



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 05:58 PM GMT

PDB ID : 1V0F  
Title : ENDOSIALIDASE OF BACTERIOPHAGE K1F IN COMPLEX WITH OLIGOMERIC ALPHA-2,8-SIALIC ACID  
Authors : Stummeyer, K.; Dickmanns, A.; Muehlenhoff, M.; Gerady-Schahn, R.; Ficner, R.  
Deposited on : 2004-03-28  
Resolution : 2.55 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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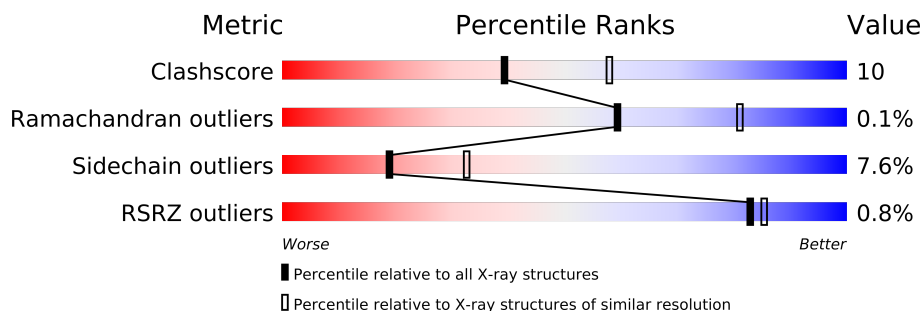
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.55 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	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

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	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SLB	E	1685	-	X

## 2 Entry composition i

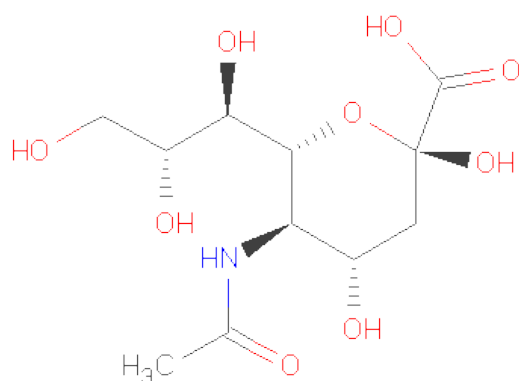
There are 5 unique types of molecules in this entry. The entry contains 32580 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

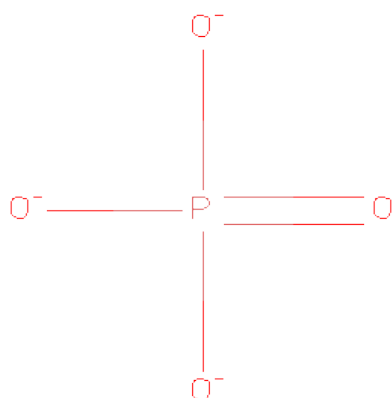
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	B	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	C	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	D	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	E	666	Total	C	N	O	S	0	0	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 SUGAR (5-N-ACETYL-BETA-D-NEURAMINICACID) (three-letter code: SLB) (formula:  $C_{11}H_{19}NO_9$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	11	1	9		
2	B	1	Total	C	N	O	0	0
			21	11	1	9		
2	C	1	Total	C	N	O	0	0
			21	11	1	9		
2	D	1	Total	C	N	O	0	0
			21	11	1	9		
2	E	1	Total	C	N	O	0	0
			21	11	1	9		
2	F	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	2	Total	C	N	O	0	0
			41	22	2	17		
4	D	2	Total	C	N	O	0	0
			41	22	2	17		
4	E	2	Total	C	N	O	0	0
			41	22	2	17		

- Molecule 5 is water.

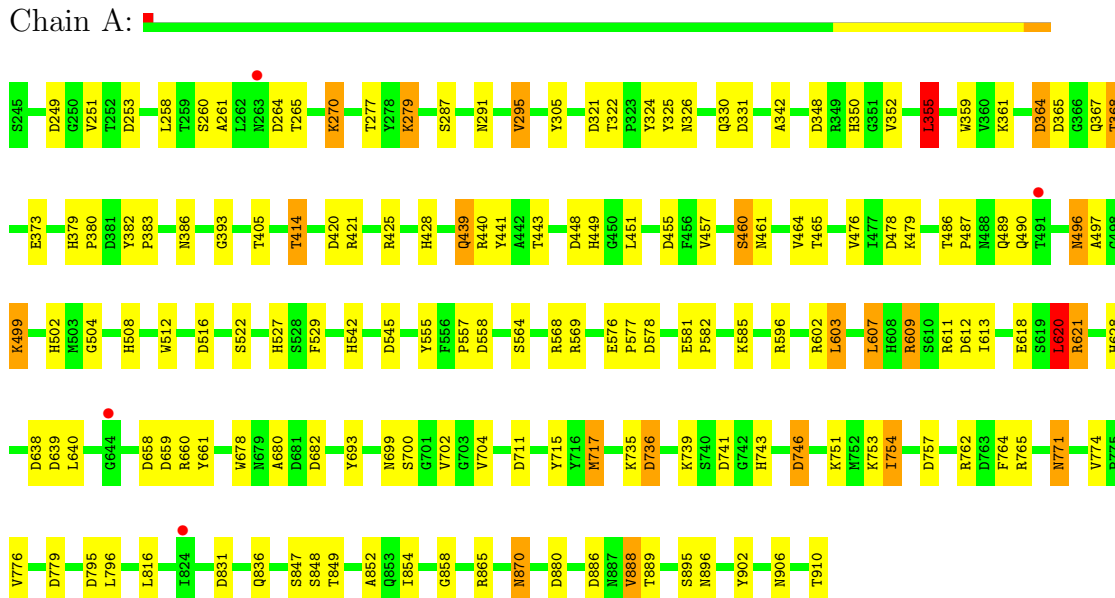
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	176	Total	O	0	0
			176	176		
5	B	178	Total	O	0	0
			178	178		
5	C	130	Total	O	0	0
			130	130		
5	D	167	Total	O	0	0
			167	167		
5	E	130	Total	O	0	0
			130	130		
5	F	140	Total	O	0	0
			140	140		

### 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.

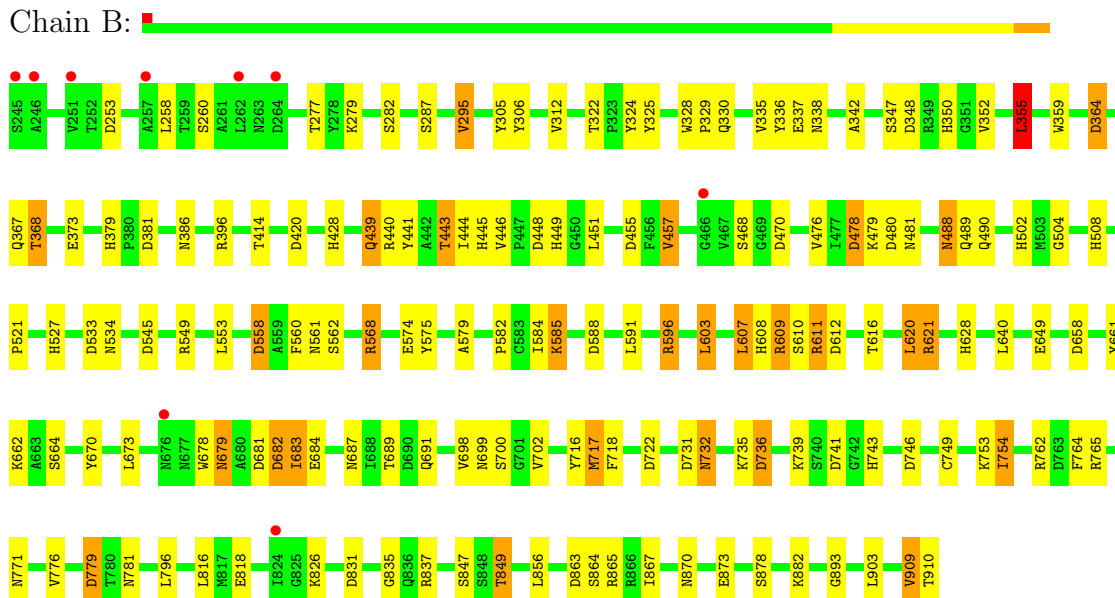
#### • Molecule 1: ENDO-ALPHA-SIALIDASE

Chain A:



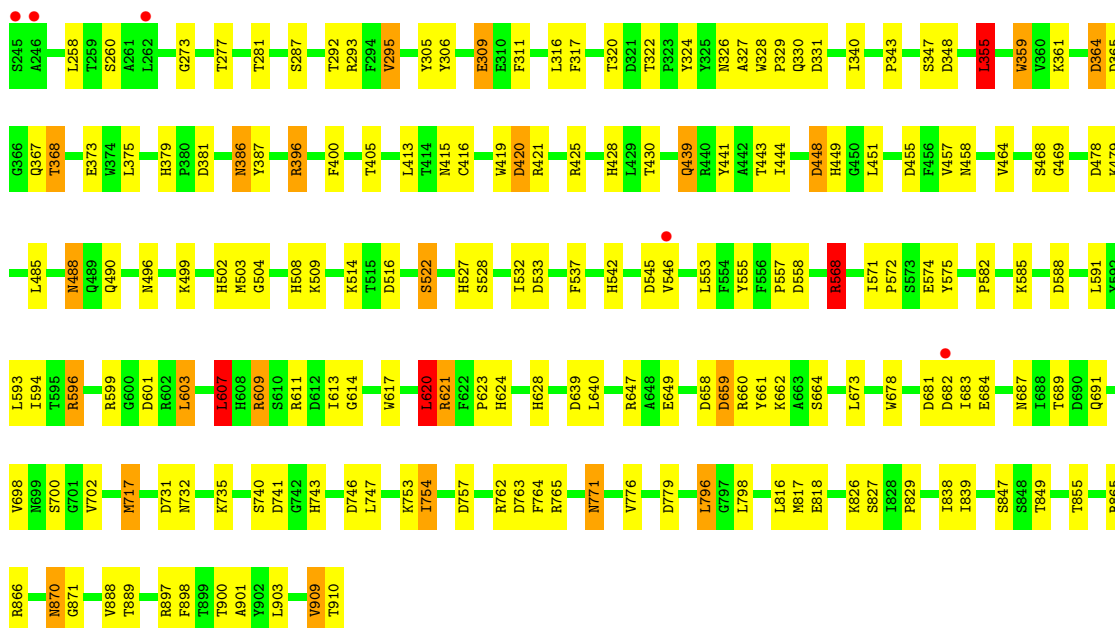
#### • Molecule 1: ENDO-ALPHA-SIALIDASE

Chain B:



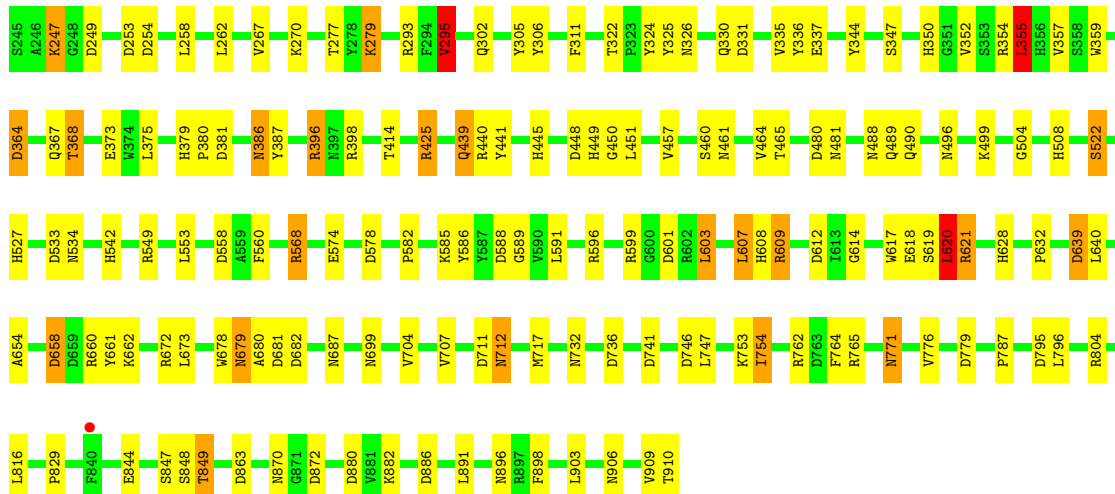
- Molecule 1: ENDO-ALPHA-SIALIDASE

Chain C:



