



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 11:37 PM GMT

PDB ID : 1VRH
Title : HRV14/SDZ 880-061 COMPLEX
Authors : Oren, D.A.; Zhang, A.; Arnold, E.
Deposited on : 1996-02-26
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

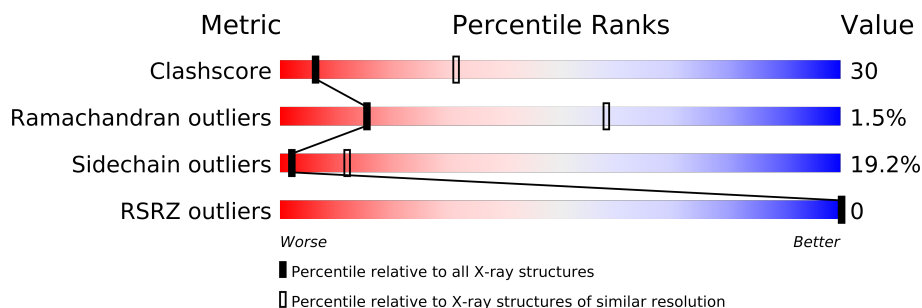
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. 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	1	289	
2	2	262	
3	3	236	
4	4	68	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6294 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 RHINOVIRUS 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	273	Total	C	N	O	S	0	0	0
			2170	1373	375	414	8			

- Molecule 2 is a protein called RHINOVIRUS 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	255	Total	C	N	O	S	0	0	0
			1952	1238	330	372	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	170	LEU	ILE	ENGINEERED	UNP P03303

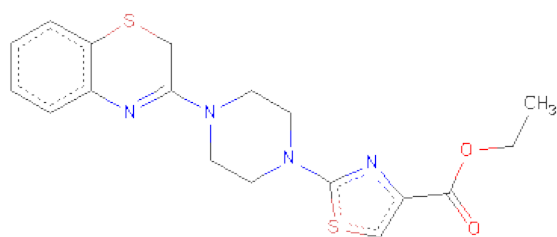
- Molecule 3 is a protein called RHINOVIRUS 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	236	Total	C	N	O	S	0	0	0
			1849	1184	305	353	7			

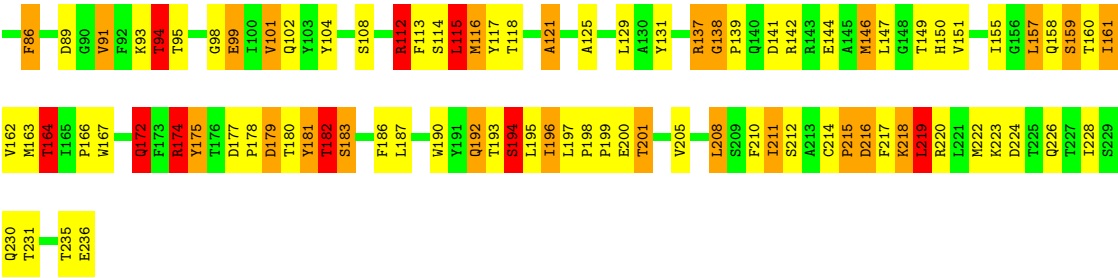
- Molecule 4 is a protein called RHINOVIRUS 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	40	Total	C	N	O	S	0	0	0
			297	186	47	62	2			

- Molecule 5 is 2-[4-(2H-1,4-BENZOTHAZINE-3-YL)-PIPERAZINE-1-LY]-1,3-THIAZOLE-4-CARBOXYLICACID ETHYLESTER (three-letter code: SD8) (formula: C₁₈H₂₀N₄O₂S₂).

