:ARG:HH12	1:F:367:GLN:NE2	2.04	0.53
1:E:342:ALA:HB2	1:E:717:MET:CE	2.39	0.53
1:B:503:MET:HG2	1:B:504:GLY:CA	2.38	0.53
1:F:440:ARG:HE	1:F:489:GLN:HE21	1.55	0.53
1:E:439:GLN:HE22	1:E:441:TYR:H	1.56	0.53
1:A:336:TYR:CE2	1:A:337:GLU:HG3	2.43	0.53
1:A:368:THR:HG23	3:A:2099:HOH:O	2.08	0.52
1:A:457:VAL:HA	1:A:504:GLY:O	2.09	0.52
1:E:620:LEU:HD21	1:E:680:ALA:CB	2.39	0.52
1:A:628:HIS:HE1	1:A:658:ASP:OD1	1.92	0.52
1:F:325:TYR:OH	1:F:350:HIS:HE1	1.93	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:628:HIS:HE1	1:F:658:ASP:OD1	1.93	0.52
1:F:771:ASN:ND2	1:F:776:VAL:H	2.08	0.52
1:B:325:TYR:OH	1:B:350:HIS:HE1	1.92	0.52
1:C:368:THR:HG22	3:C:2081:HOH:O	2.09	0.52
1:C:396:ARG:HB3	1:C:560:PHE:CZ	2.45	0.52
1:A:277:THR:HG22	1:A:295:VAL:HG22	1.92	0.52
1:D:396:ARG:HB3	1:D:560:PHE:CZ	2.44	0.52
1:C:325:TYR:OH	1:C:350:HIS:CE1	2.62	0.52
1:E:428:HIS:ND1	1:E:502:HIS:HD2	2.07	0.52
1:B:367:GLN:HE21	1:C:765:ARG:NH1	2.03	0.51
1:A:542:HIS:HE1	3:A:2159:HOH:O	1.92	0.51
1:D:261:ALA:O	1:D:265:THR:HG23	2.10	0.51
1:A:325:TYR:OH	1:A:350:HIS:CE1	2.61	0.51
1:D:765:ARG:HH12	1:E:367:GLN:NE2	1.99	0.51
1:D:457:VAL:HA	1:D:504:GLY:O	2.11	0.51
1:A:886:ASP:OD2	1:C:897:ARG:NH1	2.43	0.51
1:D:542:HIS:HD2	3:D:2237:HOH:O	1.94	0.51
1:E:732:ASN:HD21	1:E:736:ASP:H	1.59	0.51
1:B:279:LYS:HA	1:B:295:VAL:HG23	1.93	0.51
1:B:818:GLU:HB3	2:B:1685:PO4:O2	2.11	0.51
1:F:628:HIS:HD2	3:F:2283:HOH:O	1.93	0.50
1:B:607:LEU:HB3	1:B:620:LEU:HD22	1.92	0.50
1:A:779:ASP:HB2	3:C:2102:HOH:O	2.10	0.50
1:A:330:GLN:HB2	1:A:527:HIS:HE1	1.76	0.50
1:C:771:ASN:ND2	1:C:776:VAL:H	2.09	0.50
1:E:714:ILE:HG22	1:E:754:ILE:HD13	1.92	0.50
1:E:325:TYR:OH	1:E:350:HIS:HE1	1.95	0.50
1:E:628:HIS:HE1	1:E:658:ASP:OD1	1.94	0.50
1:E:396:ARG:HD2	1:E:534:ASN:ND2	2.26	0.50
1:E:553:LEU:HD22	1:E:591:LEU:HD21	1.93	0.50
1:A:650:ASN:ND2	3:A:2325:HOH:O	2.44	0.50
1:C:445:HIS:HD2	1:C:481:ASN:HD21	1.60	0.50
1:C:818:GLU:HB3	2:C:1685:PO4:O4	2.11	0.50
1:D:330:GLN:HE21	1:D:527:HIS:CE1	2.30	0.50
1:A:661:TYR:CZ	1:A:698:VAL:HB	2.47	0.50
1:D:325:TYR:OH	1:D:350:HIS:HE1	1.94	0.50
1:F:350:HIS:CE1	1:F:699:ASN:HB3	2.46	0.49
1:F:743:HIS:HD2	3:F:2391:HOH:O	1.94	0.49
3:A:2109:HOH:O	1:B:779:ASP:HB2	2.11	0.49
1:D:379:HIS:H	1:D:386:ASN:ND2	2.11	0.49
1:F:621:ARG:CD	3:F:2297:HOH:O	2.49	0.49
1:B:330:GLN:HE21	1:B:527:HIS:CE1	2.30	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:379:HIS:H	1:B:386:ASN:ND2	2.10	0.49