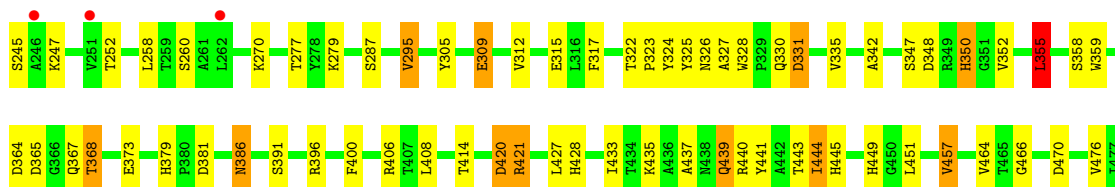
- Molecule 1: ENDO-ALPHA-SIALIDASE

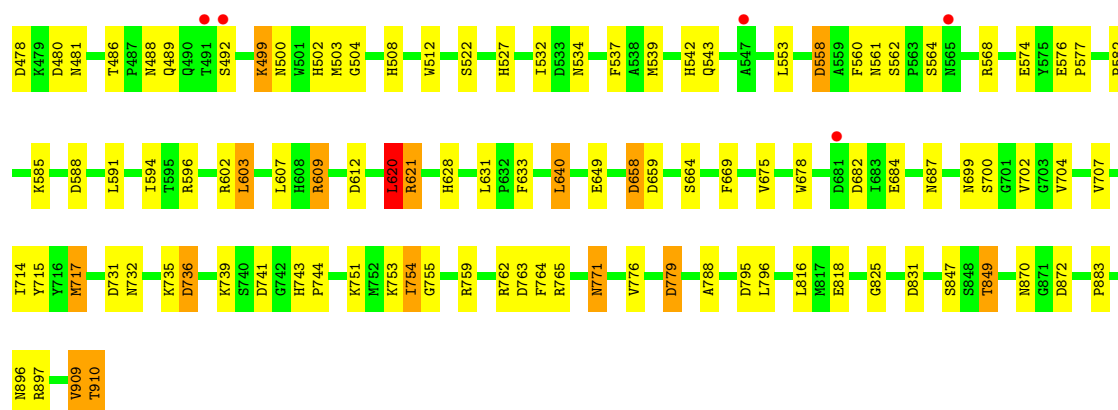
Chain D:



- Molecule 1: ENDO-ALPHA-SIALIDASE

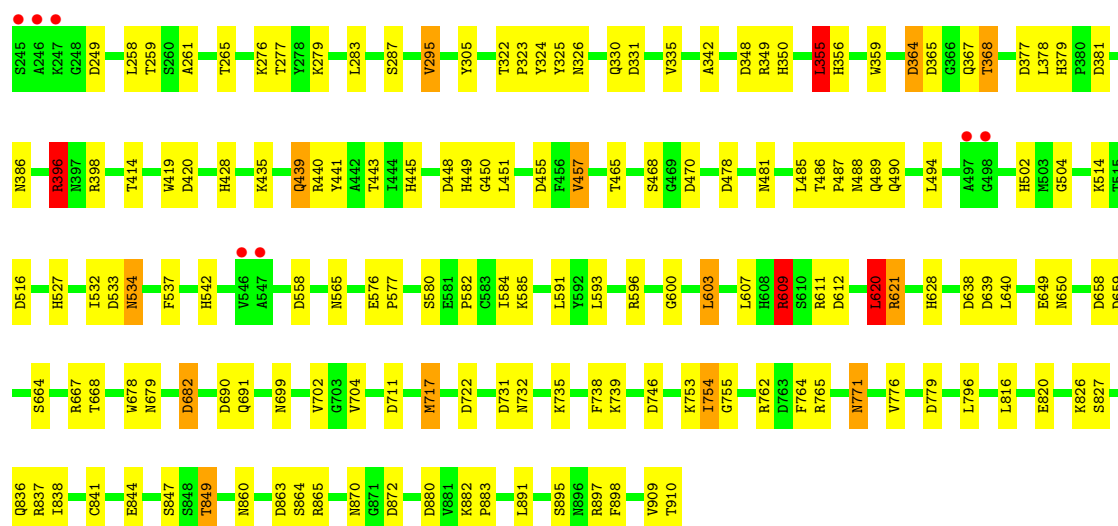
Chain E:





● 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, $\alpha$ , $\beta$ , $\gamma$	99.54Å 131.40Å 346.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.55 30.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	88.4 (30.00-2.55) 88.1 (30.00-2.55)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.28 (at 2.54Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.180 , 0.232 0.198 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 0.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 130768 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	32580	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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, SIA, SLB

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	0.72	0/5376	0.94	31/7325 (0.4%)
1	B	0.72	0/5376	0.94	28/7325 (0.4%)
1	C	0.70	0/5376	0.94	29/7325 (0.4%)
1	D	0.73	0/5376	0.95	31/7325 (0.4%)
1	E	0.69	0/5376	0.92	23/7325 (0.3%)
1	F	0.71	0/5376	0.94	33/7325 (0.5%)
All	All	0.71	0/32256	0.94	175/43950 (0.4%)

There are no bond length outliers.

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	ASP	CB-CG-OD2	9.56	126.91	118.30
1	E	355	LEU	CA-CB-CG	9.49	137.13	115.30
1	F	638	ASP	CB-CG-OD2	8.38	125.84	118.30
1	D	682	ASP	CB-CG-OD2	8.26	125.74	118.30
1	C	545	ASP	CB-CG-OD2	8.15	125.64	118.30
1	A	620	LEU	CA-CB-CG	8.15	134.04	115.30
1	E	558	ASP	CB-CG-OD2	8.15	125.63	118.30
1	E	612	ASP	CB-CG-OD2	8.07	125.57	118.30
1	B	355	LEU	CA-CB-CG	8.00	133.70	115.30
1	C	355	LEU	CA-CB-CG	8.00	133.69	115.30
1	C	639	ASP	CB-CG-OD2	7.99	125.49	118.30
1	B	478	ASP	CB-CG-OD2	7.96	125.46	118.30
1	B	620	LEU	CA-CB-CG	7.85	133.35	115.30
1	D	253	ASP	CB-CG-OD2	7.83	125.35	118.30
1	E	348	ASP	CB-CG-OD2	7.77	125.29	118.30
1	C	731	ASP	CB-CG-OD2	7.71	125.24	118.30
1	F	746	ASP	CB-CG-OD2	7.69	125.22	118.30
1	B	420	ASP	CB-CG-OD2	7.59	125.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	872	ASP	CB-CG-OD2	7.58	125.12	118.30
1	D	795	ASP	CB-CG-OD2	7.52	125.07	118.30
1	B	558	ASP	CB-CG-OD2	7.44	125.00	118.30
1	A	355	LEU	CA-CB-CG	7.43	132.38	115.30
1	A	558	ASP	CB-CG-OD2	7.32	124.89	118.30
1	C	620	LEU	CA-CB-CG	7.30	132.08	115.30
1	F	722	ASP	CB-CG-OD2	7.17	124.75	118.30
1	D	620	LEU	CA-CB-CG	7.15	131.74	115.30
1	D	639	ASP	CB-CG-OD2	7.12	124.71	118.30
1	F	478	ASP	CB-CG-OD2	7.09	124.69	118.30
1	F	355	LEU	CA-CB-CG	7.07	131.57	115.30
1	B	253	ASP	CB-CG-OD2	7.03	124.63	118.30
1	D	711	ASP	CB-CG-OD2	6.98	124.58	118.30
1	C	558	ASP	CB-CG-OD2	6.92	124.53	118.30
1	F	455	ASP	CB-CG-OD2	6.90	124.51	118.30
1	B	480	ASP	CB-CG-OD2	6.88	124.50	118.30
1	D	578	ASP	CB-CG-OD2	6.86	124.47	118.30
1	A	348	ASP	CB-CG-OD2	6.83	124.45	118.30
1	E	736	ASP	CB-CG-OD1	6.74	124.36	118.30
1	E	682	ASP	CB-CG-OD2	6.68	124.32	118.30
1	C	533	ASP	CB-CG-OD2	6.67	124.30	118.30
1	F	731	ASP	CB-CG-OD2	6.65	124.29	118.30
1	D	355	LEU	CA-CB-CG	6.63	130.54	115.30
1	E	620	LEU	CA-CB-CG	6.62	130.54	115.30
1	A	249	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	253	ASP	CB-CG-OD2	6.59	124.24	118.30
1	B	863	ASP	CB-CG-OD2	6.56	124.21	118.30
1	F	711	ASP	CB-CG-OD2	6.56	124.20	118.30
1	D	658	ASP	CB-CG-OD2	6.56	124.20	118.30
1	A	478	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	865	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	741	ASP	CB-CG-OD2	6.51	124.16	118.30
1	F	639	ASP	CB-CG-OD2	6.46	124.11	118.30
1	B	731	ASP	CB-CG-OD2	6.46	124.11	118.30
1	A	455	ASP	CB-CG-OD2	6.44	124.10	118.30
1	D	872	ASP	CB-CG-OD2	6.44	124.10	118.30
1	F	863	ASP	CB-CG-OD2	6.43	124.09	118.30
1	D	746	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	545	ASP	CB-CG-OD2	6.42	124.08	118.30
1	E	478	ASP	CB-CG-OD2	6.41	124.07	118.30
1	E	420	ASP	CB-CG-OD2	6.39	124.05	118.30
1	B	381	ASP	CB-CG-OD2	6.37	124.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	448	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	795	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	639	ASP	CB-CG-OD2	6.32	123.99	118.30
1	E	365	ASP	CB-CG-OD2	6.32	123.99	118.30
1	C	746	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	612	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	741	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	588	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	757	ASP	CB-CG-OD2	6.27	123.95	118.30
1	F	364	ASP	CB-CG-OD2	6.25	123.93	118.30
1	B	545	ASP	CB-CG-OD2	6.25	123.92	118.30
1	D	558	ASP	CB-CG-OD2	6.25	123.92	118.30
1	F	558	ASP	CB-CG-OD2	6.24	123.91	118.30
1	D	480	ASP	CB-CG-OD2	6.17	123.85	118.30
1	E	588	ASP	CB-CG-OD2	6.15	123.83	118.30
1	E	831	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	420	ASP	CB-CG-OD2	6.14	123.83	118.30
1	C	364	ASP	CB-CG-OD2	6.12	123.80	118.30
1	C	659	ASP	CB-CG-OD2	6.08	123.78	118.30
1	B	736	ASP	CB-CG-OD1	6.08	123.77	118.30
1	F	348	ASP	CB-CG-OD2	6.04	123.74	118.30
1	F	377	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	746	ASP	CB-CG-OD2	6.03	123.72	118.30
1	D	381	ASP	CB-CG-OD2	6.02	123.72	118.30
1	F	381	ASP	CB-CG-OD2	6.02	123.72	118.30
1	F	620	LEU	CA-CB-CG	6.02	129.14	115.30
1	B	607	LEU	CA-CB-CG	6.01	129.12	115.30
1	D	601	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	365	ASP	CB-CG-OD2	5.98	123.68	118.30
1	D	612	ASP	CB-CG-OD2	5.97	123.67	118.30
1	F	880	ASP	CB-CG-OD2	5.94	123.65	118.30
1	C	607	LEU	CA-CB-CG	5.94	128.95	115.30
1	F	331	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	588	ASP	CB-CG-OD2	5.87	123.58	118.30
1	D	364	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	682	ASP	CB-CG-OD2	5.83	123.54	118.30
1	B	533	ASP	CB-CG-OD2	5.83	123.54	118.30
1	C	455	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	264	ASP	CB-CG-OD2	5.81	123.53	118.30
1	D	863	ASP	CB-CG-OD2	5.79	123.52	118.30
1	C	348	ASP	CB-CG-OD2	5.76	123.49	118.30
1	B	348	ASP	CB-CG-OD2	5.75	123.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	448	ASP	CB-CG-OD2	5.68	123.41	118.30
1	E	331	ASP	CB-CG-OD2	5.67	123.41	118.30
1	B	746	ASP	CB-CG-OD2	5.65	123.38	118.30
1	E	470	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	321	ASP	CB-CG-OD2	5.62	123.36	118.30
1	F	396	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	C	568	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	D	331	ASP	CB-CG-OD2	5.61	123.35	118.30
1	D	588	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	831	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	364	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	638	ASP	CB-CG-OD2	5.58	123.33	118.30
1	D	804	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	E	731	ASP	CB-CG-OD2	5.55	123.29	118.30
1	B	455	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	596	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	C	865	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	831	ASP	CB-CG-OD2	5.51	123.26	118.30
1	D	354	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	F	516	ASP	CB-CG-OD2	5.51	123.25	118.30
1	A	516	ASP	CB-CG-OD1	5.50	123.25	118.30
1	C	601	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	381	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	865	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	420	ASP	CB-CG-OD2	5.49	123.24	118.30
1	E	381	ASP	CB-CG-OD2	5.49	123.24	118.30
1	F	609	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	F	249	ASP	CB-CG-OD2	5.47	123.23	118.30
1	E	659	ASP	CB-CG-OD2	5.45	123.21	118.30
1	C	681	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	611	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	F	779	ASP	CB-CG-OD2	5.43	123.19	118.30
1	E	779	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	682	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	470	ASP	CB-CG-OD2	5.39	123.16	118.30
1	E	658	ASP	CB-CG-OD2	5.38	123.14	118.30
1	E	480	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	516	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	736	ASP	CB-CG-OD2	5.32	123.09	118.30
1	F	682	ASP	CB-CG-OD2	5.31	123.08	118.30
1	D	249	ASP	CB-CG-OD2	5.31	123.08	118.30
1	F	365	ASP	CB-CG-OD2	5.29	123.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	448	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	612	ASP	CB-CG-OD2	5.28	123.06	118.30
1	E	795	ASP	CB-CG-OD2	5.28	123.05	118.30
1	F	420	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	578	ASP	CB-CG-OD2	5.25	123.02	118.30
1	D	295	VAL	CB-CA-C	-5.23	101.47	111.40
1	F	659	ASP	CB-CG-OD2	5.23	123.00	118.30
1	F	612	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	722	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	880	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	421	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	711	ASP	CB-CG-OD2	5.18	122.97	118.30
1	D	533	ASP	CB-CG-OD2	5.17	122.96	118.30
1	F	690	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	779	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	659	ASP	CB-CG-OD2	5.15	122.94	118.30
1	F	448	ASP	CB-CG-OD2	5.15	122.93	118.30
1	E	741	ASP	CB-CG-OD2	5.14	122.93	118.30
1	C	478	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	787	PRO	N-CD-CG	-5.11	95.53	103.20
1	C	757	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	596	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	A	880	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	254	ASP	CB-CG-OD2	5.04	122.84	118.30
1	D	425	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	A	682	ASP	CB-CG-OD2	5.04	122.83	118.30
1	F	533	ASP	CB-CG-OD2	5.04	122.84	118.30
1	F	470	ASP	CB-CG-OD2	5.04	122.83	118.30
1	E	872	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	365	ASP	CB-CG-OD2	5.01	122.81	118.30
1	D	741	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	104	0
1	B	5230	0	4942	110	0
1	C	5230	0	4942	113	0
1	D	5230	0	4942	103	0
1	E	5230	0	4942	117	0
1	F	5230	0	4942	95	0
2	A	21	0	18	0	0
2	B	21	0	18	0	0
2	C	21	0	18	0	0
2	D	21	0	18	0	0
2	E	21	0	18	0	0
2	F	21	0	18	1	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
3	F	10	0	0	0	0
4	C	41	0	34	0	0
4	D	41	0	34	2	0
4	E	41	0	34	1	0
5	A	176	0	0	11	0
5	B	178	0	0	12	0
5	C	130	0	0	6	0
5	D	167	0	0	11	0
5	E	130	0	0	15	0
5	F	140	0	0	15	0
All	All	32580	0	29862	590	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 10.