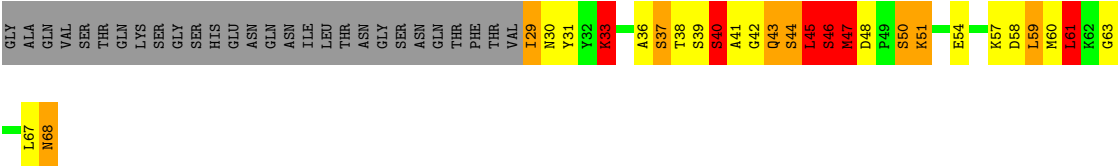


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	1	1	26	18	4	2	2	0	0



● Molecule 4: RHINOVIRUS 14

Chain 4:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	445.10Å 445.10Å 445.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00 50.72 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00) 25.4 (50.72-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.06 (at 3.01Å)	Xtriage
Refinement program	?	Depositor
R, R_{free}	(Not available) , (Not available) 0.198 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 96.1	EDS
Estimated twinning fraction	0.116 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	0 of 147189 reflections	Xtriage
F_o, F_c correlation	0.11	EDS
Total number of atoms	6294	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 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SD8

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	1	1.89	42/2228 (1.9%)	2.42	126/3031 (4.2%)
2	2	1.85	32/2001 (1.6%)	2.17	78/2735 (2.9%)
3	3	1.77	21/1898 (1.1%)	2.18	77/2597 (3.0%)
4	4	2.30	13/302 (4.3%)	2.46	21/406 (5.2%)
All	All	1.87	108/6429 (1.7%)	2.28	302/8769 (3.4%)