1:E:897:ARG:NE	3:E:2451:HOH:O	2.45	0.49
1:D:428:HIS:ND1	1:D:502:HIS:HD2	2.10	0.49
1:B:295:VAL:HG13	1:B:305:TYR:CD2	2.47	0.49
1:D:295:VAL:CG1	1:D:305:TYR:CE2	2.94	0.49
1:E:445:HIS:CD2	1:E:481:ASN:HD21	2.30	0.49
1:E:499:LYS:HE3	1:E:500:ASN:N	2.11	0.49
1:B:700:SER:OG	1:B:702:VAL:HG13	2.13	0.49
1:C:488:ASN:ND2	1:C:490:GLN:HE22	2.11	0.49
1:C:295:VAL:HG13	1:C:305:TYR:CD2	2.48	0.49
1:E:330:GLN:HB2	1:E:527:HIS:CE1	2.45	0.49
1:B:679:ASN:HD21	1:B:681:ASP:CG	2.17	0.49
1:F:826:LYS:HB2	1:F:838:ILE:HG13	1.95	0.49
1:E:765:ARG:NH1	1:F:367:GLN:HE21	2.05	0.48
1:C:330:GLN:HB2	1:C:527:HIS:CE1	2.44	0.48
1:C:542:HIS:HD2	3:C:2248:HOH:O	1.95	0.48
1:B:522:SER:OG	1:B:522:SER:O	2.32	0.48
1:B:576:GLU:N	1:B:577:PRO:CD	2.77	0.48
1:E:336:TYR:CE2	1:E:337:GLU:HG3	2.49	0.48
1:F:330:GLN:HB2	1:F:527:HIS:HE1	1.79	0.48
1:A:359:TRP:CE3	1:A:375:LEU:HD11	2.49	0.48
1:D:440:ARG:HE	1:D:489:GLN:NE2	2.09	0.48
1:A:330:GLN:HE21	1:A:527:HIS:CE1	2.32	0.48
1:E:714:ILE:CG2	1:E:754:ILE:HD13	2.44	0.47
1:B:743:HIS:HD2	3:B:2423:HOH:O	1.97	0.47
1:A:618:GLU:HG2	1:A:678:TRP:NE1	2.30	0.47
1:E:368:THR:HG22	3:E:2072:HOH:O	2.13	0.47
1:B:628:HIS:HD2	3:B:2311:HOH:O	1.98	0.47
1:A:489:GLN:O	1:E:548:PRO:HG3	2.14	0.47
1:A:621:ARG:HD2	3:A:2307:HOH:O	2.10	0.47
1:D:350:HIS:CD2	3:D:2192:HOH:O	2.65	0.47
1:E:870:ASN:C	1:E:870:ASN:HD22	2.18	0.47
1:A:465:THR:HB	1:A:490:GLN:HE22	1.80	0.47
1:E:735:LYS:O	1:E:743:HIS:HE1	1.98	0.47
1:E:689:THR:HG23	1:E:691:GLN:HE22	1.80	0.47
1:E:443:THR:HG22	3:E:2135:HOH:O	2.14	0.47
1:E:247:LYS:HG3	1:E:252:THR:HG21	1.96	0.47
1:D:753:LYS:HE2	1:D:755:GLY:O	2.15	0.47
1:A:396:ARG:HD2	1:A:534:ASN:ND2	2.30	0.47
1:E:379:HIS:H	1:E:386:ASN:HD22	1.62	0.47
1:E:576:GLU:N	1:E:577:PRO:CD	2.78	0.47
1:B:439:GLN:HE22	1:B:441:TYR:HB2	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:607:LEU:HB3	1:D:620:LEU:HD22	1.96	0.47
1:D:335:VAL:HG11	3:D:2373:HOH:O	2.16	0.47
1:D:576:GLU:N	1:D:577:PRO:CD	2.78	0.47
1:F:305:TYR:CZ	1:F:684:GLU:HG2	2.50	0.46
1:A:322:THR:HB	1:A:326:ASN:OD1	2.15	0.46
1:F:364:ASP:OD1	1:F:368:THR:CG2	2.63	0.46
1:A:628:HIS:HD2	3:A:2288:HOH:O	1.98	0.46
1:B:735:LYS:O	1:B:743:HIS:HE1	1.98	0.46
1:F:279:LYS:HE2	3:F:2002:HOH:O	2.13	0.46
1:B:888:VAL:HG12	1:B:889:THR:HG23	1.96	0.46
1:E:609:ARG:HG2	1:E:678:TRP:CZ2	2.50	0.46
1:B:330:GLN:HB2	1:B:527:HIS:CE1	2.50	0.46
