



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:37 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 X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

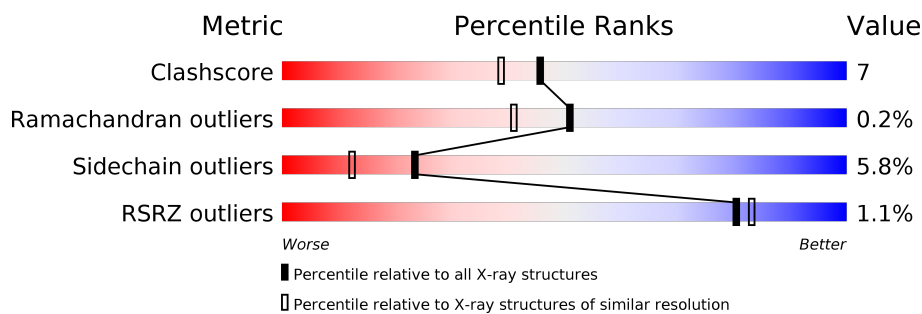
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (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 ≥ 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	666	<div> <div>3%</div> <div>82% 15% .</div> </div>
1	B	666	<div> <div>82% 14% ..</div> </div>
1	C	666	<div> <div>% 84% 13% .</div> </div>
1	D	666	<div> <div>80% 17% ..</div> </div>
1	E	666	<div> <div>2% 81% 16% .</div> </div>
1	F	666	<div> <div>% 81% 16% ..</div> </div>

2 Entry composition [i](#)

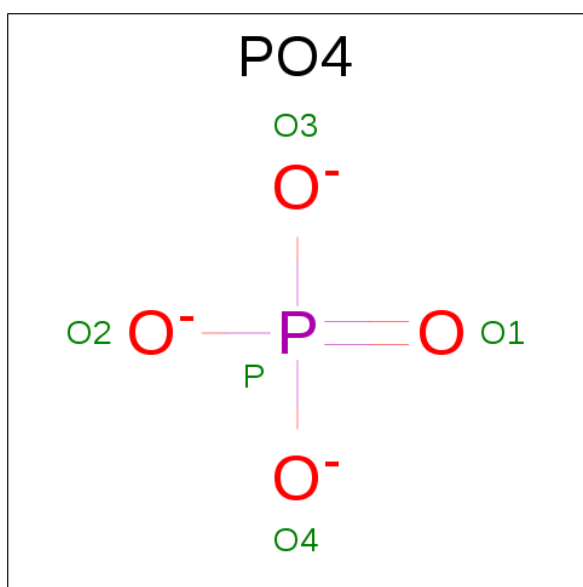
There are 3 unique types of molecules in this entry. The entry contains 34485 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 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: O₄P).



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

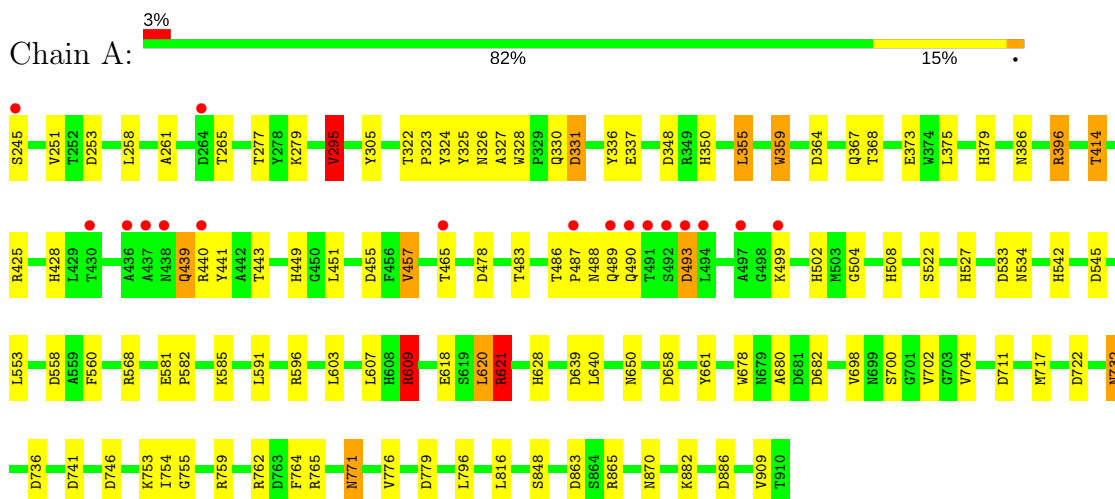
- Molecule 3 is water.