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	1	0	3
2	2	0	2
All	All	0	5

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	170	SER	CB-OG	-14.37	1.23	1.42
1	1	153	VAL	C-N	-12.15	1.11	1.34
1	1	285	ASP	CA-CB	11.83	1.79	1.53
4	4	42	GLY	N-CA	11.70	1.63	1.46
4	4	40	SER	CB-OG	10.76	1.56	1.42
1	1	198	ASN	C-N	10.24	1.57	1.34
2	2	256	SER	CB-OG	10.24	1.55	1.42
1	1	95	GLU	CB-CG	10.13	1.71	1.52
4	4	44	SER	CB-OG	9.98	1.55	1.42
1	1	117	GLU	CD-OE1	9.36	1.35	1.25
4	4	41	ALA	C-O	9.35	1.41	1.23
1	1	128	TYR	C-N	9.19	1.55	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	175	SER	CB-OG	-9.12	1.30	1.42
1	1	38	GLU	CB-CG	-9.09	1.34	1.52
1	1	63	SER	CB-OG	-8.77	1.30	1.42
3	3	21	SER	CA-CB	8.69	1.66	1.52
2	2	248	CYS	CB-SG	-8.64	1.67	1.82
3	3	57	ASN	CA-CB	8.41	1.75	1.53
2	2	40	GLU	CD-OE1	8.24	1.34	1.25
1	1	288	SER	CA-CB	8.05	1.65	1.52
2	2	52	LYS	CE-NZ	7.91	1.68	1.49
3	3	1	GLY	N-CA	7.85	1.57	1.46
2	2	219	SER	CA-CB	-7.69	1.41	1.52
3	3	63	GLU	CD-OE1	7.67	1.34	1.25
1	1	283	LYS	N-CA	7.66	1.61	1.46
2	2	136	GLU	CB-CG	7.53	1.66	1.52
4	4	33	LYS	CE-NZ	7.45	1.67	1.49
3	3	108	SER	CB-OG	7.45	1.51	1.42
1	1	282	ARG	CD-NE	7.37	1.58	1.46
1	1	234	GLU	CD-OE1	7.37	1.33	1.25
1	1	139	SER	CB-OG	7.26	1.51	1.42
2	2	152	ARG	CD-NE	7.25	1.58	1.46
2	2	152	ARG	CZ-NH2	7.11	1.42	1.33
2	2	194	ASN	CA-CB	7.01	1.71	1.53
4	4	46	SER	CB-OG	6.95	1.51	1.42
3	3	164	THR	C-O	6.90	1.36	1.23
4	4	51	LYS	CE-NZ	6.79	1.66	1.49
1	1	143	SER	CB-OG	6.78	1.51	1.42
2	2	256	SER	C-O	6.72	1.36	1.23
3	3	61	LYS	CE-NZ	6.69	1.65	1.49
1	1	72	GLY	C-O	6.58	1.34	1.23
1	1	81	GLU	CD-OE1	6.49	1.32	1.25
1	1	30	LYS	CE-NZ	6.46	1.65	1.49
2	2	8	GLY	N-CA	6.41	1.55	1.46
1	1	283	LYS	CE-NZ	6.35	1.65	1.49
3	3	138	GLY	N-CA	6.33	1.55	1.46
1	1	52	GLU	C-O	6.32	1.35	1.23
2	2	12	ARG	NE-CZ	6.32	1.41	1.33
2	2	87	LYS	CB-CG	-6.31	1.35	1.52
3	3	194	SER	CB-OG	-6.26	1.34	1.42
1	1	30	LYS	CD-CE	6.24	1.66	1.51
4	4	33	LYS	CD-CE	6.12	1.66	1.51
3	3	50	ASP	CA-CB	-6.08	1.40	1.53