All (590) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:490:GLN:HG3	5:B:2041:HOH:O	1.51	1.09
1:E:499:LYS:HE2	1:E:500:ASN:H	1.21	1.04
1:A:765:ARG:HH12	1:C:367:GLN:HE21	1.07	0.98
1:F:449:HIS:HD2	1:F:451:LEU:H	1.07	0.98
1:C:449:HIS:HD2	1:C:451:LEU:H	1.00	0.96
1:B:367:GLN:HE21	1:C:765:ARG:HH12	1.12	0.95
1:A:449:HIS:HD2	1:A:451:LEU:H	1.10	0.94

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:449:HIS:CD2	1:C:451:LEU:H	1.86	0.92
1:A:367:GLN:HE21	1:B:765:ARG:HH12	0.93	0.91
1:A:771:ASN:HD21	1:A:776:VAL:H	1.18	0.90
1:D:449:HIS:HD2	1:D:451:LEU:H	1.20	0.89
1:E:449:HIS:HD2	1:E:451:LEU:H	1.21	0.88
1:F:449:HIS:CD2	1:F:451:LEU:H	1.91	0.88
1:B:449:HIS:HD2	1:B:451:LEU:H	1.22	0.88
1:E:542:HIS:HD2	5:E:2038:HOH:O	1.56	0.87
1:B:682:ASP:HB2	5:B:2107:HOH:O	1.75	0.87
1:D:347:SER:HB3	1:D:355:LEU:HB2	1.57	0.87
1:B:771:ASN:HD21	1:B:776:VAL:H	1.20	0.86
1:D:765:ARG:NH1	1:E:367:GLN:HE21	1.74	0.86
1:D:765:ARG:HH12	1:E:367:GLN:HE21	0.89	0.86
1:E:765:ARG:HH12	1:F:367:GLN:HE21	1.25	0.83
1:B:440:ARG:HE	1:B:489:GLN:HE21	1.25	0.82
1:A:367:GLN:NE2	1:B:765:ARG:HH12	1.77	0.82
1:C:609:ARG:HG2	1:C:678:TRP:CH2	2.15	0.81
1:F:322:THR:HG21	5:F:2012:HOH:O	1.80	0.81
1:C:322:THR:HG22	1:C:324:TYR:H	1.46	0.81
1:E:440:ARG:HD2	5:E:2031:HOH:O	1.79	0.80
1:A:368:THR:HG22	5:A:2028:HOH:O	1.81	0.80
1:A:449:HIS:CD2	1:A:451:LEU:H	1.96	0.80
1:D:771:ASN:HD21	1:D:776:VAL:H	1.28	0.80
1:E:449:HIS:CD2	1:E:451:LEU:H	1.99	0.80
1:D:490:GLN:HG3	5:D:2042:HOH:O	1.83	0.79
1:B:611:ARG:HD3	5:B:2093:HOH:O	1.82	0.79
1:D:322:THR:HG22	1:D:324:TYR:H	1.47	0.79
1:B:449:HIS:CD2	1:B:451:LEU:H	2.01	0.78
1:C:779:ASP:HB2	5:C:2102:HOH:O	1.82	0.78
1:D:295:VAL:HG13	1:D:305:TYR:CE2	2.19	0.78
1:A:439:GLN:HE22	1:A:441:TYR:HB2	1.48	0.78
1:D:440:ARG:HE	1:D:489:GLN:HE21	1.32	0.78
1:D:882:LYS:HE3	5:D:2158:HOH:O	1.84	0.78
1:E:499:LYS:HE2	1:E:500:ASN:N	1.98	0.77
1:D:765:ARG:HH12	1:E:367:GLN:NE2	1.75	0.77
1:A:542:HIS:HD2	5:A:2063:HOH:O	1.68	0.77
1:C:295:VAL:HG13	1:C:305:TYR:CE2	2.19	0.77
1:D:542:HIS:HD2	5:D:2059:HOH:O	1.68	0.77
1:A:771:ASN:ND2	1:A:776:VAL:H	1.83	0.76
1:D:368:THR:HG21	5:E:2005:HOH:O	1.84	0.76
1:D:367:GLN:HE22	1:D:764:PHE:H	1.32	0.76
1:A:270:LYS:HE2	5:A:2002:HOH:O	1.87	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:602:ARG:HH11	1:A:602:ARG:HG3	1.51	0.75
1:E:714:ILE:HG22	1:E:754:ILE:HD13	1.68	0.75
1:F:440:ARG:HE	1:F:489:GLN:HE21	1.34	0.74
1:E:609:ARG:HG2	1:E:678:TRP:CH2	2.22	0.74
1:F:322:THR:HG22	1:F:324:TYR:H	1.53	0.74
1:F:295:VAL:HG13	1:F:305:TYR:CE2	2.22	0.74
1:E:499:LYS:CE	1:E:500:ASN:H	1.98	0.74
1:A:367:GLN:HE21	1:B:765:ARG:NH1	1.79	0.72
1:A:448:ASP:OD2	1:A:479:LYS:NZ	2.22	0.72
1:E:364:ASP:OD1	1:E:368:THR:HB	1.89	0.72
1:C:673:LEU:HD12	1:C:683:ILE:HD12	1.71	0.72
1:C:449:HIS:HD2	1:C:451:LEU:N	1.84	0.72
1:C:364:ASP:OD1	1:C:368:THR:HB	1.90	0.72
1:F:771:ASN:HD21	1:F:776:VAL:H	1.38	0.71
1:B:743:HIS:HD2	5:B:2131:HOH:O	1.74	0.71
1:C:870:ASN:HD22	1:C:870:ASN:C	1.94	0.71
1:B:771:ASN:ND2	1:B:776:VAL:H	1.89	0.70
1:B:609:ARG:HG2	1:B:678:TRP:CH2	2.26	0.70
1:B:439:GLN:HE22	1:B:441:TYR:HB2	1.56	0.70
1:E:322:THR:HG22	1:E:324:TYR:H	1.54	0.70
1:C:448:ASP:OD2	1:C:479:LYS:NZ	2.23	0.69
1:E:367:GLN:HE22	1:E:764:PHE:H	1.37	0.69
1:F:367:GLN:HE22	1:F:764:PHE:H	1.37	0.69
1:D:844:GLU:HG2	5:D:2149:HOH:O	1.91	0.69
1:B:379:HIS:H	1:B:386:ASN:ND2	1.91	0.69
5:A:2012:HOH:O	1:B:368:THR:HG21	1.93	0.69
1:C:740:SER:OG	1:C:741:ASP:N	2.26	0.69
1:A:295:VAL:HG13	1:A:305:TYR:CE2	2.27	0.68
1:D:679:ASN:ND2	1:D:681:ASP:H	1.92	0.68
1:F:753:LYS:HE2	1:F:755:GLY:O	1.93	0.68
1:E:779:ASP:HB2	5:E:2094:HOH:O	1.93	0.68
1:B:364:ASP:OD1	1:B:368:THR:HB	1.94	0.68
1:D:779:ASP:HB2	5:D:2131:HOH:O	1.94	0.68
1:D:367:GLN:HE21	1:F:765:ARG:HH12	1.40	0.67
1:A:440:ARG:HE	1:A:489:GLN:HE21	1.42	0.67
1:E:350:HIS:CE1	1:E:699:ASN:HB3	2.29	0.67
1:A:367:GLN:HE22	1:A:764:PHE:H	1.42	0.67
1:C:689:THR:HG23	1:C:691:GLN:HE22	1.59	0.67
1:E:421:ARG:HD2	1:E:512:TRP:CD2	2.29	0.67
1:A:322:THR:HG22	1:A:324:TYR:H	1.60	0.66
1:F:628:HIS:HD2	5:F:2066:HOH:O	1.77	0.66
1:E:532:ILE:HG12	1:E:537:PHE:HA	1.76	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:330:GLN:HE21	1:F:527:HIS:HE1	1.44	0.66
1:D:771:ASN:ND2	1:D:776:VAL:H	1.94	0.66
1:A:527:HIS:HD2	1:A:582:PRO:O	1.79	0.66
1:A:291:ASN:HB2	5:C:2002:HOH:O	1.95	0.66
1:E:603:LEU:HG	1:E:621:ARG:HD3	1.78	0.66
1:D:847:SER:OG	1:D:849:THR:HB	1.95	0.65
1:E:373:GLU:OE2	1:E:508:HIS:HE1	1.78	0.65
1:A:886:ASP:OD2	1:C:897:ARG:NH1	2.29	0.65
1:A:486:THR:HB	1:A:487:PRO:HD3	1.79	0.65
1:F:330:GLN:HE21	1:F:527:HIS:CE1	2.14	0.65
1:D:662:LYS:HE3	5:D:2084:HOH:O	1.97	0.65
1:F:449:HIS:HD2	1:F:451:LEU:N	1.89	0.65
5:D:2010:HOH:O	1:F:368:THR:HG21	1.97	0.65
1:D:765:ARG:HD3	5:D:2126:HOH:O	1.97	0.64
1:B:373:GLU:OE2	1:B:508:HIS:HE1	1.80	0.64
1:C:322:THR:HB	1:C:326:ASN:OD1	1.97	0.64
1:E:427:LEU:N	1:E:503:MET:O	2.23	0.64
1:D:712:ASN:HD22	1:D:712:ASN:H	1.46	0.64
1:B:322:THR:HG22	1:B:324:TYR:H	1.62	0.64
1:D:609:ARG:HG2	1:D:678:TRP:CH2	2.33	0.64
1:B:443:THR:HG22	5:B:2045:HOH:O	1.96	0.64
1:F:609:ARG:HG2	1:F:678:TRP:CH2	2.33	0.63
1:B:558:ASP:OD1	1:B:561:ASN:HB2	1.98	0.63
1:A:368:THR:HG21	5:C:2006:HOH:O	1.98	0.63
1:D:886:ASP:OD2	1:E:897:ARG:NH1	2.32	0.63
1:A:906:ASN:OD1	1:C:909:VAL:HG11	1.98	0.63
1:E:309:GLU:OE1	1:E:309:GLU:HA	1.97	0.63
1:D:449:HIS:CD2	1:D:451:LEU:H	2.09	0.62
1:A:364:ASP:OD1	1:A:368:THR:HB	1.99	0.62
1:B:322:THR:HG21	5:B:2012:HOH:O	1.98	0.62
1:C:771:ASN:HD21	1:C:776:VAL:H	1.47	0.62
1:B:527:HIS:HD2	1:B:582:PRO:O	1.82	0.62
1:A:896:ASN:HB2	1:B:882:LYS:HD2	1.81	0.62
1:B:440:ARG:HE	1:B:489:GLN:NE2	1.98	0.62
1:A:373:GLU:OE2	1:A:508:HIS:HE1	1.83	0.61
1:E:439:GLN:HE22	1:E:441:TYR:HB2	1.64	0.61
1:B:818:GLU:HB3	3:B:1686:PO4:O2	2.00	0.61
1:D:553:LEU:HD22	1:D:591:LEU:HD21	1.81	0.61
1:E:714:ILE:CG2	1:E:754:ILE:HD13	2.30	0.61
1:C:373:GLU:OE2	1:C:508:HIS:HE1	1.84	0.60
1:F:580:SER:HB3	5:F:2058:HOH:O	2.02	0.60
1:C:439:GLN:NE2	1:C:441:TYR:H	1.99	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:847:SER:OG	1:A:849:THR:HB	2.02	0.60
1:B:367:GLN:NE2	1:C:765:ARG:HH12	1.93	0.60
1:B:835:GLY:O	1:B:837:ARG:HG2	2.01	0.60
1:A:609:ARG:HG2	1:A:678:TRP:CH2	2.36	0.60
1:D:632:PRO:HB2	1:D:707:VAL:HG23	1.84	0.60
1:B:396:ARG:HB3	1:B:560:PHE:CZ	2.37	0.60
1:D:527:HIS:HD2	1:D:582:PRO:O	1.85	0.59
1:E:368:THR:HG21	5:F:2009:HOH:O	2.03	0.59
1:A:277:THR:HG22	1:A:295:VAL:HG22	1.85	0.59
1:B:396:ARG:NH2	1:B:534:ASN:O	2.32	0.59
1:D:439:GLN:HE22	1:D:441:TYR:HB2	1.67	0.59
1:C:273:GLY:HA3	1:C:292:THR:OG1	2.03	0.59
1:A:486:THR:HB	1:A:487:PRO:CD	2.33	0.59
1:E:759:ARG:HD3	5:F:2080:HOH:O	2.03	0.58
1:A:886:ASP:OD1	1:C:897:ARG:NH1	2.37	0.58
1:F:668:THR:OG1	1:F:691:GLN:NE2	2.36	0.58
1:F:628:HIS:HE1	1:F:658:ASP:OD1	1.87	0.58
1:C:488:ASN:ND2	1:C:490:GLN:HE22	2.02	0.58
1:C:439:GLN:HE22	1:C:441:TYR:HB2	1.67	0.58
1:C:700:SER:OG	1:C:702:VAL:HG13	2.04	0.58
1:E:527:HIS:HD2	1:E:582:PRO:O	1.86	0.58
1:F:295:VAL:HG13	1:F:305:TYR:CD2	2.39	0.58
1:C:607:LEU:HB3	1:C:620:LEU:HD22	1.87	0.57
1:C:330:GLN:HE21	1:C:527:HIS:CE1	2.21	0.57
1:C:735:LYS:O	1:C:743:HIS:HE1	1.86	0.57
1:A:854:ILE:HD12	1:B:856:LEU:HD21	1.85	0.57
1:B:277:THR:CG2	1:B:295:VAL:HG22	2.35	0.57
1:B:295:VAL:HG13	1:B:305:TYR:CE2	2.40	0.57
1:B:350:HIS:CE1	1:B:699:ASN:HB3	2.39	0.57
1:A:576:GLU:N	1:A:577:PRO:HD2	2.20	0.57
1:B:428:HIS:ND1	1:B:502:HIS:HD2	2.03	0.57
1:E:277:THR:HG22	1:E:295:VAL:HG22	1.86	0.57
1:A:325:TYR:OH	1:A:350:HIS:HE1	1.87	0.57
1:C:367:GLN:HE22	1:C:764:PHE:H	1.53	0.57
1:E:305:TYR:CZ	1:E:684:GLU:HG2	2.40	0.57
1:C:419:TRP:CE2	1:C:514:LYS:HD3	2.39	0.57
1:F:603:LEU:HB3	1:F:621:ARG:CZ	2.35	0.56
4:D:1688:SIA:H6	4:D:1688:SIA:O1B	2.05	0.56
1:D:396:ARG:HB3	1:D:560:PHE:CZ	2.40	0.56
1:B:610:SER:HB2	1:B:616:THR:O	2.06	0.56
1:B:488:ASN:C	1:B:488:ASN:HD22	2.08	0.56
1:D:553:LEU:CD2	1:D:591:LEU:HD21	2.36	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:444:ILE:HG22	1:B:446:VAL:HG23	1.88	0.56
1:A:779:ASP:HB2	5:A:2155:HOH:O	2.06	0.56
1:E:457:VAL:HA	1:E:504:GLY:O	2.05	0.56
1:F:325:TYR:OH	1:F:350:HIS:HE1	1.89	0.56
1:A:352:VAL:HB	1:A:386:ASN:HB3	1.88	0.56
1:A:736:ASP:HB3	1:A:739:LYS:HG3	1.88	0.56
1:B:445:HIS:HD2	1:B:481:ASN:ND2	2.04	0.56
1:A:428:HIS:ND1	1:A:502:HIS:HD2	2.04	0.56
1:A:440:ARG:HE	1:A:489:GLN:NE2	2.03	0.56
1:F:439:GLN:HE22	1:F:441:TYR:HB2	1.71	0.56
1:B:445:HIS:CD2	1:B:481:ASN:HD21	2.23	0.55
1:A:602:ARG:NH1	1:A:602:ARG:HG3	2.21	0.55
1:B:287:SER:OG	1:C:753:LYS:HE3	2.05	0.55
1:E:277:THR:CG2	1:E:295:VAL:HG22	2.36	0.55
1:A:628:HIS:HE1	1:A:658:ASP:OD1	1.88	0.55
1:C:818:GLU:HB3	3:C:1687:PO4:O4	2.05	0.55
1:F:765:ARG:HD2	5:F:2112:HOH:O	2.05	0.55
1:C:888:VAL:HG12	1:C:889:THR:HG23	1.87	0.55
1:C:277:THR:HG22	1:C:295:VAL:HG22	1.87	0.55
1:D:586:TYR:OH	1:D:589:GLY:HA2	2.05	0.55
1:E:327:ALA:HB3	1:E:328:TRP:CE3	2.42	0.55
1:D:490:GLN:CG	5:D:2042:HOH:O	2.47	0.55
1:B:732:ASN:HD21	1:B:736:ASP:H	1.53	0.55
1:D:373:GLU:OE2	1:D:508:HIS:HE1	1.89	0.55
1:A:602:ARG:NE	5:A:2082:HOH:O	2.37	0.54
1:A:379:HIS:H	1:A:386:ASN:ND2	2.05	0.54
1:B:847:SER:OG	1:B:849:THR:HB	2.07	0.54