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

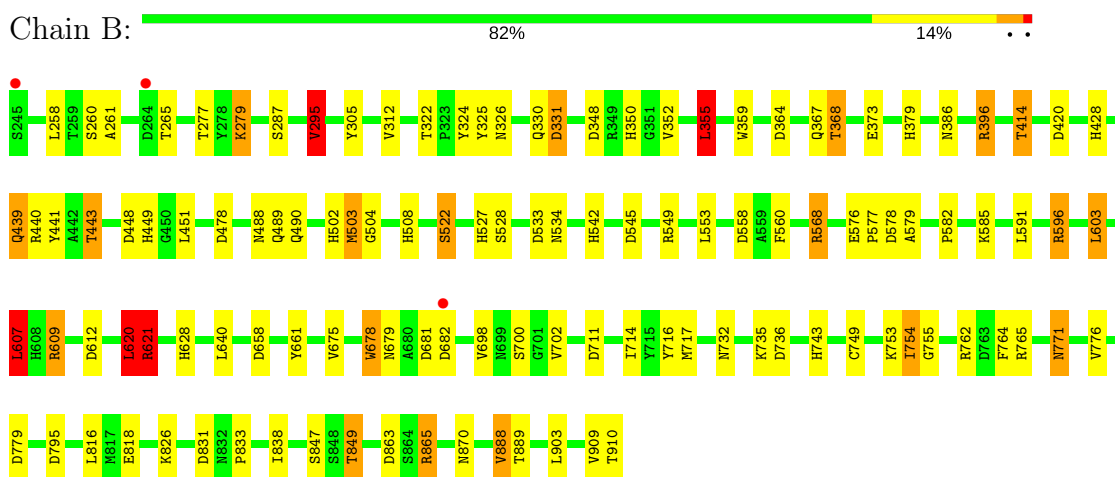
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