1:D:542:HIS:HE1	3:D:2153:HOH:O	1.97	0.46
1:A:330:GLN:HE21	1:A:527:HIS:HE1	1.62	0.46
1:B:325:TYR:OH	1:B:350:HIS:CE1	2.68	0.46
1:D:367:GLN:HE21	1:F:765:ARG:NH1	2.11	0.46
1:A:542:HIS:HD2	3:A:2233:HOH:O	1.98	0.46
1:B:367:GLN:NE2	1:C:765:ARG:HH12	2.04	0.46
1:D:759:ARG:HD3	3:E:2293:HOH:O	2.15	0.46
1:B:330:GLN:HE21	1:B:527:HIS:HE1	1.62	0.45
1:D:689:THR:HG23	1:D:691:GLN:HE22	1.81	0.45
1:E:779:ASP:HB2	3:F:2099:HOH:O	2.15	0.45
1:F:396:ARG:HB3	1:F:560:PHE:CZ	2.52	0.45
1:D:439:GLN:HE22	1:D:441:TYR:HB2	1.81	0.45
1:D:330:GLN:HB2	1:D:527:HIS:HE1	1.82	0.45
1:D:503:MET:HG2	1:D:504:GLY:HA3	1.98	0.45
1:A:848:SER:O	1:B:865:ARG:NE	2.50	0.45
1:C:740:SER:OG	1:C:741:ASP:N	2.47	0.45
1:E:542:HIS:CD2	1:E:581:GLU:H	2.35	0.45
1:F:576:GLU:N	1:F:577:PRO:CD	2.80	0.45
1:D:679:ASN:ND2	1:D:681:ASP:H	2.15	0.45
1:A:373:GLU:OE2	1:A:508:HIS:HE1	1.98	0.45
1:C:322:THR:HG22	1:C:324:TYR:N	2.27	0.45
1:B:568:ARG:HD2	3:B:2288:HOH:O	2.16	0.45
1:F:553:LEU:HD21	1:F:591:LEU:HD21	1.96	0.45
1:F:330:GLN:HA	1:F:331:ASP:HA	1.83	0.45
1:F:331:ASP:HB3	1:F:528:SER:HA	1.99	0.45
1:C:700:SER:HG	1:C:702:VAL:HG13	1.82	0.45
1:D:403:ILE:HG13	1:D:419:TRP:CD2	2.52	0.45
1:B:322:THR:HB	1:B:326:ASN:OD1	2.17	0.44
1:A:379:HIS:H	1:A:386:ASN:ND2	2.16	0.44
1:D:700:SER:OG	1:D:702:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:330:GLN:HA	1:C:331:ASP:HA	1.75	0.44
1:D:277:THR:HG22	1:D:295:VAL:HG22	1.99	0.44
3:B:2047:HOH:O	1:C:368:THR:CG2	2.59	0.44
1:E:628:HIS:HD2	3:E:2242:HOH:O	1.99	0.44
1:E:753:LYS:HE3	1:F:287:SER:OG	2.17	0.44
1:D:322:THR:HB	1:D:326:ASN:OD1	2.16	0.44
1:F:379:HIS:H	1:F:386:ASN:HD22	1.65	0.44
1:A:700:SER:OG	1:A:702:VAL:HG13	2.17	0.44
1:F:326:ASN:ND2	3:F:2048:HOH:O	2.48	0.44
1:D:848:SER:O	1:F:865:ARG:NE	2.51	0.44
1:F:910:THR:HB	3:F:2507:HOH:O	2.17	0.44
1:C:342:ALA:HB2	1:C:717:MET:CE	2.48	0.44
1:D:712:ASN:ND2	1:D:712:ASN:H	2.14	0.44
1:D:621:ARG:CD	3:D:2296:HOH:O	2.65	0.44
1:C:689:THR:HG23	1:C:691:GLN:HE22	1.83	0.43
1:F:609:ARG:HG2	1:F:678:TRP:CZ2	2.50	0.43
1:F:609:ARG:HD2	1:F:618:GLU:OE2	2.18	0.43
1:D:542:HIS:CD2	1:D:581:GLU:H	2.36	0.43
1:C:753:LYS:HE2	1:C:755:GLY:O	2.17	0.43
1:C:305:TYR:CE1	1:C:684:GLU:HG2	2.54	0.43
1:C:322:THR:HB	1:C:326:ASN:OD1	2.18	0.43
1:D:754:ILE:HA	1:D:754:ILE:HD12	1.82	0.43
1:D:650:ASN:ND2	3:D:2323:HOH:O	2.42	0.43
1:E:322:THR:HG21	3:E:2047:HOH:O	2.17	0.43
1:A:330:GLN:HA	1:A:331:ASP:HA	1.79	0.43