1:D:330:GLN:HE21	1:D:527:HIS:CE1	2.25	0.54
1:F:457:VAL:HA	1:F:504:GLY:O	2.07	0.54
1:A:607:LEU:HB3	1:A:620:LEU:HD22	1.90	0.54
1:E:466:GLY:HA3	1:E:486:THR:HB	1.90	0.54
1:B:909:VAL:HA	1:C:903:LEU:O	2.08	0.54
1:D:460:SER:OG	4:D:1688:SIA:H4	2.07	0.54
1:E:342:ALA:HB2	1:E:717:MET:HE2	1.89	0.54
1:B:445:HIS:HD2	1:B:481:ASN:HD21	1.55	0.54
1:F:532:ILE:HG12	1:F:537:PHE:HA	1.89	0.54
1:A:613:ILE:O	1:A:613:ILE:HG22	2.08	0.54
1:F:486:THR:HB	1:F:487:PRO:HD2	1.90	0.54
1:E:715:TYR:CE1	1:E:751:LYS:HG3	2.42	0.54
1:B:367:GLN:HE22	1:B:764:PHE:H	1.56	0.54
1:C:386:ASN:ND2	1:C:387:TYR:H	2.06	0.54
1:E:440:ARG:HE	1:E:489:GLN:HE21	1.56	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:277:THR:HG22	1:D:295:VAL:HG22	1.90	0.53
1:B:277:THR:HG22	1:B:295:VAL:HG22	1.89	0.53
1:C:405:THR:HB	1:C:415:ASN:HB3	1.91	0.53
5:E:2110:HOH:O	1:F:844:GLU:HG2	2.07	0.53
1:E:433:ILE:HG12	1:E:444:ILE:HG23	1.90	0.53
1:E:910:THR:HG22	1:F:897:ARG:HH11	1.74	0.53
1:C:628:HIS:HE1	1:C:658:ASP:OD1	1.90	0.53
1:A:342:ALA:HB2	1:A:717:MET:HE2	1.90	0.53
1:D:306:TYR:HD1	1:D:687:ASN:HD22	1.54	0.53
1:A:465:THR:HB	1:A:490:GLN:HE22	1.73	0.53
1:F:650:ASN:HA	1:F:667:ARG:NH2	2.24	0.53
1:D:367:GLN:HE21	1:F:765:ARG:NH1	2.07	0.53
1:E:379:HIS:H	1:E:386:ASN:ND2	2.06	0.53
1:F:368:THR:HG22	5:F:2024:HOH:O	2.07	0.52
1:E:352:VAL:HA	1:E:355:LEU:HD23	1.91	0.52
1:C:771:ASN:ND2	1:C:776:VAL:H	2.07	0.52
1:A:287:SER:OG	1:B:753:LYS:HE3	2.09	0.52
1:A:522:SER:HB3	1:A:568:ARG:HH22	1.74	0.52
1:A:771:ASN:HD21	1:A:776:VAL:N	1.96	0.52
1:D:352:VAL:HA	1:D:355:LEU:HD23	1.90	0.52
1:A:464:VAL:HG23	1:A:496:ASN:HB3	1.91	0.52
1:C:293:ARG:HD3	1:C:311:PHE:CE2	2.45	0.52
1:F:330:GLN:HB2	1:F:527:HIS:HE1	1.74	0.52
1:E:330:GLN:HB2	1:E:527:HIS:HE1	1.75	0.52
1:B:700:SER:OG	1:B:702:VAL:HG13	2.09	0.51
1:B:903:LEU:HA	1:C:898:PHE:O	2.10	0.51
1:E:400:PHE:CD1	1:E:420:ASP:HB3	2.45	0.51
1:E:620:LEU:HD23	1:E:620:LEU:C	2.31	0.51
1:A:693:TYR:HE1	5:A:2105:HOH:O	1.91	0.51
1:D:379:HIS:ND1	1:D:380:PRO:HD2	2.25	0.51
1:E:322:THR:HG21	5:E:2009:HOH:O	2.09	0.51
1:C:522:SER:HB3	1:C:568:ARG:NH2	2.25	0.51
1:A:261:ALA:O	1:A:265:THR:HG23	2.10	0.51
1:A:555:TYR:O	1:A:557:PRO:HD3	2.10	0.51
1:F:398:ARG:HD2	1:F:450:GLY:O	2.10	0.51
1:A:774:VAL:O	1:A:776:VAL:HG23	2.10	0.51
1:E:373:GLU:OE2	1:E:508:HIS:CE1	2.62	0.51
1:A:393:GLY:HA3	1:A:529:PHE:CD2	2.46	0.51
1:C:359:TRP:CE3	1:C:375:LEU:HD11	2.46	0.51
1:E:396:ARG:HD3	1:E:534:ASN:O	2.10	0.51
1:C:305:TYR:CZ	1:C:684:GLU:HG2	2.45	0.51
1:E:322:THR:HB	1:E:326:ASN:OD1	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:765:ARG:CD	5:F:2112:HOH:O	2.58	0.51
1:D:330:GLN:HG3	1:D:330:GLN:O	2.10	0.51
1:C:396:ARG:CG	1:C:396:ARG:O	2.58	0.51
1:F:379:HIS:H	1:F:386:ASN:ND2	2.09	0.51
1:C:527:HIS:HD2	1:C:582:PRO:O	1.94	0.50
1:F:439:GLN:NE2	1:F:441:TYR:H	2.09	0.50
1:E:433:ILE:HG22	1:E:464:VAL:HG21	1.92	0.50
1:E:347:SER:HB3	1:E:355:LEU:HB2	1.94	0.50
1:D:732:ASN:HD21	1:D:736:ASP:H	1.60	0.50
5:A:2032:HOH:O	1:B:779:ASP:HB2	2.10	0.50
1:A:449:HIS:HD2	1:A:451:LEU:N	1.93	0.50
1:B:743:HIS:CD2	5:B:2131:HOH:O	2.55	0.50
1:D:325:TYR:OH	1:D:350:HIS:HE1	1.94	0.50
1:C:870:ASN:HD22	1:C:871:GLY:N	2.09	0.50
1:A:277:THR:CG2	1:A:295:VAL:HG22	2.42	0.50
1:A:660:ARG:O	1:A:661:TYR:HB2	2.11	0.50
1:A:765:ARG:HH12	1:C:367:GLN:NE2	1.91	0.50
1:D:440:ARG:NE	1:D:489:GLN:HE21	2.06	0.50
1:B:373:GLU:OE2	1:B:508:HIS:CE1	2.64	0.50
1:C:628:HIS:HD2	5:C:2058:HOH:O	1.95	0.50
1:E:594:ILE:HD12	1:E:633:PHE:CD2	2.47	0.50
1:D:386:ASN:ND2	1:D:387:TYR:H	2.10	0.50
1:D:322:THR:HB	1:D:326:ASN:OD1	2.12	0.50
1:A:522:SER:HB3	1:A:568:ARG:NH2	2.26	0.50
1:D:896:ASN:HB2	1:F:882:LYS:HD2	1.94	0.50
1:F:837:ARG:NH2	2:F:1685:SLB:H111	2.26	0.50
1:E:628:HIS:HE1	1:E:658:ASP:OD1	1.95	0.50
1:E:771:ASN:HD21	1:E:776:VAL:H	1.58	0.49
1:D:352:VAL:HB	1:D:386:ASN:HB3	1.94	0.49
1:A:888:VAL:HG12	1:A:889:THR:HG23	1.94	0.49
1:D:465:THR:HG21	1:D:490:GLN:HE21	1.77	0.49
5:A:2012:HOH:O	1:B:368:THR:CG2	2.56	0.49
1:E:669:PHE:CE1	1:E:687:ASN:HB2	2.47	0.49
1:C:413:LEU:HD21	1:C:416:CYS:SG	2.53	0.49
1:A:527:HIS:CD2	1:A:582:PRO:O	2.60	0.49
1:F:428:HIS:ND1	1:F:502:HIS:HD2	2.11	0.49
1:A:700:SER:OG	1:A:702:VAL:HG13	2.11	0.49
1:B:347:SER:HB3	1:B:355:LEU:HD22	1.95	0.49
1:B:603:LEU:HB3	1:B:621:ARG:CZ	2.42	0.49
1:C:367:GLN:HE22	1:C:763:ASP:HA	1.77	0.49
1:D:765:ARG:NH1	5:D:2126:HOH:O	2.25	0.49
1:A:609:ARG:HG2	1:A:678:TRP:CZ2	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:396:ARG:HD3	1:B:534:ASN:O	2.13	0.49
1:A:620:LEU:HD21	1:A:680:ALA:HB2	1.94	0.49
1:E:352:VAL:HB	1:E:386:ASN:HB3	1.94	0.49
1:D:293:ARG:HD3	1:D:311:PHE:CE2	2.48	0.49
1:E:736:ASP:HB3	1:E:739:LYS:HG2	1.94	0.49
1:B:568:ARG:HD2	5:B:2082:HOH:O	2.12	0.49
1:C:295:VAL:HG13	1:C:305:TYR:CD2	2.47	0.49
1:D:753:LYS:HE3	1:E:287:SER:OG	2.12	0.49
1:B:649:GLU:HB3	1:B:664:SER:HB2	1.94	0.49
1:A:497:ALA:HB2	5:A:2057:HOH:O	2.13	0.49
1:E:449:HIS:HD2	1:E:451:LEU:N	2.01	0.49
1:E:558:ASP:OD1	1:E:561:ASN:HB2	2.13	0.48
1:B:661:TYR:CZ	1:B:698:VAL:HB	2.48	0.48
1:D:603:LEU:HB3	1:D:621:ARG:CZ	2.43	0.48
1:E:277:THR:HG22	1:E:295:VAL:CG2	2.43	0.48
1:D:460:SER:HB3	1:D:461:ASN:ND2	2.28	0.48
1:C:571:ILE:HB	1:C:572:PRO:HD2	1.95	0.48
1:F:603:LEU:HG	1:F:621:ARG:HD3	1.94	0.48
1:F:350:HIS:CE1	1:F:699:ASN:HB3	2.48	0.48
1:E:628:HIS:HD2	5:E:2045:HOH:O	1.96	0.48
1:C:614:GLY:HA2	1:C:617:TRP:CZ2	2.48	0.48
1:A:352:VAL:O	1:A:355:LEU:HB3	2.13	0.48
1:C:532:ILE:HG12	1:C:537:PHE:HA	1.95	0.48
1:D:679:ASN:HD22	1:D:680:ALA:N	2.11	0.48
1:A:753:LYS:HE3	1:C:287:SER:OG	2.14	0.48
1:E:700:SER:OG	1:E:702:VAL:HG13	2.13	0.48
1:D:357:VAL:HG12	1:D:375:LEU:HD12	1.96	0.48
1:F:342:ALA:HB2	1:F:717:MET:HE2	1.96	0.48
1:B:305:TYR:CE1	1:B:684:GLU:HB3	2.49	0.48
1:E:342:ALA:HB2	1:E:717:MET:CE	2.44	0.48
1:B:521:PRO:HA	5:B:2071:HOH:O	2.14	0.48
1:D:906:ASN:OD1	1:E:909:VAL:HG11	2.14	0.48
1:E:609:ARG:HG2	1:E:678:TRP:CZ2	2.48	0.48
1:E:744:PRO:HD2	5:E:2087:HOH:O	2.14	0.48
1:E:428:HIS:ND1	1:E:502:HIS:HD2	2.11	0.47
1:E:433:ILE:CG2	1:E:464:VAL:HG21	2.44	0.47
1:F:379:HIS:H	1:F:386:ASN:HD22	1.63	0.47
1:F:419:TRP:CD1	1:F:514:LYS:HG2	2.48	0.47
1:B:673:LEU:HD12	1:B:683:ILE:HD12	1.95	0.47
1:B:330:GLN:HB2	1:B:527:HIS:HE1	1.80	0.47
1:B:527:HIS:CD2	1:B:582:PRO:O	2.66	0.47
1:B:673:LEU:HD12	1:B:683:ILE:CD1	2.45	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:503:MET:HG2	1:C:504:GLY:HA3	1.96	0.47
1:E:788:ALA:HB2	1:F:738:PHE:CD1	2.50	0.47
1:D:396:ARG:HD3	1:D:534:ASN:O	2.15	0.47
1:E:735:LYS:O	1:E:743:HIS:HE1	1.97	0.47
1:B:328:TRP:N	1:B:329:PRO:HD3	2.29	0.47
1:E:649:GLU:HB2	1:E:664:SER:HB2	1.96	0.47
1:F:435:LYS:HB3	1:F:494:LEU:HB2	1.96	0.47
1:D:848:SER:O	1:F:865:ARG:NE	2.47	0.47
1:B:689:THR:HG23	1:B:691:GLN:HE22	1.79	0.47
1:B:771:ASN:HD21	1:B:776:VAL:N	2.02	0.47
1:D:712:ASN:ND2	1:D:712:ASN:H	2.11	0.47
1:E:753:LYS:HE2	1:E:755:GLY:O	2.15	0.47
1:A:405:THR:HB	1:A:414:THR:HG22	1.96	0.47
1:D:440:ARG:HE	1:D:489:GLN:NE2	2.05	0.47
1:B:878:SER:HB2	1:C:871:GLY:O	2.15	0.47
1:E:847:SER:OG	1:E:849:THR:HB	2.15	0.47
1:B:325:TYR:OH	1:B:350:HIS:HE1	1.97	0.46
1:B:457:VAL:HA	1:B:504:GLY:O	2.15	0.46
1:B:379:HIS:HB2	1:B:386:ASN:HD22	1.79	0.46
1:F:847:SER:OG	1:F:849:THR:HB	2.14	0.46
1:F:682:ASP:HB2	5:F:2082:HOH:O	2.15	0.46
1:E:445:HIS:HD2	1:E:481:ASN:HD21	1.62	0.46
1:C:320:THR:HG23	1:C:747:LEU:HB2	1.96	0.46
1:C:428:HIS:ND1	1:C:502:HIS:HD2	2.14	0.46
1:B:549:ARG:HD3	1:B:579:ALA:O	2.16	0.46
1:A:870:ASN:ND2	1:B:865:ARG:HH22	2.13	0.46
1:C:661:TYR:CZ	1:C:698:VAL:HB	2.50	0.46
1:A:852:ALA:HB1	1:B:867:ILE:HG12	1.96	0.46
1:A:886:ASP:CG	1:C:897:ARG:NH1	2.69	0.46
1:C:306:TYR:HD1	1:C:687:ASN:HD22	1.62	0.46
1:D:398:ARG:HD2	1:D:450:GLY:O	2.15	0.46
1:E:367:GLN:NE2	1:E:763:ASP:HA	2.31	0.46
1:B:445:HIS:CD2	1:B:481:ASN:ND2	2.82	0.46
1:E:743:HIS:O	5:E:2085:HOH:O	2.20	0.46
1:D:464:VAL:HG23	1:D:496:ASN:HB3	1.97	0.46
1:D:754:ILE:HA	1:D:754:ILE:HD12	1.44	0.46
1:C:607:LEU:HD13	1:C:678:TRP:CH2	2.50	0.46
1:E:440:ARG:HE	1:E:489:GLN:NE2	2.14	0.46
1:A:322:THR:HB	1:A:326:ASN:OD1	2.16	0.46
1:C:340:ILE:CG2	1:C:717:MET:HE1	2.46	0.46
1:F:440:ARG:HG2	1:F:489:GLN:HB3	1.96	0.46
1:F:439:GLN:HE22	1:F:441:TYR:H	1.62	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:771:ASN:ND2	1:E:776:VAL:H	2.13	0.46
1:C:347:SER:HB3	1:C:355:LEU:HB2	1.97	0.46
1:D:367:GLN:NE2	1:F:765:ARG:HH12	2.12	0.46
1:A:460:SER:HB3	1:A:461:ASN:ND2	2.31	0.46
1:A:382:TYR:CG	1:A:383:PRO:HA	2.51	0.46
1:F:527:HIS:HD2	1:F:582:PRO:O	1.98	0.46
1:C:464:VAL:HG23	1:C:496:ASN:HB3	1.98	0.46
1:C:826:LYS:HB2	1:C:838:ILE:HG13	1.97	0.46
1:A:852:ALA:HB1	1:B:867:ILE:CG1	2.46	0.45
1:F:295:VAL:CG1	1:F:305:TYR:CE2	2.98	0.45
1:D:620:LEU:C	1:D:620:LEU:HD23	2.36	0.45
1:E:391:SER:OG	1:E:539:MET:HG2	2.16	0.45
1:F:609:ARG:HG2	1:F:678:TRP:CZ3	2.51	0.45
1:C:441:TYR:CZ	1:C:485:LEU:HD13	2.52	0.45
1:C:827:SER:O	1:C:829:PRO:HD3	2.16	0.45
1:F:325:TYR:OH	1:F:350:HIS:CE1	2.69	0.45
1:C:661:TYR:OH	1:C:698:VAL:HB	2.16	0.45
1:F:620:LEU:HD23	1:F:620:LEU:C	2.37	0.45
1:C:322:THR:HG22	1:C:324:TYR:N	2.23	0.45
1:F:679:ASN:C	1:F:679:ASN:OD1	2.55	0.45