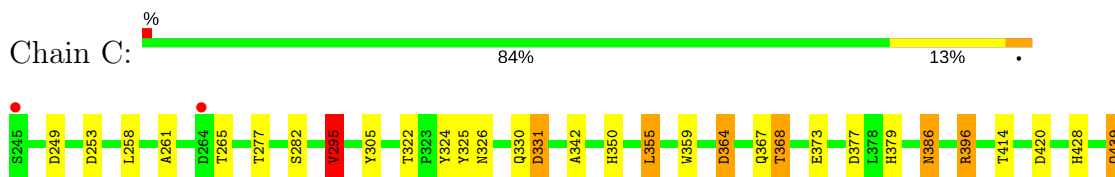
• Molecule 1: ENDO-ALPHA-SIALIDASE

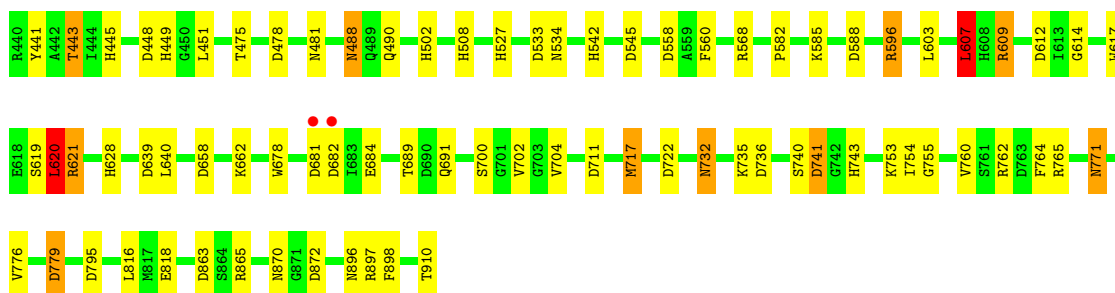


• Molecule 1: ENDO-ALPHA-SIALIDASE



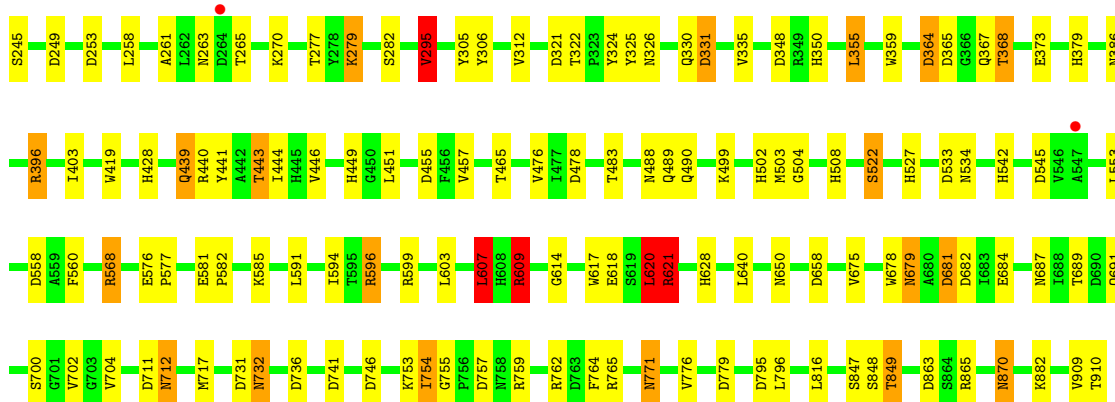
• Molecule 1: ENDO-ALPHA-SIALIDASE





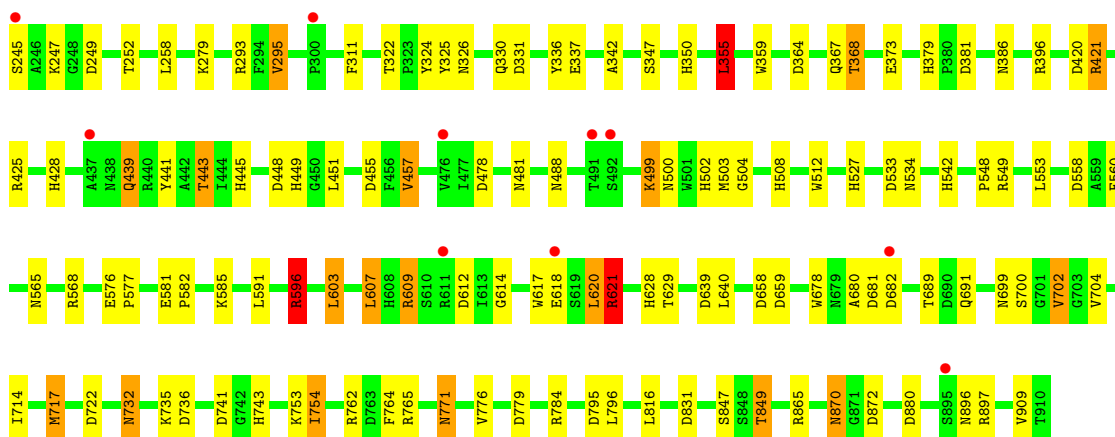
• Molecule 1: ENDO-ALPHA-SIALIDASE

Chain D: 80% 17% . .



• Molecule 1: ENDO-ALPHA-SIALIDASE

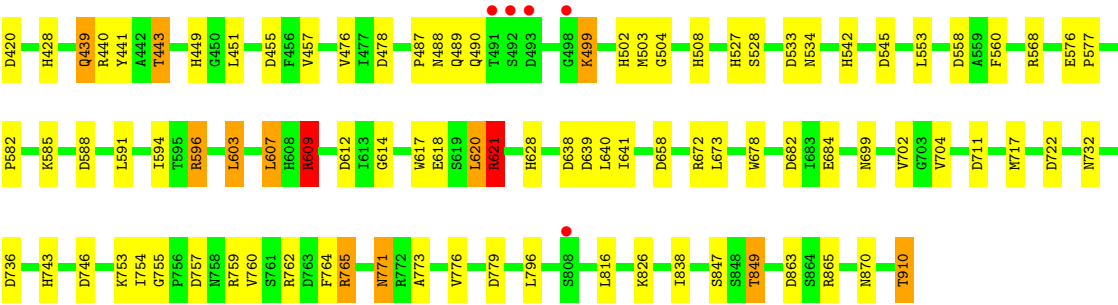
Chain E: 2% 81% 16% .