1	1	144	SER	N-CA	6.03	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	108	SER	CA-CB	-6.02	1.44	1.52
4	4	54	GLU	CD-OE1	5.97	1.32	1.25
2	2	102	GLY	N-CA	5.97	1.55	1.46
1	1	94	ARG	CD-NE	5.94	1.56	1.46
3	3	99	GLU	CB-CG	-5.94	1.40	1.52
1	1	285	ASP	N-CA	-5.79	1.34	1.46
2	2	168	ASP	C-O	5.69	1.34	1.23
2	2	11	ASP	CA-CB	5.69	1.66	1.53
1	1	175	SER	CA-CB	-5.64	1.44	1.52
4	4	37	SER	CB-OG	-5.64	1.34	1.42
3	3	45	GLU	CD-OE1	5.64	1.31	1.25
3	3	172	GLN	CG-CD	-5.62	1.38	1.51
4	4	63	GLY	N-CA	5.60	1.54	1.46
2	2	187	GLN	N-CA	5.59	1.57	1.46
2	2	235	THR	C-N	-5.58	1.23	1.34
3	3	222	MET	CG-SD	5.57	1.95	1.81
1	1	139	SER	CA-CB	5.55	1.61	1.52
4	4	45	LEU	C-N	5.53	1.46	1.34
2	2	219	SER	CB-OG	-5.49	1.35	1.42
1	1	276	GLU	CD-OE1	5.45	1.31	1.25
2	2	236	PRO	C-O	5.43	1.34	1.23
2	2	262	GLN	CD-OE1	5.41	1.35	1.24
2	2	187	GLN	CB-CG	-5.38	1.38	1.52
1	1	73	ARG	C-O	5.38	1.33	1.23
2	2	54	SER	CA-CB	-5.37	1.44	1.52
4	4	50	SER	CB-OG	5.37	1.49	1.42
1	1	267	GLY	C-O	5.36	1.32	1.23
1	1	94	ARG	NE-CZ	5.34	1.40	1.33
1	1	246	ARG	CZ-NH2	5.27	1.40	1.33
1	1	117	GLU	CD-OE2	-5.26	1.19	1.25
1	1	251	GLU	CA-CB	-5.26	1.42	1.53
1	1	175	SER	N-CA	5.25	1.56	1.46
2	2	40	GLU	CB-CG	5.24	1.62	1.52
3	3	33	ARG	CZ-NH2	5.22	1.39	1.33
3	3	118	THR	CB-OG1	5.22	1.53	1.43
2	2	68	SER	CB-OG	-5.20	1.35	1.42
2	2	120	GLY	N-CA	5.18	1.53	1.46
2	2	161	GLU	CA-CB	-5.17	1.42	1.53
2	2	136	GLU	CD-OE1	5.16	1.31	1.25
2	2	74	GLY	C-O	5.16	1.31	1.23
2	2	12	ARG	CZ-NH2	5.13	1.39	1.33
3	3	77	ASN	C-O	5.13	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	38	GLY	CA-C	-5.11	1.43	1.51
1	1	143	SER	C-O	5.10	1.33	1.23
2	2	58	THR	C-O	5.09	1.33	1.23
1	1	26	LYS	CB-CG	-5.08	1.38	1.52
1	1	202	ASP	CA-CB	-5.08	1.42	1.53
1	1	68	GLU	CD-OE2	-5.08	1.20	1.25
1	1	283	LYS	CD-CE	5.08	1.64	1.51
3	3	86	PHE	CA-CB	-5.04	1.42	1.53
1	1	88	THR	CB-OG1	5.02	1.53	1.43
3	3	30	PRO	N-CD	-5.02	1.40	1.47
1	1	288	SER	C-O	5.01	1.32	1.23
2	2	38	TRP	CG-CD1	5.01	1.43	1.36