1:E:553:LEU:HD22	1:E:591:LEU:HD21	1.98	0.45
1:F:322:THR:HG23	1:F:323:PRO:HD2	1.99	0.45
1:D:712:ASN:HB3	5:D:2122:HOH:O	2.16	0.45
1:F:826:LYS:HB2	1:F:838:ILE:HG13	1.99	0.45
1:F:739:LYS:CD	5:F:2098:HOH:O	2.65	0.45
1:E:883:PRO:HD3	1:F:898:PHE:CZ	2.51	0.45
1:C:659:ASP:OD1	1:C:662:LYS:HE3	2.17	0.45
1:C:870:ASN:ND2	1:C:870:ASN:C	2.61	0.45
1:B:739:LYS:HE3	5:B:2126:HOH:O	2.15	0.44
1:B:584:ILE:O	1:B:585:LYS:HD2	2.17	0.44
1:C:305:TYR:CE1	1:C:684:GLU:HG2	2.52	0.44
1:E:910:THR:HB	5:E:2126:HOH:O	2.18	0.44
1:E:553:LEU:CD2	1:E:591:LEU:HD21	2.47	0.44
1:C:458:ASN:HA	1:C:469:GLY:O	2.17	0.44
1:C:796:LEU:HG	1:C:798:LEU:HD21	1.99	0.44
1:C:754:ILE:HA	1:C:754:ILE:HD12	1.59	0.44
1:D:457:VAL:HA	1:D:504:GLY:O	2.17	0.44
1:F:322:THR:HB	1:F:326:ASN:OD1	2.18	0.44
1:C:343:PRO:HA	1:C:359:TRP:HB3	1.99	0.44
1:A:848:SER:O	1:B:865:ARG:NE	2.50	0.44
1:C:430:THR:HA	1:C:499:LYS:O	2.17	0.44
1:A:836:GLN:HG2	1:A:858:GLY:HA3	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:449:HIS:HE1	1:B:478:ASP:O	2.00	0.44
1:E:732:ASN:HA	5:E:2081:HOH:O	2.17	0.44
1:C:613:ILE:O	1:C:613:ILE:HG22	2.18	0.44
1:A:428:HIS:ND1	1:A:502:HIS:CD2	2.84	0.44
1:B:826:LYS:HD2	1:C:817:MET:O	2.16	0.44
1:C:593:LEU:HD23	1:C:593:LEU:C	2.38	0.44
1:C:574:GLU:HG3	1:C:575:TYR:CD2	2.52	0.44
1:A:279:LYS:HA	1:A:295:VAL:HG23	1.99	0.44
1:F:364:ASP:OD1	1:F:368:THR:HB	2.16	0.44
1:C:379:HIS:H	1:C:386:ASN:ND2	2.14	0.44
1:F:378:LEU:HA	1:F:386:ASN:HD21	1.83	0.44
1:D:247:LYS:HA	1:D:247:LYS:HD3	1.73	0.44
1:E:322:THR:HG23	1:E:323:PRO:HD2	1.98	0.44
1:A:603:LEU:HB3	1:A:621:ARG:CZ	2.48	0.44
1:A:902:TYR:CD1	1:B:893:GLY:HA2	2.52	0.44
1:F:326:ASN:ND2	5:F:2012:HOH:O	2.51	0.44
1:F:771:ASN:ND2	1:F:776:VAL:H	2.12	0.44
1:B:305:TYR:CD1	1:B:305:TYR:N	2.86	0.44
1:A:848:SER:HB2	1:B:865:ARG:NH2	2.33	0.44
1:D:898:PHE:CE1	1:F:883:PRO:HD3	2.53	0.44
1:E:247:LYS:HG3	1:E:252:THR:HG21	2.00	0.44
1:B:306:TYR:HD1	1:B:687:ASN:HD22	1.66	0.44
1:F:277:THR:HG22	1:F:295:VAL:HG22	2.00	0.44
1:B:379:HIS:H	1:B:386:ASN:HD22	1.65	0.44
1:D:330:GLN:HB2	1:D:527:HIS:HE1	1.83	0.44
1:C:330:GLN:HA	1:C:331:ASP:HA	1.82	0.44
1:C:330:GLN:HB2	1:C:527:HIS:HE1	1.83	0.43
1:D:350:HIS:CE1	1:D:699:ASN:HB3	2.53	0.43
1:A:457:VAL:HA	1:A:504:GLY:O	2.17	0.43
1:A:735:LYS:O	1:A:743:HIS:HE1	2.00	0.43
1:F:445:HIS:HD2	1:F:481:ASN:HD21	1.66	0.43
1:D:614:GLY:HA2	1:D:617:TRP:CZ2	2.53	0.43
1:B:449:HIS:HD2	1:B:451:LEU:N	2.03	0.43
1:C:400:PHE:CD1	1:C:420:ASP:HB3	2.53	0.43
1:C:839:ILE:HG12	1:C:855:THR:HG23	2.00	0.43
1:C:542:HIS:HD2	5:C:2047:HOH:O	2.00	0.43
1:F:754:ILE:HA	1:F:754:ILE:HD12	1.62	0.43
1:C:847:SER:OG	1:C:849:THR:HB	2.17	0.43
1:E:367:GLN:HE22	1:E:763:ASP:HA	1.82	0.43
1:D:445:HIS:HD2	1:D:481:ASN:HD21	1.66	0.43
1:A:342:ALA:HB2	1:A:717:MET:CE	2.49	0.43
1:C:457:VAL:HA	1:C:504:GLY:O	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:267:VAL:HB	5:F:2007:HOH:O	2.18	0.43
1:D:609:ARG:HD2	1:D:618:GLU:OE1	2.19	0.43
1:B:277:THR:HG22	1:B:295:VAL:CG2	2.49	0.43
1:B:649:GLU:CB	1:B:664:SER:HB2	2.49	0.43
1:D:903:LEU:HA	1:F:898:PHE:O	2.19	0.43
1:E:315:GLU:HB3	5:E:2004:HOH:O	2.18	0.43
1:D:522:SER:HB3	1:D:568:ARG:NH2	2.33	0.43
1:F:283:LEU:HA	1:F:283:LEU:HD23	1.86	0.43
1:C:735:LYS:O	1:C:743:HIS:CE1	2.71	0.43
1:A:576:GLU:N	1:A:577:PRO:CD	2.81	0.43
1:A:325:TYR:OH	1:A:350:HIS:CE1	2.70	0.43
1:E:771:ASN:HA	1:E:771:ASN:HD22	1.70	0.43
1:F:542:HIS:HD2	5:F:2057:HOH:O	2.01	0.43
1:F:396:ARG:HD3	1:F:534:ASN:O	2.19	0.43
1:E:542:HIS:CD2	5:E:2038:HOH:O	2.44	0.43
1:D:765:ARG:O	1:E:317:PHE:HA	2.19	0.43
1:D:882:LYS:HD2	1:E:896:ASN:HB2	2.01	0.43
1:D:364:ASP:OD1	1:D:368:THR:HB	2.19	0.43
1:E:707:VAL:HA	1:E:715:TYR:O	2.19	0.43
1:E:352:VAL:HG11	1:E:406:ARG:HB2	2.01	0.43
1:F:576:GLU:N	1:F:577:PRO:CD	2.82	0.43
1:B:679:ASN:HD21	1:B:681:ASP:CG	2.21	0.43
1:F:349:ARG:HB3	1:F:735:LYS:HD3	2.01	0.43
1:C:367:GLN:NE2	1:C:763:ASP:HA	2.34	0.43
1:A:715:TYR:CE1	1:A:751:LYS:HD2	2.54	0.43
1:D:603:LEU:HG	1:D:621:ARG:HD3	2.01	0.42
1:C:649:GLU:HB2	1:C:664:SER:HB2	2.01	0.42
1:A:421:ARG:HD2	1:A:512:TRP:CD2	2.54	0.42
1:C:327:ALA:HB3	1:C:328:TRP:CE3	2.53	0.42
1:F:836:GLN:OE1	1:F:860:ASN:HB2	2.18	0.42
1:D:607:LEU:HB3	1:D:620:LEU:HD22	2.00	0.42
1:E:818:GLU:HA	1:F:827:SER:OG	2.19	0.42
1:C:316:LEU:HD22	1:C:689:THR:OG1	2.19	0.42
1:E:330:GLN:HA	1:E:331:ASP:HA	1.82	0.42
1:B:338:ASN:HB2	5:B:2017:HOH:O	2.18	0.42
1:E:437:ALA:HB2	1:E:492:SER:C	2.39	0.42
1:B:754:ILE:HA	1:B:754:ILE:HD12	1.88	0.42
1:A:754:ILE:HA	1:A:754:ILE:HD12	1.51	0.42
1:E:270:LYS:HD3	1:E:270:LYS:HA	1.92	0.42
1:E:576:GLU:N	1:E:577:PRO:CD	2.83	0.42
1:E:435:LYS:HB3	5:E:2029:HOH:O	2.19	0.42
4:E:1688:SIA:H6	4:E:1688:SIA:O1B	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:883:PRO:HD3	1:F:898:PHE:CE1	2.55	0.42
1:B:396:ARG:HB3	1:B:560:PHE:HZ	1.82	0.42
1:A:379:HIS:ND1	1:A:380:PRO:HD2	2.35	0.42
1:A:870:ASN:HD22	1:A:870:ASN:C	2.23	0.42
1:C:660:ARG:O	1:C:661:TYR:HB2	2.20	0.42
1:F:649:GLU:HB3	1:F:664:SER:HB2	2.02	0.42
1:C:900:THR:OG1	1:C:901:ALA:N	2.52	0.42
1:C:594:ILE:HG12	1:C:607:LEU:HD23	2.02	0.42
1:F:440:ARG:NE	1:F:489:GLN:HE21	2.09	0.42
1:D:330:GLN:HE21	1:D:527:HIS:HE1	1.68	0.42
1:D:586:TYR:CZ	1:D:589:GLY:HA2	2.55	0.42
1:F:600:GLY:HA3	5:F:2077:HOH:O	2.19	0.42
1:D:639:ASP:OD1	1:D:672:ARG:HD3	2.19	0.42
1:A:326:ASN:HB2	1:A:746:ASP:HA	2.01	0.42
1:A:379:HIS:CG	1:A:380:PRO:HD2	2.54	0.42
1:E:640:LEU:HD22	1:E:675:VAL:HG12	2.02	0.42
1:A:765:ARG:O	1:C:317:PHE:HA	2.20	0.41
1:A:569:ARG:HD2	1:A:613:ILE:O	2.20	0.41
1:B:336:TYR:CE2	1:B:337:GLU:HG3	2.55	0.41
1:B:628:HIS:HE1	1:B:658:ASP:OD1	2.03	0.41
1:D:891:LEU:HD22	1:F:891:LEU:HD21	2.02	0.41
1:D:608:HIS:CE1	1:D:619:SER:HG	2.30	0.41
1:C:647:ARG:HH11	1:C:647:ARG:HG3	1.83	0.41
1:F:277:THR:CG2	1:F:295:VAL:HG22	2.50	0.41
1:E:368:THR:HG22	5:E:2019:HOH:O	2.21	0.41
1:B:352:VAL:HA	1:B:355:LEU:HD23	2.02	0.41
1:E:445:HIS:CD2	1:E:481:ASN:HD21	2.38	0.41
1:C:468:SER:HA	5:C:2130:HOH:O	2.19	0.41
1:D:628:HIS:HE1	1:D:658:ASP:OD1	2.03	0.41
1:A:324:TYR:HB2	1:A:326:ASN:HD21	1.84	0.41
1:E:305:TYR:N	1:E:305:TYR:CD1	2.89	0.41
1:C:647:ARG:NH1	1:C:647:ARG:HG3	2.35	0.41
1:C:555:TYR:CZ	1:C:557:PRO:HA	2.55	0.41
1:B:342:ALA:HB2	1:B:717:MET:CE	2.51	0.41
1:B:553:LEU:HD22	1:B:591:LEU:HD21	2.01	0.41
1:E:631:LEU:HA	1:E:631:LEU:HD23	1.89	0.41
1:D:279:LYS:HA	1:D:295:VAL:HG23	2.02	0.41
1:A:350:HIS:CE1	1:A:699:ASN:HB3	2.54	0.41
1:D:325:TYR:OH	1:D:350:HIS:CE1	2.72	0.41
1:B:779:ASP:OD1	1:B:781:ASN:N	2.53	0.41
1:D:336:TYR:CE2	1:D:337:GLU:HG3	2.55	0.41
5:A:2170:HOH:O	1:B:864:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:330:GLN:HA	1:A:331:ASP:HA	1.82	0.41
1:E:325:TYR:OH	1:E:350:HIS:HE1	2.03	0.41
1:E:295:VAL:HG13	1:E:305:TYR:CE2	2.55	0.41
1:B:628:HIS:HD2	5:B:2088:HOH:O	2.04	0.41
1:D:439:GLN:NE2	1:D:441:TYR:H	2.19	0.41
1:B:873:GLU:OE2	1:C:866:ARG:HB2	2.21	0.41
1:F:261:ALA:O	1:F:265:THR:HG23	2.20	0.41
1:E:825:GLY:HA2	1:F:841:CYS:O	2.21	0.41
1:C:553:LEU:HD22	1:C:591:LEU:HD21	2.02	0.41
1:B:771:ASN:HD22	1:B:771:ASN:HA	1.74	0.41
1:B:330:GLN:HB2	1:B:527:HIS:CE1	2.56	0.41
1:E:640:LEU:HD12	1:E:640:LEU:HA	1.95	0.41
1:D:262:LEU:HA	1:D:262:LEU:HD23	1.89	0.41
1:C:309:GLU:HA	1:C:309:GLU:OE1	2.20	0.41
1:E:367:GLN:HE22	1:E:764:PHE:N	2.12	0.41
1:E:765:ARG:HH12	1:F:367:GLN:NE2	2.05	0.41
1:C:603:LEU:HB3	1:C:621:ARG:CZ	2.51	0.41
1:C:623:PRO:HB2	1:C:624:HIS:CD2	2.56	0.41
1:F:593:LEU:C	1:F:593:LEU:HD23	2.41	0.40
1:D:673:LEU:HA	1:D:673:LEU:HD23	1.86	0.40
1:A:542:HIS:CD2	1:A:581:GLU:H	2.39	0.40
1:B:735:LYS:O	1:B:743:HIS:HE1	2.04	0.40
1:D:553:LEU:CD2	1:D:591:LEU:CD2	2.99	0.40
1:E:396:ARG:HB3	1:E:560:PHE:CZ	2.56	0.40
1:E:753:LYS:HE3	1:F:287:SER:OG	2.21	0.40
1:C:328:TRP:N	1:C:329:PRO:HD3	2.36	0.40
1:F:355:LEU:HD13	1:F:356:HIS:N	2.35	0.40
1:D:660:ARG:O	1:D:661:TYR:HB2	2.20	0.40
1:F:490:GLN:HG2	5:F:2049:HOH:O	2.21	0.40
1:B:716:TYR:O	1:B:749:CYS:HA	2.20	0.40
1:D:829:PRO:HB3	1:F:820:GLU:HA	2.03	0.40
1:D:522:SER:HB3	1:D:568:ARG:HH21	1.86	0.40
1:E:522:SER:HB2	1:E:568:ARG:NH2	2.37	0.40
1:B:575:TYR:CG	1:B:608:HIS:HE1	2.39	0.40
1:D:302:GLN:HE22	1:D:654:ALA:HB3	1.87	0.40
1:D:344:TYR:CD2	1:D:747:LEU:HD11	2.56	0.40
1:A:499:LYS:HD2	1:A:499:LYS:HA	1.90	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%)	631 (95%)	31 (5%)	2 (0%)	50	71
1	B	664/666 (100%)	630 (95%)	34 (5%)	0	100	100
1	C	664/666 (100%)	629 (95%)	35 (5%)	0	100	100
1	D	664/666 (100%)	631 (95%)	32 (5%)	1 (0%)	56	78
1	E	664/666 (100%)	634 (96%)	28 (4%)	2 (0%)	50	71
1	F	664/666 (100%)	630 (95%)	34 (5%)	0	100	100
All	All	3984/3996 (100%)	3785 (95%)	194 (5%)	5 (0%)	59	81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	496	ASN
1	D	704	VAL
1	E	350	HIS
1	E	704	VAL
1	A	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%)	527 (93%)	37 (7%)	24	40
1	B	564/564 (100%)	519 (92%)	45 (8%)	17	30
1	C	564/564 (100%)	523 (93%)	41 (7%)	20	35
1	D	564/564 (100%)	523 (93%)	41 (7%)	20	35
1	E	564/564 (100%)	518 (92%)	46 (8%)	17	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	564/564 (100%)	518 (92%)	46 (8%)	17	29
All	All	3384/3384 (100%)	3128 (92%)	256 (8%)	19	33