• Molecule 1: ENDO-ALPHA-SIALIDASE

Chain F: 81% 16% . .





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.166 , 0.202 0.174 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34485	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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 7.

All (447) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ALA:O	1:B:265:THR:HG23	1.71	0.91
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:C:609:ARG:HG2	1:C:678:TRP:CH2	2.19	0.76
1:F:367:GLN:HE22	1:F:764:PHE:H	1.33	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:443:THR:HG21	3:B:2183:HOH:O	1.91	0.71
1:E:499:LYS:CE	1:E:500:ASN:H	2.02	0.71
1:D:449:HIS:CD2	1:D:451:LEU:H	2.08	0.71
3:B:2047:HOH:O	1:C:368:THR:HG21	1.92	0.70
1:F:322:THR:HG22	1:F:324:TYR:H	1.56	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:322:THR:HG22	1:C:324:TYR:H	1.56	0.70
1:C:373:GLU:OE2	1:C:508:HIS:HE1	1.75	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:A:322:THR:HG21	3:A:2056:HOH:O	1.91	0.69
1:A:771:ASN:HD21	1:A:776:VAL:H	1.40	0.69
1:F:588:ASP:HB3	3:F:2278:HOH:O	1.92	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:A:553:LEU:HD22	1:A:591:LEU:HD21	1.74	0.68
1:F:732:ASN:HD21	1:F:736:ASP:H	1.41	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:621:ARG:CD	3:A:2307:HOH:O	2.41	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: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:A:414:THR:HG21	3:A:2141:HOH:O	1.96	0.66
1:F:847:SER:OG	1:F:849:THR:HB	1.95	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:B:771:ASN:HD21	1:B:776:VAL:H	1.45	0.65
1:E:439:GLN:HE22	1:E:441:TYR:HB2	1.62	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:396:ARG:HD3	1:D:534:ASN:O	1.99	0.63
1:D:367:GLN:HE21	1:F:765:ARG:HH12	1.46	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:553:LEU:CD2	1:A:591:LEU:HD21	2.29	0.63
1:A:765:ARG:NH1	1:C:367:GLN:HE21	1.95	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:B:373:GLU:OE2	1:B:508:HIS:HE1	1.82	0.61
1:C:439:GLN:NE2	1:C:441:TYR:H	1.98	0.61
1:C:449:HIS:CD2	1:C:451:LEU:H	2.09	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:B:396:ARG:HB3	1:B:560:PHE:CZ	2.37	0.59
1:C:527:HIS:HD2	1:C:582:PRO:O	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:609:ARG:HG2	1:C:678:TRP:CZ2	2.38	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
1:E:439:GLN:NE2	1:E:441:TYR:H	2.00	0.59
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:445:HIS:HD2	1:E:481:ASN:HD21	1.51	0.58
1:E:847:SER:OG	1:E:849:THR:HB	2.04	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:A:428:HIS:ND1	1:A:502:HIS:HD2	2.01	0.58
1:D:322:THR:HG22	1:D:324:TYR:H	1.69	0.58
1:E:771:ASN:ND2	1:E:776:VAL:H	2.02	0.57
1:F:277:THR:HG22	1:F:295:VAL:HG22	1.84	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:F:527:HIS:HD2	1:F:582:PRO:O	1.88	0.56
1:B:322:THR:HG22	1:B:324:TYR:H	1.70	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:373:GLU:OE2	1:E:508:HIS:HE1	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:621:ARG:HD2	3:E:2254:HOH:O	2.07	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