1:F:503:MET:HG2	1:F:504:GLY:HA3	2.01	0.43
1:E:293:ARG:HD3	1:E:311:PHE:CE2	2.54	0.43
1:B:603:LEU:HB3	1:B:621:ARG:CZ	2.49	0.43
1:B:439:GLN:NE2	1:B:441:TYR:H	2.16	0.43
1:E:743:HIS:HD2	3:E:2182:HOH:O	2.01	0.43
1:B:903:LEU:HA	1:C:898:PHE:O	2.19	0.43
1:C:324:TYR:HB2	1:C:326:ASN:HD21	1.83	0.43
1:F:753:LYS:HE2	1:F:755:GLY:O	2.19	0.43
1:C:614:GLY:HA2	1:C:617:TRP:CZ2	2.54	0.43
1:D:522:SER:HB3	1:D:568:ARG:NH2	2.33	0.43
1:C:735:LYS:O	1:C:743:HIS:HE1	2.02	0.43
1:E:596:ARG:HG3	1:E:629:THR:O	2.18	0.42
1:C:732:ASN:HD21	1:C:736:ASP:H	1.66	0.42
1:B:414:THR:CG2	3:B:2109:HOH:O	2.67	0.42
1:A:759:ARG:HD3	3:C:2339:HOH:O	2.18	0.42
1:A:486:THR:HB	1:A:487:PRO:CD	2.50	0.42
1:D:443:THR:HB	1:D:483:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:784:ARG:HD3	1:F:773:ALA:O	2.19	0.42
1:D:465:THR:CB	1:D:490:GLN:NE2	2.82	0.42
1:E:330:GLN:HA	1:E:331:ASP:HA	1.79	0.42
1:F:330:GLN:HE21	1:F:527:HIS:HE1	1.64	0.42
1:A:568:ARG:HG2	3:A:2262:HOH:O	2.20	0.42
1:D:594:ILE:HG12	1:D:607:LEU:HD23	2.01	0.42
1:D:609:ARG:NH1	1:D:675:VAL:O	2.53	0.42
1:D:324:TYR:HB2	1:D:326:ASN:HD21	1.84	0.42
1:B:379:HIS:H	1:B:386:ASN:HD22	1.68	0.42
1:E:897:ARG:NH2	3:E:2451:HOH:O	2.52	0.42
1:D:330:GLN:HE21	1:D:527:HIS:HE1	1.66	0.42
1:F:399:LEU:O	1:F:420:ASP:HA	2.20	0.42
1:E:350:HIS:CE1	1:E:699:ASN:HB3	2.55	0.42
1:B:553:LEU:HD22	1:B:591:LEU:HD21	2.02	0.42
1:B:324:TYR:HB2	1:B:326:ASN:HD21	1.85	0.42
1:A:330:GLN:HB2	1:A:527:HIS:CE1	2.54	0.42
1:E:421:ARG:HD2	1:E:512:TRP:CD2	2.54	0.42
1:D:325:TYR:OH	1:D:350:HIS:CE1	2.73	0.41
1:A:753:LYS:HE2	1:A:755:GLY:O	2.20	0.41
1:D:330:GLN:HA	1:D:331:ASP:HA	1.80	0.41
1:E:325:TYR:OH	1:E:350:HIS:CE1	2.73	0.41
1:C:607:LEU:HB3	1:C:620:LEU:HD22	2.02	0.41
1:B:352:VAL:HA	1:B:355:LEU:HD23	2.02	0.41
1:D:444:ILE:HG22	1:D:446:VAL:HG23	2.02	0.41
1:E:771:ASN:HA	1:E:771:ASN:HD22	1.76	0.41
1:F:325:TYR:OH	1:F:350:HIS:CE1	2.74	0.41
1:A:439:GLN:HE22	1:A:441:TYR:HB2	1.85	0.41
1:B:716:TYR:O	1:B:749:CYS:HA	2.20	0.41
1:E:618:GLU:HG2	1:E:678:TRP:NE1	2.36	0.41
1:A:542:HIS:CD2	1:A:581:GLU:H	2.39	0.41
1:E:700:SER:OG	1:E:702:VAL:HG13	2.20	0.41
1:B:549:ARG:HD3	1:B:579:ALA:O	2.21	0.41
1:A:327:ALA:HB3	1:A:328:TRP:CE3	2.56	0.41
1:E:542:HIS:HD2	3:E:2202:HOH:O	2.03	0.41
1:D:609:ARG:HD2	1:D:618:GLU:OE1	2.21	0.41
1:B:661:TYR:CZ	1:B:698:VAL:HB	2.56	0.41
1:B:330:GLN:HA	1:B:331:ASP:HA	1.81	0.41
1:C:379:HIS:H	1:C:386:ASN:ND2	2.19	0.41