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	VAL
1	A	258	LEU
1	A	260	SER
1	A	270	LYS
1	A	279	LYS
1	A	295	VAL
1	A	355	LEU
1	A	359	TRP
1	A	361	LYS
1	A	368	THR
1	A	414	THR
1	A	425	ARG
1	A	439	GLN
1	A	443	THR
1	A	460	SER
1	A	476	VAL
1	A	499	LYS
1	A	564	SER
1	A	585	LYS
1	A	596	ARG
1	A	603	LEU
1	A	607	LEU
1	A	609	ARG
1	A	618	GLU
1	A	620	LEU
1	A	621	ARG
1	A	640	LEU
1	A	717	MET
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	888	VAL
1	A	895	SER

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Mol	Chain	Res	Type
1	A	910	THR
1	B	258	LEU
1	B	260	SER
1	B	279	LYS
1	B	282	SER
1	B	295	VAL
1	B	312	VAL
1	B	335	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	457	VAL
1	B	468	SER
1	B	476	VAL
1	B	479	LYS
1	B	488	ASN
1	B	562	SER
1	B	568	ARG
1	B	574	GLU
1	B	585	LYS
1	B	596	ARG
1	B	603	LEU
1	B	607	LEU
1	B	609	ARG
1	B	611	ARG
1	B	620	LEU
1	B	621	ARG
1	B	640	LEU
1	B	662	LYS
1	B	670	TYR
1	B	679	ASN
1	B	683	ILE
1	B	717	MET
1	B	718	PHE
1	B	732	ASN
1	B	754	ILE
1	B	762	ARG
1	B	796	LEU
1	B	816	LEU