1:B:542:HIS:HD2	3:B:2263:HOH:O	1.89	0.55
1:E:364:ASP:OD1	1:E:368:THR:HB	2.06	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:B:621:ARG:CD	3:B:2325:HOH:O	2.54	0.55
1:B:732:ASN:HD21	1:B:736:ASP:H	1.54	0.55
1:B:826:LYS:HB2	1:B:838:ILE:HG13	1.89	0.55
1:E:457:VAL:HA	1:E:504:GLY:O	2.07	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:B:753:LYS:HE2	1:B:755:GLY:O	2.07	0.55
1:D:368:THR:HG21	3:E:2041:HOH: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:B:628:HIS:HE1	1:B:658:ASP:OD1	1.90	0.54
1:F:534:ASN:HB2	3:F:2242:HOH:O	2.07	0.54
1:C:396:ARG:HD3	1:C:534:ASN:O	2.07	0.54
1:D:373:GLU:OE2	1:D:508:HIS:HE1	1.89	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: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:B:503:MET:HG2	1:B:504:GLY:HA2	1.90	0.53
1:C:439:GLN:HE22	1:C:441:TYR:H	1.56	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:B:503:MET:HG2	1:B:504:GLY:CA	2.38	0.53
1:E:342:ALA:HB2	1:E:717:MET:CE	2.39	0.53
1:F:440:ARG:HE	1:F:489:GLN:HE21	1.55	0.53
1:A:336:TYR:CE2	1:A:337:GLU:HG3	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:439:GLN:HE22	1:E:441:TYR:H	1.56	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
1:F:628:HIS:HE1	1:F:658:ASP:OD1	1.93	0.52
1:B:325:TYR:OH	1:B:350:HIS:HE1	1.92	0.52
1:F:771:ASN:ND2	1:F:776:VAL:H	2.08	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:C:325:TYR:OH	1:C:350:HIS:CE1	2.62	0.52
1:D:396:ARG:HB3	1:D:560:PHE:CZ	2.44	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:A:886:ASP:OD2	1:C:897:ARG:NH1	2.43	0.51
1:D:457:VAL:HA	1:D:504:GLY:O	2.11	0.51
1:D:765:ARG:HH12	1:E:367:GLN:NE2	1.99	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:A:779:ASP:HB2	3:C:2102:HOH:O	2.10	0.50
1:B:607:LEU:HB3	1:B:620:LEU:HD22	1.92	0.50
1:F:628:HIS:HD2	3:F:2283:HOH:O	1.93	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:325:TYR:OH	1:E:350:HIS:HE1	1.95	0.50
1:E:714:ILE:HG22	1:E:754:ILE:HD13	1.92	0.50
1:E:628:HIS:HE1	1:E:658:ASP:OD1	1.94	0.50
1:A:650:ASN:ND2	3:A:2325:HOH:O	2.44	0.50
1:C:818:GLU:HB3	2:C:1685:PO4:O4	2.11	0.50
1:C:445:HIS:HD2	1:C:481:ASN:HD21	1.60	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:661:TYR:CZ	1:A:698:VAL:HB	2.47	0.50
1:D:330:GLN:HE21	1:D:527:HIS:CE1	2.30	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:TYR:OH	1:D:350:HIS:HE1	1.94	0.50
3:A:2109:HOH:O	1:B:779:ASP:HB2	2.11	0.49
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
1:D:379:HIS:H	1:D:386:ASN:ND2	2.11	0.49
1:B:379:HIS:H	1:B:386:ASN:ND2	2.10	0.49
1:B:330:GLN:HE21	1:B:527:HIS:CE1	2.30	0.49
1:F:621:ARG:CD	3:F:2297:HOH:O	2.49	0.49
1:D:428:HIS:ND1	1:D:502:HIS:HD2	2.10	0.49
1:E:897:ARG:NE	3:E:2451:HOH:O	2.45	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: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:E:499:LYS:HE3	1:E:500:ASN:N	2.11	0.49