1:E:379:HIS:HB2	1:E:386:ASN:HA	2.03	0.41
1:C:621:ARG:CD	3:C:2307:HOH:O	2.64	0.41
1:D:465:THR:HB	1:D:490:GLN:NE2	2.36	0.41
1:D:779:ASP:HB2	3:E:2089:HOH:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:499:LYS:HD2	1:F:499:LYS:HA	1.63	0.41
1:D:609:ARG:HD2	1:D:618:GLU:HB2	2.03	0.41
1:A:440:ARG:HE	1:A:489:GLN:HE21	1.68	0.41
1:B:287:SER:OG	1:C:753:LYS:HE3	2.21	0.41
1:A:882:LYS:HD2	1:C:896:ASN:HB2	2.03	0.41
1:C:439:GLN:HE22	1:C:441:TYR:HB2	1.85	0.40
1:D:306:TYR:HD1	1:D:687:ASN:HD22	1.68	0.40
1:E:614:GLY:HA2	1:E:617:TRP:CZ2	2.56	0.40
1:E:764:PHE:HB3	1:F:316:LEU:HD23	2.02	0.40
1:F:379:HIS:HB2	1:F:386:ASN:HA	2.04	0.40
1:C:386:ASN:HA	1:C:386:ASN:HD22	1.71	0.40
1:B:331:ASP:HB3	1:B:528:SER:HA	2.02	0.40
1:E:553:LEU:HD21	1:E:591:LEU:HD21	2.03	0.40
1:D:614:GLY:HA2	1:D:617:TRP:CZ2	2.56	0.40
1:E:347:SER:HB3	1:E:355:LEU:HB2	2.03	0.40
1:C:662:LYS:HB3	3:C:2334:HOH:O	2.22	0.40
1:F:614:GLY:HA2	1:F:617:TRP:CZ2	2.56	0.40
1:B:714:ILE:HG22	1:B:754:ILE:HD13	2.04	0.40
1:D:870:ASN:C	1:D:870:ASN:HD22	2.25	0.40
1:D:527:HIS:CD2	1:D:582:PRO:O	2.71	0.40
1:F:641:ILE:HG12	1:F:672:ARG:HG2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	664/666 (100%)	642 (97%)	21 (3%)	1 (0%)	56	44
1	B	664/666 (100%)	640 (96%)	23 (4%)	1 (0%)	56	44
1	C	664/666 (100%)	642 (97%)	21 (3%)	1 (0%)	56	44
1	D	664/666 (100%)	639 (96%)	24 (4%)	1 (0%)	56	44
1	E	664/666 (100%)	636 (96%)	27 (4%)	1 (0%)	56	44
1	F	664/666 (100%)	639 (96%)	24 (4%)	1 (0%)	56	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3984/3996 (100%)	3838 (96%)	140 (4%)	6 (0%)	56	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	678	TRP
1	A	704	VAL
1	C	704	VAL
1	E	704	VAL
1	D	704	VAL
1	F	704	VAL

### 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	564/564 (100%)	534 (95%)	30 (5%)	32	18
1	B	564/564 (100%)	532 (94%)	32 (6%)	29	15
1	C	564/564 (100%)	534 (95%)	30 (5%)	32	18
1	D	564/564 (100%)	525 (93%)	39 (7%)	22	10
1	E	564/564 (100%)	532 (94%)	32 (6%)	29	15
1	F	564/564 (100%)	531 (94%)	33 (6%)	28	14
All	All	3384/3384 (100%)	3188 (94%)	196 (6%)	28	15

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	SER
1	A	251	VAL
1	A	258	LEU
1	A	295	VAL
1	A	323	PRO
1	A	355	LEU
1	A	359	TRP
1	A	414	THR

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Mol	Chain	Res	Type
1	A	425	ARG
1	A	439	GLN
1	A	457	VAL
1	A	488	ASN
1	A	493	ASP