All (302) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	246	ARG	NE-CZ-NH1	22.42	131.51	120.30
1	1	256	ARG	NE-CZ-NH2	20.34	130.47	120.30
1	1	123	ARG	NE-CZ-NH1	19.14	129.87	120.30
2	2	255	ARG	NE-CZ-NH2	-18.73	110.93	120.30
2	2	87	LYS	CA-CB-CG	17.62	152.17	113.40
1	1	285	ASP	CB-CG-OD1	-17.61	102.45	118.30
3	3	137	ARG	NE-CZ-NH1	-16.95	111.83	120.30
1	1	256	ARG	NE-CZ-NH1	-16.83	111.89	120.30
1	1	94	ARG	NE-CZ-NH2	-16.52	112.04	120.30
3	3	216	ASP	CB-CG-OD2	16.06	132.75	118.30
1	1	129	THR	O-C-N	-15.93	97.21	122.70
1	1	153	VAL	CB-CA-C	-15.46	82.03	111.40
1	1	282	ARG	NE-CZ-NH2	-14.18	113.21	120.30
2	2	255	ARG	NE-CZ-NH1	14.18	127.39	120.30
1	1	129	THR	CA-C-N	14.02	148.05	117.20
1	1	165	ASP	CB-CG-OD2	13.05	130.05	118.30
2	2	168	ASP	CB-CG-OD1	-12.85	106.74	118.30
1	1	128	TYR	O-C-N	12.55	142.78	122.70
1	1	185	ARG	NE-CZ-NH1	12.36	126.48	120.30
3	3	50	ASP	CA-CB-CG	12.22	140.29	113.40
1	1	94	ARG	CD-NE-CZ	-12.02	106.78	123.60
1	1	128	TYR	C-N-CA	-11.84	92.11	121.70
2	2	11	ASP	CB-CG-OD1	-11.72	107.75	118.30
2	2	194	ASN	N-CA-CB	-11.57	89.77	110.60
2	2	193	THR	C-N-CA	11.36	150.10	121.70
3	3	174	ARG	NE-CZ-NH2	-11.35	114.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	170	SER	CA-CB-OG	11.11	141.19	111.20
2	2	152	ARG	NE-CZ-NH2	-11.11	114.75	120.30
3	3	215	PRO	C-N-CA	11.00	149.20	121.70
4	4	48	ASP	CB-CG-OD1	-10.92	108.47	118.30
4	4	41	ALA	CA-C-N	10.88	137.96	116.20
3	3	19	ARG	NE-CZ-NH2	10.82	125.71	120.30
3	3	33	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	1	285	ASP	CB-CG-OD2	10.59	127.83	118.30
1	1	285	ASP	CA-CB-CG	-10.47	90.36	113.40
3	3	50	ASP	CB-CG-OD1	10.46	127.71	118.30
2	2	151	GLU	CA-CB-CG	10.41	136.29	113.40
1	1	282	ARG	CD-NE-CZ	-10.06	109.51	123.60
1	1	246	ARG	CD-NE-CZ	10.06	137.68	123.60
1	1	246	ARG	NE-CZ-NH2	-9.97	115.32	120.30
1	1	208	ASP	CB-CG-OD1	-9.91	109.38	118.30
3	3	57	ASN	N-CA-CB	-9.82	92.92	110.60
3	3	146	MET	CG-SD-CE	9.80	115.88	100.20
3	3	216	ASP	CB-CG-OD1	-9.73	109.55	118.30
1	1	113	ARG	NE-CZ-NH2	-9.71	115.44	120.30
2	2	88	ASP	CB-CG-OD1	-9.71	109.56	118.30
1	1	128	TYR	CA-C-N	-9.45	96.41	117.20
1	1	54	ARG	CD-NE-CZ	-9.36	110.50	123.60
1	1	242	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	1	66	ASP	CB-CG-OD2	-9.21	110.01	118.30
3	3	57	ASN	CB-CA-C	-9.04	92.31	110.40
2	2	11	ASP	CA-CB-CG	-8.99	93.62	113.40
3	3	137	ARG	NE-CZ-NH2	8.88	124.74	120.30
1	1	38	GLU	CA-CB-CG	8.86	132.90	113.40
3	3	112	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	1	165	ASP	CB-CG-OD1	-8.57	110.59	118.30
3	3	182	THR	CA-CB-CG2	8.56	124.39	112.40
1	1	285	ASP	N-CA-CB	-8.54	95.23	110.60
1	1	268	ARG	CD-NE-CZ	-8.46	111.76	123.60
1	1	175	SER	CB-CA-C	8.42	126.09	110.10
1	1	123	ARG	CD-NE-CZ	8.38	135.34	123.60
1	1	63	SER	CB-CA-C	-8.38	94.19	110.10
1	1	165	ASP	CB-CA-C	-8.36	93.69	110.40
1	1	285	ASP	CB-CA-C	-8.30	93.80	110.40
2	2	250	GLU	CA-CB-CG	8.30	131.66	113.40
2	2	152	ARG	NE-CZ-NH1	8.25	124.43	120.30
3	3	172	GLN	CB-CG-CD	8.23	133.00	111.60
1	1	251	GLU	CA-CB-CG	8.19	131.41	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	45	LEU	N-CA-CB	-8.14	94.11	110.40
3	3	224	ASP	CB-CG-OD1	-8.06	111.05	118.30
4	4	48	ASP	OD1-CG-OD2	8.05	138.60	123.30
2	2	11	ASP	OD1-CG-OD2	8.02	138.54	123.30