1:B:679:ASN:HD21	1:B:681:ASP:CG	2.17	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: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:B:522:SER:OG	1:B:522:SER:O	2.32	0.48
1:C:542:HIS:HD2	3:C:2248:HOH:O	1.95	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:A:359:TRP:CE3	1:A:375:LEU:HD11	2.49	0.48
1:F:330:GLN:HB2	1:F:527:HIS:HE1	1.79	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:B:743:HIS:HD2	3:B:2423:HOH:O	1.97	0.47
1:E:714:ILE:CG2	1:E:754:ILE:HD13	2.44	0.47
1:A:489:GLN:O	1:E:548:PRO:HG3	2.14	0.47
1:A:618:GLU:HG2	1:A:678:TRP:NE1	2.30	0.47
1:B:628:HIS:HD2	3:B:2311:HOH:O	1.98	0.47
1:E:368:THR:HG22	3:E:2072:HOH:O	2.13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:443:THR:HG22	3:E:2135:HOH:O	2.14	0.47
1:E:689:THR:HG23	1:E:691:GLN:HE22	1.80	0.47
1:D:753:LYS:HE2	1:D:755:GLY:O	2.15	0.47
1:E:247:LYS:HG3	1:E:252:THR:HG21	1.96	0.47
1:A:396:ARG:HD2	1:A:534:ASN:ND2	2.30	0.47
1:B:439:GLN:HE22	1:B:441:TYR:HB2	1.80	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:D:607:LEU:HB3	1:D:620:LEU:HD22	1.96	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:A:322:THR:HB	1:A:326:ASN:OD1	2.15	0.46
1:F:305:TYR:CZ	1:F:684:GLU:HG2	2.50	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:A:542:HIS:HD2	3:A:2233:HOH:O	1.98	0.46
1:D:367:GLN:HE21	1:F:765:ARG:NH1	2.11	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:D:439:GLN:HE22	1:D:441:TYR:HB2	1.81	0.45
1:F:396:ARG:HB3	1:F:560:PHE:CZ	2.52	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:D:503:MET:HG2	1:D:504:GLY:HA3	1.98	0.45
1:D:330:GLN:HB2	1:D:527:HIS:HE1	1.82	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:A:373:GLU:OE2	1:A:508:HIS:HE1	1.98	0.45
1:D:679:ASN:ND2	1:D:681:ASP:H	2.15	0.45
1:B:568:ARG:HD2	3:B:2288:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:THR:HG22	1:C:324:TYR:N	2.27	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: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:F:553:LEU:HD21	1:F:591:LEU:HD21	1.96	0.45
1:A:379:HIS:H	1:A:386:ASN:ND2	2.16	0.44
1:B:322:THR:HB	1:B:326:ASN:OD1	2.17	0.44
1:D:700:SER:OG	1:D:702:VAL:HG13	2.17	0.44
1:C:330:GLN:HA	1:C:331:ASP:HA	1.75	0.44
3:B:2047:HOH:O	1:C:368:THR:CG2	2.59	0.44
1:D:277:THR:HG22	1:D:295:VAL:HG22	1.99	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:A:700:SER:OG	1:A:702:VAL:HG13	2.17	0.44
1:F:379:HIS:H	1:F:386:ASN:HD22	1.65	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:C:342:ALA:HB2	1:C:717:MET:CE	2.48	0.44
1:F:910:THR:HB	3:F:2507:HOH:O	2.17	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:C:753:LYS:HE2	1:C:755:GLY:O	2.17	0.43
1:D:542:HIS:CD2	1:D:581:GLU:H	2.36	0.43
1:F:609:ARG:HD2	1:F:618:GLU:OE2	2.18	0.43
1:C:322:THR:HB	1:C:326:ASN:OD1	2.18	0.43
1:C:305:TYR:CE1	1:C:684:GLU:HG2	2.54	0.43
1:D:650:ASN:ND2	3:D:2323:HOH:O	2.42	0.43
1:D:754:ILE:HA	1:D:754:ILE:HD12	1.82	0.43
1:A:330:GLN:HA	1:A:331:ASP:HA	1.79	0.43
1:E:293:ARG:HD3	1:E:311:PHE:CE2	2.54	0.43
1:E:322:THR:HG21	3:E:2047:HOH:O	2.17	0.43
1:F:503:MET:HG2	1:F:504:GLY:HA3	2.01	0.43
1:B:439:GLN:NE2	1:B:441:TYR:H	2.16	0.43