1	A	499	LYS
1	A	522	SER
1	A	585	LYS
1	A	603	LEU
1	A	607	LEU
1	A	609	ARG
1	A	621	ARG
1	A	640	LEU
1	A	717	MET
1	A	732	ASN
1	A	754	ILE
1	A	762	ARG
1	A	771	ASN
1	A	796	LEU
1	A	816	LEU
1	A	870	ASN
1	A	909	VAL
1	B	258	LEU
1	B	260	SER
1	B	279	LYS
1	B	295	VAL
1	B	312	VAL
1	B	355	LEU
1	B	359	TRP
1	B	368	THR
1	B	414	THR
1	B	439	GLN
1	B	443	THR
1	B	488	ASN
1	B	522	SER
1	B	585	LYS
1	B	596	ARG
1	B	603	LEU
1	B	607	LEU
1	B	609	ARG
1	B	620	LEU
1	B	621	ARG

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Mol	Chain	Res	Type
1	B	640	LEU
1	B	717	MET
1	B	754	ILE
1	B	762	ARG
1	B	771	ASN
1	B	816	LEU
1	B	833	PRO
1	B	849	THR
1	B	870	ASN
1	B	888	VAL
1	B	909	VAL
1	B	910	THR
1	C	258	LEU
1	C	282	SER
1	C	295	VAL
1	C	355	LEU
1	C	359	TRP
1	C	368	THR
1	C	386	ASN
1	C	414	THR
1	C	439	GLN
1	C	443	THR
1	C	488	ASN
1	C	568	ARG
1	C	585	LYS
1	C	596	ARG
1	C	603	LEU
1	C	607	LEU
1	C	609	ARG
1	C	619	SER
1	C	620	LEU
1	C	621	ARG
1	C	640	LEU
1	C	717	MET
1	C	732	ASN
1	C	754	ILE
1	C	760	VAL
1	C	762	ARG
1	C	771	ASN
1	C	816	LEU
1	C	870	ASN
1	C	910	THR

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Mol	Chain	Res	Type
1	D	245	SER
1	D	258	LEU
1	D	270	LYS
1	D	279	LYS
1	D	282	SER
1	D	295	VAL
1	D	312	VAL
1	D	355	LEU
1	D	359	TRP
1	D	368	THR
1	D	439	GLN
1	D	443	THR
1	D	476	VAL
1	D	488	ASN
1	D	499	LYS
1	D	522	SER
1	D	568	ARG
1	D	585	LYS
1	D	596	ARG
1	D	599	ARG
1	D	603	LEU
1	D	607	LEU
1	D	609	ARG
1	D	620	LEU
1	D	621	ARG
1	D	640	LEU
1	D	679	ASN
1	D	712	ASN
1	D	717	MET
1	D	732	ASN
1	D	754	ILE
1	D	762	ARG
1	D	771	ASN
1	D	796	LEU
1	D	816	LEU
1	D	849	THR
1	D	870	ASN
1	D	909	VAL
1	D	910	THR
1	E	258	LEU
1	E	279	LYS
1	E	295	VAL

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Mol	Chain	Res	Type
1	E	355	LEU
1	E	359	TRP
1	E	368	THR
1	E	421	ARG
1	E	425	ARG
1	E	439	GLN
1	E	443	THR
1	E	457	VAL
1	E	488	ASN
1	E	499	LYS
1	E	568	ARG
1	E	585	LYS
1	E	596	ARG
1	E	603	LEU
1	E	607	LEU
1	E	609	ARG
1	E	621	ARG
1	E	640	LEU
1	E	702	VAL
1	E	717	MET
1	E	732	ASN
1	E	754	ILE
1	E	762	ARG
1	E	771	ASN
1	E	796	LEU
1	E	816	LEU
1	E	849	THR
1	E	870	ASN
1	E	909	VAL
1	F	258	LEU
1	F	295	VAL
1	F	312	VAL
1	F	355	LEU
1	F	359	TRP
1	F	439	GLN
1	F	443	THR
1	F	476	VAL
1	F	487	PRO
1	F	488	ASN
1	F	499	LYS
1	F	568	ARG
1	F	585	LYS

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Mol	Chain	Res	Type
1	F	596	ARG
1	F	603	LEU
1	F	607	LEU
1	F	609	ARG