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Mol	Chain	Res	Type
1	B	849	THR
1	B	870	ASN
1	B	909	VAL
1	B	910	THR
1	C	258	LEU
1	C	260	SER
1	C	281	THR
1	C	295	VAL
1	C	309	GLU
1	C	355	LEU
1	C	359	TRP
1	C	361	LYS
1	C	368	THR
1	C	386	ASN
1	C	396	ARG
1	C	425	ARG
1	C	439	GLN
1	C	443	THR
1	C	444	ILE
1	C	488	ASN
1	C	509	LYS
1	C	522	SER
1	C	528	SER
1	C	546	VAL
1	C	568	ARG
1	C	585	LYS
1	C	596	ARG
1	C	599	ARG
1	C	603	LEU
1	C	607	LEU
1	C	609	ARG
1	C	611	ARG
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	762	ARG
1	C	771	ASN
1	C	796	LEU
1	C	816	LEU

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Mol	Chain	Res	Type
1	C	870	ASN
1	C	909	VAL
1	C	910	THR
1	D	247	LYS
1	D	258	LEU
1	D	270	LYS
1	D	279	LYS
1	D	295	VAL
1	D	335	VAL
1	D	355	LEU
1	D	359	TRP
1	D	368	THR
1	D	386	ASN
1	D	396	ARG
1	D	414	THR
1	D	425	ARG
1	D	439	GLN
1	D	488	ASN
1	D	499	LYS
1	D	522	SER
1	D	549	ARG
1	D	568	ARG
1	D	574	GLU
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	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

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Mol	Chain	Res	Type
1	D	909	VAL
1	D	910	THR
1	E	245	SER
1	E	258	LEU
1	E	260	SER
1	E	279	LYS
1	E	295	VAL
1	E	309	GLU
1	E	312	VAL
1	E	335	VAL
1	E	355	LEU
1	E	358	SER
1	E	359	TRP
1	E	368	THR
1	E	386	ASN
1	E	408	LEU
1	E	414	THR
1	E	421	ARG
1	E	439	GLN
1	E	443	THR
1	E	444	ILE
1	E	457	VAL
1	E	476	VAL
1	E	488	ASN
1	E	499	LYS
1	E	543	GLN
1	E	562	SER
1	E	564	SER
1	E	574	GLU
1	E	585	LYS
1	E	596	ARG
1	E	602	ARG
1	E	603	LEU
1	E	607	LEU
1	E	609	ARG
1	E	620	LEU
1	E	621	ARG
1	E	640	LEU
1	E	717	MET
1	E	754	ILE
1	E	762	ARG
1	E	771	ASN

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Mol	Chain	Res	Type
1	E	796	LEU
1	E	816	LEU
1	E	849	THR
1	E	870	ASN
1	E	909	VAL
1	E	910	THR
1	F	258	LEU
1	F	259	THR
1	F	276	LYS
1	F	279	LYS
1	F	295	VAL
1	F	335	VAL
1	F	355	LEU
1	F	359	TRP
1	F	368	THR
1	F	396	ARG
1	F	414	THR
1	F	439	GLN
1	F	443	THR
1	F	457	VAL
1	F	465	THR
1	F	468	SER
1	F	485	LEU
1	F	488	ASN
1	F	534	ASN
1	F	565	ASN
1	F	584	ILE
1	F	585	LYS
1	F	591	LEU
1	F	596	ARG
1	F	603	LEU
1	F	607	LEU
1	F	609	ARG
1	F	611	ARG
1	F	620	LEU
1	F	621	ARG
1	F	640	LEU
1	F	702	VAL
1	F	704	VAL
1	F	717	MET
1	F	732	ASN
1	F	754	ILE

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Mol	Chain	Res	Type
1	F	762	ARG
1	F	771	ASN
1	F	796	LEU
1	F	816	LEU
1	F	849	THR
1	F	864	SER
1	F	870	ASN
1	F	895	SER
1	F	909	VAL
1	F	910	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (163) 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	439	GLN
1	A	445	HIS
1	A	449	HIS
1	A	461	ASN
1	A	481	ASN
1	A	489	GLN
1	A	490	GLN
1	A	502	HIS
1	A	508	HIS
1	A	527	HIS
1	A	542	HIS
1	A	561	ASN
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	860	ASN
1	A	870	ASN

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Mol	Chain	Res	Type
1	B	263	ASN
1	B	350	HIS
1	B	367	GLN
1	B	386	ASN
1	B	397	ASN
1	B	439	GLN
1	B	445	HIS
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	625	ASN
1	B	628	HIS
1	B	677	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	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	489	GLN
1	C	502	HIS
1	C	508	HIS
1	C	527	HIS
1	C	542	HIS

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Mol	Chain	Res	Type
1	C	624	HIS
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
1	D	508	HIS
1	D	527	HIS
1	D	542	HIS
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

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Mol	Chain	Res	Type
1	E	263	ASN
1	E	350	HIS
1	E	367	GLN
1	E	386	ASN
1	E	439	GLN
1	E	449	HIS
1	E	461	ASN
1	E	481	ASN
1	E	488	ASN
1	E	489	GLN
1	E	502	HIS
1	E	508	HIS
1	E	527	HIS
1	E	561	ASN
1	E	625	ASN
1	E	628	HIS
1	E	650	ASN
1	E	676	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	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	489	GLN
1	F	502	HIS
1	F	508	HIS
1	F	527	HIS
1	F	542	HIS
1	F	625	ASN

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Mol	Chain	Res	Type
1	F	628	HIS
1	F	650	ASN
1	F	691	GLN
1	F	732	ASN
1	F	743	HIS
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 ⓘ

6 carbohydrates 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	$\# Z  > 2$
4	SIA	C	1686	4	21,21,21	2.45	7 (33%)	31,31,31	2.11	6 (19%)
4	SIA	C	1688	4	20,20,21	5.76	4 (20%)	23,28,31	2.19	4 (17%)
4	SIA	D	1686	4	21,21,21	2.71	6 (28%)	31,31,31	2.25	10 (32%)
4	SIA	D	1688	4	20,20,21	6.01	5 (25%)	23,28,31	3.23	5 (21%)
4	SIA	E	1686	4	21,21,21	3.40	7 (33%)	31,31,31	1.55	7 (22%)
4	SIA	E	1688	4	20,20,21	5.55	5 (25%)	23,28,31	2.72	8 (34%)

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
4	SIA	C	1686	4	-	0/20/38/38	0/1/1/1
4	SIA	C	1688	4	-	0/15/34/38	0/1/1/1
4	SIA	D	1686	4	-	0/20/38/38	0/1/1/1
4	SIA	D	1688	4	-	0/15/34/38	0/1/1/1
4	SIA	E	1686	4	-	0/20/38/38	0/1/1/1
4	SIA	E	1688	4	-	0/15/34/38	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1688	SIA	O6-C2	26.03	1.51	1.28
4	C	1688	SIA	O6-C2	24.91	1.50	1.28
4	E	1688	SIA	O6-C2	23.85	1.49	1.28
4	E	1686	SIA	O6-C2	11.65	1.53	1.42
4	D	1686	SIA	C4-C5	6.85	1.59	1.53
4	C	1686	SIA	O6-C2	6.28	1.48	1.42
4	E	1686	SIA	O2-C2	5.89	1.47	1.39
4	D	1686	SIA	O2-C2	5.81	1.47	1.39
4	D	1686	SIA	C3-C2	5.31	1.59	1.51
4	E	1686	SIA	O6-C6	4.62	1.52	1.44
4	C	1686	SIA	O2-C2	4.45	1.45	1.39
4	E	1686	SIA	C3-C2	4.13	1.57	1.51
4	C	1688	SIA	C4-C5	4.08	1.56	1.53
4	E	1688	SIA	C4-C5	4.02	1.56	1.53
4	D	1686	SIA	C3-C4	3.93	1.59	1.53
4	C	1686	SIA	C3-C2	3.91	1.57	1.51
4	C	1686	SIA	C4-C5	3.55	1.56	1.53
4	C	1686	SIA	C3-C4	3.13	1.58	1.53
4	C	1686	SIA	O6-C6	3.09	1.49	1.44
4	D	1688	SIA	C4-C5	3.00	1.55	1.53
4	D	1688	SIA	C7-C6	2.90	1.56	1.52
4	D	1688	SIA	O1B-C1	-2.70	1.21	1.30
4	E	1686	SIA	C3-C4	2.67	1.57	1.53
4	C	1688	SIA	C7-C6	2.61	1.56	1.52
4	E	1688	SIA	C7-C6	2.58	1.56	1.52
4	E	1688	SIA	O1B-C1	-2.55	1.22	1.30
4	D	1686	SIA	O6-C6	2.48	1.48	1.44
4	D	1686	SIA	C5-N5	2.39	1.49	1.45
4	E	1688	SIA	C3-C2	2.38	1.54	1.46
4	D	1688	SIA	C3-C2	2.20	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1688	SIA	C3-C2	2.16	1.54	1.46
4	C	1686	SIA	C5-N5	2.12	1.49	1.45
4	E	1686	SIA	C5-N5	2.09	1.49	1.45
4	E	1686	SIA	C4-C5	2.06	1.54	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1688	SIA	O6-C2-C3	-10.84	110.74	124.91
4	E	1688	SIA	O6-C2-C3	-9.36	112.68	124.91
4	C	1688	SIA	O6-C2-C3	-8.65	113.61	124.91
4	D	1688	SIA	O6-C6-C5	-7.20	101.28	110.29
4	D	1686	SIA	O6-C2-C3	-7.06	106.05	110.22
4	C	1686	SIA	C7-C6-C5	-6.79	104.23	114.24
4	C	1686	SIA	O6-C6-C7	6.13	114.24	106.34
4	D	1688	SIA	O6-C6-C7	6.00	116.86	105.73
4	E	1688	SIA	O6-C6-C5	-5.84	102.98	110.29
4	D	1686	SIA	O6-C6-C5	-4.88	104.94	109.55
4	D	1686	SIA	C3-C4-C5	3.93	115.27	110.72
4	D	1686	SIA	O2-C2-C3	3.30	114.48	109.67
4	C	1688	SIA	C7-C6-C5	3.28	119.08	114.24
4	D	1686	SIA	C2-O6-C6	-3.20	109.05	113.93
4	E	1688	SIA	C4-C5-C6	3.05	116.86	108.99
4	D	1688	SIA	C7-C6-C5	-3.00	109.82	114.24
4	E	1686	SIA	O6-C6-C7	3.00	110.20	106.34
4	D	1686	SIA	O6-C6-C7	2.87	110.03	106.34
4	E	1688	SIA	C3-C4-C5	2.82	114.28	110.41
4	E	1686	SIA	C2-O6-C6	2.78	118.16	113.93
4	D	1686	SIA	O2-C2-C1	-2.59	105.47	109.86
4	E	1686	SIA	C3-C2-C1	-2.58	109.25	113.58
4	E	1688	SIA	C7-C6-C5	2.56	118.02	114.24
4	E	1686	SIA	C7-C6-C5	-2.52	110.52	114.24
4	C	1686	SIA	C3-C2-C1	-2.47	109.43	113.58
4	D	1686	SIA	C7-C6-C5	-2.42	110.67	114.24
4	E	1688	SIA	C5-N5-C10	-2.38	116.67	123.02
4	E	1686	SIA	O1A-C1-C2	-2.28	120.31	123.48
4	E	1688	SIA	C3-C2-C1	-2.25	108.50	121.08
4	D	1686	SIA	C4-C5-N5	2.22	115.03	110.12
4	E	1688	SIA	O6-C6-C7	2.20	109.80	105.73
4	C	1688	SIA	C3-C4-C5	2.15	113.37	110.41
4	C	1686	SIA	O2-C2-O6	-2.15	106.23	109.95
4	C	1688	SIA	C6-C5-N5	-2.05	107.40	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1688	SIA	C8-C7-C6	2.04	116.94	112.99
4	E	1686	SIA	O8-C8-C9	-2.03	104.46	109.20
4	E	1686	SIA	C2-C3-C4	2.03	114.55	110.75
4	C	1686	SIA	O1A-C1-C2	-2.02	120.68	123.48
4	C	1686	SIA	O2-C2-C1	-2.01	106.46	109.86
4	D	1686	SIA	C2-C3-C4	2.01	114.51	110.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