1:B:603:LEU:HB3	1:B:621:ARG:CZ	2.49	0.43
1:B:903:LEU:HA	1:C:898:PHE:O	2.19	0.43
1:E:743:HIS:HD2	3:E:2182:HOH:O	2.01	0.43
1:C:324:TYR:HB2	1:C:326:ASN:HD21	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:614:GLY:HA2	1:C:617:TRP:CZ2	2.54	0.43
1:C:735:LYS:O	1:C:743:HIS:HE1	2.02	0.43
1:D:522:SER:HB3	1:D:568:ARG:NH2	2.33	0.43
1:F:753:LYS:HE2	1:F:755:GLY:O	2.19	0.43
1:B:414:THR:CG2	3:B:2109:HOH:O	2.67	0.42
1:C:732:ASN:HD21	1:C:736:ASP:H	1.66	0.42
1:E:596:ARG:HG3	1:E:629:THR:O	2.18	0.42
1:A:486:THR:HB	1:A:487:PRO:CD	2.50	0.42
1:A:759:ARG:HD3	3:C:2339:HOH:O	2.18	0.42
1:D:443:THR:HB	1:D:483:THR:HG22	2.02	0.42
1:D:465:THR:CB	1:D:490:GLN:NE2	2.82	0.42
1:E:784:ARG:HD3	1:F:773:ALA:O	2.19	0.42
1:A:568:ARG:HG2	3:A:2262:HOH:O	2.20	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:D:594:ILE:HG12	1:D:607:LEU:HD23	2.01	0.42
1:B:379:HIS:H	1:B:386:ASN:HD22	1.68	0.42
1:D:324:TYR:HB2	1:D:326:ASN:HD21	1.84	0.42
1:D:609:ARG:NH1	1:D:675:VAL:O	2.53	0.42
1:D:330:GLN:HE21	1:D:527:HIS:HE1	1.66	0.42
1:E:897:ARG:NH2	3:E:2451:HOH:O	2.52	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:A:330:GLN:HB2	1:A:527:HIS:CE1	2.54	0.42
1:B:324:TYR:HB2	1:B:326:ASN:HD21	1.85	0.42
1:E:421:ARG:HD2	1:E:512:TRP:CD2	2.54	0.42
1:A:753:LYS:HE2	1:A:755:GLY:O	2.20	0.41
1:D:325:TYR:OH	1:D:350:HIS:CE1	2.73	0.41
1:B:352:VAL:HA	1:B:355:LEU:HD23	2.02	0.41
1:C:607:LEU:HB3	1:C:620:LEU:HD22	2.02	0.41
1:D:330:GLN:HA	1:D:331:ASP:HA	1.80	0.41
1:D:444:ILE:HG22	1:D:446:VAL:HG23	2.02	0.41
1:E:325:TYR:OH	1:E:350:HIS:CE1	2.73	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: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:327:ALA:HB3	1:A:328:TRP:CE3	2.56	0.41
1:A:542:HIS:CD2	1:A:581:GLU:H	2.39	0.41
1:B:549:ARG:HD3	1:B:579:ALA:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:618:GLU:HG2	1:E:678:TRP:NE1	2.36	0.41
1:E:700:SER:OG	1:E:702:VAL:HG13	2.20	0.41
1:E:542:HIS:HD2	3:E:2202:HOH:O	2.03	0.41
1:B:661:TYR:CZ	1:B:698:VAL:HB	2.56	0.41
1:D:609:ARG:HD2	1:D:618:GLU:OE1	2.21	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: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
1:E:379:HIS:HB2	1:E:386:ASN:HA	2.03	0.41
1:F:499:LYS:HD2	1:F:499:LYS:HA	1.63	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:D:609:ARG:HD2	1:D:618:GLU: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:C:386:ASN:HA	1:C:386:ASN:HD22	1.71	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:B:331:ASP:HB3	1:B:528:SER:HA	2.02	0.40
1:C:662:LYS:HB3	3:C:2334:HOH:O	2.22	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:E:553:LEU:HD21	1:E:591:LEU:HD21	2.03	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%)	51	41
1	B	664/666 (100%)	640 (96%)	23 (4%)	1 (0%)	51	41
1	C	664/666 (100%)	642 (97%)	21 (3%)	1 (0%)	51	41
1	D	664/666 (100%)	639 (96%)	24 (4%)	1 (0%)	51	41
1	E	664/666 (100%)	636 (96%)	27 (4%)	1 (0%)	51	41
1	F	664/666 (100%)	639 (96%)	24 (4%)	1 (0%)	51	41
All	All	3984/3996 (100%)	3838 (96%)	140 (4%)	6 (0%)	51	41