1	F	620	LEU
1	F	621	ARG
1	F	640	LEU
1	F	673	LEU
1	F	702	VAL
1	F	717	MET
1	F	754	ILE
1	F	760	VAL
1	F	762	ARG
1	F	765	ARG
1	F	771	ASN
1	F	796	LEU
1	F	816	LEU
1	F	849	THR
1	F	870	ASN
1	F	910	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (174) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
1	A	338	ASN
1	A	350	HIS
1	A	367	GLN
1	A	386	ASN
1	A	397	ASN
1	A	439	GLN
1	A	445	HIS
1	A	449	HIS
1	A	461	ASN
1	A	481	ASN
1	A	488	ASN
1	A	489	GLN
1	A	490	GLN
1	A	500	ASN
1	A	502	HIS
1	A	508	HIS
1	A	527	HIS

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Mol	Chain	Res	Type
1	A	542	HIS
1	A	570	GLN
1	A	625	ASN
1	A	628	HIS
1	A	650	ASN
1	A	691	GLN
1	A	732	ASN
1	A	743	HIS
1	A	771	ASN
1	A	832	ASN
1	A	853	GLN
1	A	870	ASN
1	B	263	ASN
1	B	338	ASN
1	B	350	HIS
1	B	367	GLN
1	B	386	ASN
1	B	397	ASN
1	B	439	GLN
1	B	449	HIS
1	B	461	ASN
1	B	481	ASN
1	B	488	ASN
1	B	489	GLN
1	B	502	HIS
1	B	508	HIS
1	B	527	HIS
1	B	542	HIS
1	B	565	ASN
1	B	625	ASN
1	B	628	HIS
1	B	650	ASN
1	B	679	ASN
1	B	691	GLN
1	B	732	ASN
1	B	743	HIS
1	B	771	ASN
1	B	832	ASN
1	B	853	GLN
1	B	870	ASN
1	C	263	ASN
1	C	338	ASN

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Mol	Chain	Res	Type
1	C	350	HIS
1	C	367	GLN
1	C	386	ASN
1	C	397	ASN
1	C	439	GLN
1	C	445	HIS
1	C	449	HIS
1	C	461	ASN
1	C	481	ASN
1	C	488	ASN
1	C	502	HIS
1	C	508	HIS
1	C	527	HIS
1	C	542	HIS
1	C	561	ASN
1	C	570	GLN
1	C	625	ASN
1	C	628	HIS
1	C	650	ASN
1	C	676	ASN
1	C	691	GLN
1	C	732	ASN
1	C	743	HIS
1	C	771	ASN
1	C	832	ASN
1	C	853	GLN
1	C	870	ASN
1	D	263	ASN
1	D	338	ASN
1	D	350	HIS
1	D	367	GLN
1	D	386	ASN
1	D	397	ASN
1	D	439	GLN
1	D	445	HIS
1	D	449	HIS
1	D	461	ASN
1	D	481	ASN
1	D	488	ASN
1	D	489	GLN
1	D	490	GLN
1	D	502	HIS

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Mol	Chain	Res	Type
1	D	508	HIS
1	D	527	HIS
1	D	542	HIS
1	D	561	ASN
1	D	625	ASN
1	D	628	HIS
1	D	650	ASN
1	D	679	ASN
1	D	691	GLN
1	D	712	ASN
1	D	732	ASN
1	D	743	HIS
1	D	771	ASN
1	D	832	ASN
1	D	853	GLN
1	D	870	ASN
1	E	263	ASN
1	E	350	HIS
1	E	367	GLN
1	E	386	ASN
1	E	397	ASN
1	E	439	GLN
1	E	445	HIS
1	E	449	HIS
1	E	461	ASN
1	E	481	ASN
1	E	488	ASN
1	E	502	HIS
1	E	508	HIS
1	E	527	HIS
1	E	542	HIS
1	E	625	ASN
1	E	628	HIS
1	E	650	ASN
1	E	691	GLN
1	E	732	ASN
1	E	743	HIS
1	E	771	ASN
1	E	832	ASN
1	E	853	GLN
1	E	860	ASN
1	E	870	ASN

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Mol	Chain	Res	Type