12 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	SLB	A	1685	-	21,21,21	2.53	7 (33%)	31,31,31	1.89	4 (12%)
3	PO4	A	1686	-	4,4,4	0.38	0	6,6,6	0.34	0
2	SLB	B	1685	-	21,21,21	3.04	8 (38%)	31,31,31	2.38	10 (32%)
3	PO4	B	1686	-	4,4,4	0.58	0	6,6,6	0.32	0
2	SLB	C	1685	-	21,21,21	2.48	9 (42%)	31,31,31	1.89	9 (29%)
3	PO4	C	1687	-	4,4,4	0.31	0	6,6,6	0.31	0
2	SLB	D	1685	-	21,21,21	2.48	7 (33%)	31,31,31	2.62	8 (25%)
3	PO4	D	1687	-	4,4,4	0.57	0	6,6,6	0.31	0
2	SLB	E	1685	-	21,21,21	2.64	8 (38%)	31,31,31	2.05	9 (29%)
2	SLB	F	1685	-	21,21,21	2.20	5 (23%)	31,31,31	2.11	8 (25%)
3	PO4	F	1686	-	4,4,4	0.35	0	6,6,6	0.31	0
3	PO4	F	1687	-	4,4,4	0.33	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	SLB	A	1685	-	-	0/20/38/38	0/1/1/1
3	PO4	A	1686	-	-	0/0/0/0	0/0/0/0
2	SLB	B	1685	-	-	0/20/38/38	0/1/1/1
3	PO4	B	1686	-	-	0/0/0/0	0/0/0/0
2	SLB	C	1685	-	-	0/20/38/38	0/1/1/1
3	PO4	C	1687	-	-	0/0/0/0	0/0/0/0
2	SLB	D	1685	-	-	0/20/38/38	0/1/1/1
3	PO4	D	1687	-	-	0/0/0/0	0/0/0/0
2	SLB	E	1685	-	-	0/20/38/38	0/1/1/1
2	SLB	F	1685	-	-	0/20/38/38	0/1/1/1
3	PO4	F	1686	-	-	0/0/0/0	0/0/0/0
3	PO4	F	1687	-	-	0/0/0/0	0/0/0/0

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1685	SLB	O6-C2	7.88	1.50	1.42
2	B	1685	SLB	C2-C1	7.41	1.61	1.53
2	C	1685	SLB	O2-C2	6.70	1.48	1.39
2	F	1685	SLB	O6-C2	6.48	1.49	1.42
2	D	1685	SLB	O6-C2	6.05	1.48	1.42
2	A	1685	SLB	O6-C2	5.87	1.48	1.42
2	E	1685	SLB	O2-C2	5.35	1.46	1.39
2	E	1685	SLB	C2-C1	5.27	1.59	1.53
2	A	1685	SLB	O6-C6	4.96	1.52	1.44
2	E	1685	SLB	O6-C2	4.93	1.47	1.42
2	B	1685	SLB	O2-C2	4.49	1.45	1.39
2	B	1685	SLB	O6-C6	4.47	1.51	1.44
2	A	1685	SLB	O2-C2	4.46	1.45	1.39
2	D	1685	SLB	O2-C2	4.44	1.45	1.39
2	A	1685	SLB	C2-C1	4.22	1.58	1.53
2	E	1685	SLB	C4-C5	3.96	1.56	1.53
2	C	1685	SLB	O6-C2	3.83	1.46	1.42
2	E	1685	SLB	C3-C2	3.82	1.57	1.51
2	D	1685	SLB	C8-C7	3.76	1.61	1.53
2	D	1685	SLB	C4-C5	3.72	1.56	1.53
2	F	1685	SLB	O2-C2	3.58	1.44	1.39
2	C	1685	SLB	O6-C6	3.48	1.50	1.44
2	C	1685	SLB	C2-C1	3.34	1.57	1.53
2	F	1685	SLB	C7-C6	3.32	1.57	1.52
2	D	1685	SLB	C7-C6	3.21	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1685	SLB	C3-C2	3.19	1.56	1.51
2	D	1685	SLB	O6-C6	2.88	1.49	1.44
2	B	1685	SLB	C3-C2	2.83	1.55	1.51
2	F	1685	SLB	C6-C5	2.79	1.57	1.53
2	D	1685	SLB	C3-C2	2.78	1.55	1.51
2	C	1685	SLB	C3-C2	2.71	1.55	1.51
2	F	1685	SLB	C8-C7	2.70	1.59	1.53
2	E	1685	SLB	O6-C6	-2.68	1.39	1.44
2	E	1685	SLB	C3-C4	2.68	1.57	1.53
2	C	1685	SLB	C7-C6	2.66	1.56	1.52
2	B	1685	SLB	C3-C4	2.55	1.57	1.53
2	C	1685	SLB	C4-C5	2.42	1.55	1.53
2	C	1685	SLB	C6-C5	2.36	1.57	1.53
2	C	1685	SLB	C11-C10	2.32	1.55	1.50
2	A	1685	SLB	C4-C5	2.30	1.55	1.53
2	A	1685	SLB	C3-C4	2.30	1.56	1.53
2	B	1685	SLB	C6-C5	2.11	1.56	1.53
2	E	1685	SLB	C11-C10	2.09	1.55	1.50
2	B	1685	SLB	C7-C6	2.04	1.55	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1685	SLB	O6-C2-C3	7.76	114.80	110.22
2	F	1685	SLB	O6-C2-C3	7.56	114.68	110.22
2	A	1685	SLB	O6-C6-C5	7.08	116.23	109.55
2	D	1685	SLB	O6-C6-C5	6.99	116.14	109.55
2	B	1685	SLB	C7-C6-C5	-6.37	104.85	114.24
2	B	1685	SLB	O6-C6-C7	6.24	114.38	106.34
2	E	1685	SLB	C2-O6-C6	6.20	123.37	113.93
2	D	1685	SLB	C2-O6-C6	5.74	122.66	113.93
2	F	1685	SLB	C3-C2-C1	-4.96	105.26	113.58
2	B	1685	SLB	O2-C2-C3	-4.94	102.48	109.67
2	C	1685	SLB	O6-C6-C5	4.70	113.98	109.55
2	D	1685	SLB	C3-C2-C1	-4.27	106.42	113.58
2	B	1685	SLB	O2-C2-C1	4.07	116.78	109.86
2	E	1685	SLB	C6-C5-N5	-3.82	104.32	110.99
2	E	1685	SLB	O6-C6-C5	3.78	113.11	109.55
2	C	1685	SLB	C2-O6-C6	3.60	119.42	113.93
2	C	1685	SLB	C3-C2-C1	-3.58	107.57	113.58
2	C	1685	SLB	O1A-C1-C2	-3.23	119.00	123.48
2	E	1685	SLB	O1A-C1-C2	-3.20	119.03	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1685	SLB	C7-C6-C5	-3.20	109.52	114.24
2	E	1685	SLB	C4-C5-N5	3.06	116.88	110.12
2	F	1685	SLB	O1A-C1-C2	-3.06	119.23	123.48
2	E	1685	SLB	C7-C6-C5	-2.98	109.85	114.24
2	B	1685	SLB	O1B-C1-O1A	-2.95	114.47	123.76
2	B	1685	SLB	O1B-C1-C2	2.94	125.56	114.41
2	A	1685	SLB	C8-C7-C6	-2.87	107.42	112.99
2	A	1685	SLB	C2-O6-C6	2.69	118.02	113.93
2	D	1685	SLB	C9-C8-C7	2.66	118.42	112.38
2	F	1685	SLB	C8-C7-C6	2.61	118.05	112.99
2	F	1685	SLB	C2-O6-C6	2.60	117.89	113.93
2	E	1685	SLB	O1B-C1-C2	2.59	124.23	114.41
2	B	1685	SLB	O1A-C1-C2	-2.53	119.97	123.48
2	B	1685	SLB	O6-C6-C5	2.48	111.89	109.55
2	D	1685	SLB	O7-C7-C8	2.39	114.78	108.74
2	B	1685	SLB	C8-C7-C6	2.39	117.62	112.99
2	D	1685	SLB	C3-C4-C5	2.33	113.42	110.72
2	F	1685	SLB	C4-C5-N5	2.32	115.25	110.12
2	C	1685	SLB	C7-C6-C5	-2.26	110.91	114.24
2	E	1685	SLB	O1B-C1-O1A	-2.25	116.67	123.76
2	C	1685	SLB	O1B-C1-C2	2.20	122.75	114.41
2	F	1685	SLB	C9-C8-C7	2.18	117.32	112.38
2	C	1685	SLB	O4-C4-C3	-2.15	104.81	109.92
2	B	1685	SLB	O6-C2-C3	-2.09	108.98	110.22
2	E	1685	SLB	O2-C2-C1	2.08	113.39	109.86
2	C	1685	SLB	O2-C2-C3	2.07	112.69	109.67
2	A	1685	SLB	O6-C6-C7	2.07	109.01	106.34
2	F	1685	SLB	O2-C2-C1	2.06	113.36	109.86
2	C	1685	SLB	C4-C5-N5	2.04	114.63	110.12

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%)	-0.18	4 (0%)	86 89	17, 21, 24, 30	0
1	B	666/666 (100%)	-0.14	9 (1%)	72 75	17, 21, 23, 30	0
1	C	666/666 (100%)	-0.09	5 (0%)	83 85	17, 21, 23, 29	0
1	D	666/666 (100%)	-0.24	1 (0%)	93 95	18, 21, 23, 31	0
1	E	666/666 (100%)	-0.15	8 (1%)	75 78	18, 21, 23, 30	0
1	F	666/666 (100%)	-0.21	7 (1%)	77 80	18, 21, 23, 29	0
All	All	3996/3996 (100%)	-0.17	34 (0%)	83 83	17, 21, 23, 31	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	245	SER	4.7
1	F	245	SER	4.7
1	E	246	ALA	4.1
1	F	246	ALA	4.1
1	C	245	SER	3.2
1	A	491	THR	2.9
1	E	262	LEU	2.8
1	C	682	ASP	2.8
1	B	246	ALA	2.8
1	C	262	LEU	2.6
1	B	262	LEU	2.6
1	B	251	VAL	2.5
1	E	491	THR	2.5
1	F	247	LYS	2.5
1	B	264	ASP	2.5
1	B	466	GLY	2.5
1	C	246	ALA	2.3
1	D	840	PHE	2.3
1	A	263	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	546	VAL	2.2
1	E	492	SER	2.2
1	C	546	VAL	2.1
1	E	681	ASP	2.1
1	E	565	ASN	2.1
1	E	547	ALA	2.1
1	F	498	GLY	2.1
1	A	824	ILE	2.1
1	B	676	ASN	2.1
1	F	547	ALA	2.0
1	A	644	GLY	2.0
1	E	251	VAL	2.0
1	B	257	ALA	2.0
1	F	497	ALA	2.0
1	B	824	ILE	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 ⓘ

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
4	SIA	C	1686	21/21	0.26	6.22	36,40,43,44	0
4	SIA	E	1686	21/21	0.27	5.58	38,41,47,49	0
4	SIA	C	1688	20/21	0.18	3.04	35,38,43,45	0
4	SIA	D	1686	21/21	0.32	2.98	43,45,49,51	0
4	SIA	D	1688	20/21	0.18	2.67	35,40,42,44	0
4	SIA	E	1688	20/21	0.15	1.46	31,38,44,46	0

## 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	SLB	E	1685	21/21	0.20	2.27	32,37,44,50	0
2	SLB	B	1685	21/21	0.18	1.78	30,37,43,44	0
2	SLB	A	1685	21/21	0.21	1.75	37,42,47,48	0
2	SLB	F	1685	21/21	0.19	1.66	33,40,46,49	0
2	SLB	D	1685	21/21	0.15	0.42	33,39,42,46	0
2	SLB	C	1685	21/21	0.15	0.17	37,39,43,44	0
3	PO4	F	1687	5/5	0.13	0.11	34,36,37,39	0
3	PO4	A	1686	5/5	0.10	-0.55	33,36,38,39	0
3	PO4	C	1687	5/5	0.10	-0.62	36,37,38,40	0
3	PO4	D	1687	5/5	0.11	-1.06	35,35,37,37	0
3	PO4	B	1686	5/5	0.11	-1.12	30,33,34,34	0
3	PO4	F	1686	5/5	0.08	-1.22	38,39,39,40	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.