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%)	26	15
1	B	564/564 (100%)	532 (94%)	32 (6%)	24	13
1	C	564/564 (100%)	534 (95%)	30 (5%)	26	15
1	D	564/564 (100%)	525 (93%)	39 (7%)	18	8
1	E	564/564 (100%)	532 (94%)	32 (6%)	24	13
1	F	564/564 (100%)	531 (94%)	33 (6%)	23	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3384/3384 (100%)	3188 (94%)	196 (6%)	23	12

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	870	ASN

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 ⓘ

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	0.98	0	6,6,6	0.60	0
2	PO4	C	1685	-	4,4,4	0.82	0	6,6,6	0.43	0
2	PO4	C	1686	-	4,4,4	1.03	0	6,6,6	0.61	0
2	PO4	D	1685	-	4,4,4	1.01	0	6,6,6	0.39	0
2	PO4	F	1685	-	4,4,4	0.79	0	6,6,6	0.31	0
2	PO4	F	1686	-	4,4,4	0.83	0	6,6,6	0.50	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1685	PO4	1	0
2	C	1685	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	666/666 (100%)	-0.10	17 (2%) 56 60	8, 14, 21, 28	0
1	B	666/666 (100%)	-0.23	3 (0%) 90 92	9, 13, 20, 29	0
1	C	666/666 (100%)	-0.23	4 (0%) 89 90	9, 13, 21, 28	0
1	D	666/666 (100%)	-0.29	2 (0%) 93 94	9, 13, 20, 28	0
1	E	666/666 (100%)	-0.17	10 (1%) 74 77	9, 14, 20, 29	0
1	F	666/666 (100%)	-0.23	6 (0%) 84 86	9, 14, 20, 28	0
All	All	3996/3996 (100%)	-0.21	42 (1%) 80 83	8, 13, 21, 29	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	436	ALA	4.0
1	A	491	THR	3.9
1	B	245	SER	3.9
1	F	245	SER	3.4
1	E	492	SER	3.2
1	C	681	ASP	3.2
1	D	547	ALA	3.1
1	F	491	THR	3.0
1	A	492	SER	2.9
1	E	491	THR	2.9
1	E	611	ARG	2.8
1	A	490	GLN	2.8
1	C	682	ASP	2.7
1	E	245	SER	2.7
1	A	264	ASP	2.7
1	C	264	ASP	2.5
1	F	498	GLY	2.4
1	E	682	ASP	2.4
1	A	494	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	492	SER	2.4
1	F	808	SER	2.4
1	A	245	SER	2.3
1	A	430	THR	2.3
1	C	245	SER	2.3
1	D	264	ASP	2.3
1	A	487	PRO	2.3
1	A	437	ALA	2.2
1	A	438	ASN	2.2
1	E	476	VAL	2.2
1	A	493	ASP	2.2
1	A	499	LYS	2.2
1	B	682	ASP	2.2
1	A	497	ALA	2.1
1	E	437	ALA	2.1
1	E	895	SER	2.1
1	E	300	PRO	2.1
1	A	465	THR	2.1
1	B	264	ASP	2.1
1	A	440	ARG	2.1
1	F	493	ASP	2.1
1	A	489	GLN	2.1
1	E	618	GLU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PO4	F	1685	5/5	0.97	0.15	0.53	38,38,39,40	0
2	PO4	F	1686	5/5	0.97	0.13	0.47	39,40,40,42	0
2	PO4	B	1685	5/5	0.98	0.12	0.46	32,33,34,36	0
2	PO4	C	1685	5/5	0.98	0.11	0.14	32,33,36,38	0
2	PO4	D	1685	5/5	0.97	0.10	-0.26	36,36,39,39	0
2	PO4	C	1686	5/5	0.98	0.10	-0.39	32,34,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.