1	F	263	ASN
1	F	338	ASN
1	F	350	HIS
1	F	367	GLN
1	F	386	ASN
1	F	397	ASN
1	F	439	GLN
1	F	445	HIS
1	F	449	HIS
1	F	461	ASN
1	F	481	ASN
1	F	488	ASN
1	F	489	GLN
1	F	502	HIS
1	F	508	HIS
1	F	527	HIS
1	F	542	HIS
1	F	561	ASN
1	F	625	ASN
1	F	628	HIS
1	F	650	ASN
1	F	676	ASN
1	F	691	GLN
1	F	732	ASN
1	F	743	HIS
1	F	758	ASN
1	F	771	ASN
1	F	832	ASN
1	F	853	GLN
1	F	870	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	PO4	B	1685	-	4,4,4	0.52	0	6,6,6	0.32	0
2	PO4	C	1685	-	4,4,4	0.39	0	6,6,6	0.31	0
2	PO4	C	1686	-	4,4,4	0.60	0	6,6,6	0.32	0
2	PO4	D	1685	-	4,4,4	0.50	0	6,6,6	0.31	0
2	PO4	F	1685	-	4,4,4	0.41	0	6,6,6	0.30	0
2	PO4	F	1686	-	4,4,4	0.41	0	6,6,6	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	B	1685	-	-	0/0/0/0	0/0/0/0
2	PO4	C	1685	-	-	0/0/0/0	0/0/0/0
2	PO4	C	1686	-	-	0/0/0/0	0/0/0/0
2	PO4	D	1685	-	-	0/0/0/0	0/0/0/0
2	PO4	F	1685	-	-	0/0/0/0	0/0/0/0
2	PO4	F	1686	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	666/666 (100%)	-0.09	13 (1%) 62 63	8, 14, 21, 28	0
1	B	666/666 (100%)	-0.20	2 (0%) 91 93	9, 13, 20, 29	0
1	C	666/666 (100%)	-0.20	4 (0%) 86 88	9, 13, 21, 28	0
1	D	666/666 (100%)	-0.26	1 (0%) 93 94	9, 13, 20, 28	0
1	E	666/666 (100%)	-0.14	8 (1%) 75 78	9, 14, 20, 29	0
1	F	666/666 (100%)	-0.21	5 (0%) 83 85	9, 14, 20, 28	0
All	All	3996/3996 (100%)	-0.18	33 (0%) 83 85	8, 13, 21, 29	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	491	THR	3.8
1	A	436	ALA	3.6
1	B	245	SER	3.6
1	D	547	ALA	3.2
1	E	491	THR	3.0
1	F	245	SER	2.8
1	C	681	ASP	2.8
1	F	491	THR	2.8
1	A	492	SER	2.8
1	E	245	SER	2.7
1	E	492	SER	2.7
1	E	611	ARG	2.7
1	C	682	ASP	2.6
1	A	494	LEU	2.5
1	A	245	SER	2.5
1	E	682	ASP	2.5
1	A	264	ASP	2.4
1	C	264	ASP	2.3
1	F	492	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	493	ASP	2.3
1	A	490	GLN	2.3
1	C	245	SER	2.2
1	E	437	ALA	2.2
1	E	476	VAL	2.1
1	F	808	SER	2.1
1	A	437	ALA	2.1
1	A	477	ILE	2.1
1	F	498	GLY	2.1
1	A	465	THR	2.1
1	B	682	ASP	2.1
1	E	300	PRO	2.0
1	A	499	LYS	2.0
1	A	497	ALA	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	B	1685	5/5	0.12	0.52	32,33,34,36	0
2	PO4	F	1685	5/5	0.14	0.51	38,38,39,40	0
2	PO4	F	1686	5/5	0.13	0.36	39,40,40,42	0
2	PO4	C	1685	5/5	0.10	-0.07	32,33,36,38	0
2	PO4	D	1685	5/5	0.10	-0.20	36,36,39,39	0
2	PO4	C	1686	5/5	0.10	-0.40	32,34,35,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.