2	2	255	ARG	CA-CB-CG	8.01	131.02	113.40
1	1	38	GLU	CB-CG-CD	8.01	135.82	114.20
3	3	181	TYR	CB-CG-CD2	-8.00	116.20	121.00
1	1	95	GLU	OE1-CD-OE2	7.98	132.87	123.30
3	3	174	ARG	CD-NE-CZ	-7.84	112.62	123.60
4	4	47	MET	CA-CB-CG	-7.84	99.98	113.30
2	2	219	SER	CA-CB-OG	7.83	132.35	111.20
1	1	145	ASN	OD1-CG-ND2	7.79	139.83	121.90
3	3	21	SER	CB-CA-C	-7.70	95.47	110.10
1	1	121	TYR	CB-CG-CD1	-7.65	116.41	121.00
1	1	266	ILE	CB-CA-C	-7.64	96.31	111.60
2	2	155	ASP	CB-CG-OD1	-7.63	111.43	118.30
2	2	187	GLN	CA-CB-CG	7.59	130.09	113.40
3	3	78	GLU	OE1-CD-OE2	7.58	132.40	123.30
2	2	11	ASP	C-N-CA	7.55	140.58	121.70
1	1	277	PRO	N-CD-CG	-7.55	91.88	103.20
1	1	173	ASN	N-CA-CB	-7.54	97.03	110.60
2	2	170	LEU	CA-CB-CG	7.51	132.58	115.30
2	2	187	GLN	CB-CA-C	7.50	125.39	110.40
1	1	123	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	1	182	ASP	CB-CG-OD1	-7.47	111.58	118.30
1	1	259	ARG	CA-CB-CG	-7.36	97.21	113.40
2	2	214	ARG	NE-CZ-NH1	7.33	123.96	120.30
3	3	112	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	1	282	ARG	NH1-CZ-NH2	7.29	127.42	119.40
1	1	117	GLU	CG-CD-OE2	7.27	132.84	118.30
3	3	142	ARG	CA-CB-CG	7.20	129.24	113.40
2	2	194	ASN	CA-CB-CG	-7.16	97.64	113.40
2	2	190	ASN	CA-CB-CG	7.09	129.00	113.40
1	1	185	ARG	NH1-CZ-NH2	-7.07	111.62	119.40
2	2	256	SER	CA-C-O	-7.04	105.31	120.10
3	3	121	ALA	CB-CA-C	-7.02	99.56	110.10
3	3	137	ARG	CD-NE-CZ	-7.02	113.78	123.60
2	2	168	ASP	N-CA-CB	-7.00	98.00	110.60
3	3	28	TYR	CB-CG-CD1	-6.99	116.81	121.00
3	3	174	ARG	NH1-CZ-NH2	6.97	127.07	119.40
1	1	68	GLU	CG-CD-OE2	6.96	132.21	118.30
1	1	113	ARG	NE-CZ-NH1	6.95	123.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	41	ALA	CA-C-O	-6.95	105.51	120.10
1	1	28	THR	CB-CA-C	-6.91	92.95	111.60
1	1	42	THR	CA-CB-CG2	6.91	122.07	112.40
1	1	125	ASP	CB-CG-OD1	-6.90	112.09	118.30
1	1	26	LYS	CA-CB-CG	6.86	128.50	113.40
1	1	266	ILE	O-C-N	-6.83	111.59	123.20
2	2	136	GLU	CG-CD-OE1	-6.78	104.74	118.30
4	4	37	SER	CB-CA-C	6.76	122.95	110.10
3	3	194	SER	N-CA-CB	-6.76	100.36	110.50
3	3	163	MET	CA-CB-CG	-6.72	101.88	113.30
2	2	146	PHE	CB-CG-CD1	-6.70	116.11	120.80
3	3	216	ASP	N-CA-CB	-6.68	98.58	110.60
1	1	265	SER	N-CA-CB	-6.65	100.53	110.50
2	2	103	ARG	CD-NE-CZ	-6.64	114.31	123.60
3	3	45	GLU	CG-CD-OE2	6.62	131.54	118.30
3	3	57	ASN	CA-CB-CG	-6.59	98.90	113.40
1	1	94	ARG	NH1-CZ-NH2	6.58	126.64	119.40
2	2	87	LYS	CB-CG-CD	6.58	128.71	111.60
3	3	27	ASN	CB-CA-C	-6.58	97.25	110.40
1	1	276	GLU	OE1-CD-OE2	6.55	131.16	123.30
1	1	68	GLU	CG-CD-OE1	-6.54	105.22	118.30
2	2	203	TYR	CB-CG-CD2	6.53	124.92	121.00
1	1	53	THR	CA-CB-OG1	-6.52	95.31	109.00
1	1	288	SER	CB-CA-C	-6.52	97.72	110.10
3	3	74	ASN	CA-CB-CG	-6.50	99.11	113.40
1	1	288	SER	N-CA-CB	-6.48	100.78	110.50
4	4	45	LEU	CB-CA-C	6.48	122.50	110.20
1	1	144	SER	N-CA-CB	-6.46	100.81	110.50
3	3	183	SER	N-CA-CB	-6.45	100.82	110.50
1	1	176	VAL	CB-CA-C	-6.45	99.14	111.40
2	2	168	ASP	OD1-CG-OD2	6.45	135.55	123.30
1	1	22	SER	N-CA-CB	-6.44	100.84	110.50
3	3	55	MET	CA-CB-CG	-6.42	102.38	113.30
1	1	274	ASN	O-C-N	6.42	132.97	122.70
3	3	29	GLU	CB-CG-CD	6.41	131.51	114.20
2	2	97	PHE	CB-CG-CD1	-6.35	116.36	120.80
3	3	65	ASN	CA-CB-CG	-6.32	99.50	113.40
3	3	16	THR	N-CA-CB	-6.30	98.32	110.30
1	1	138	ASP	CB-CG-OD1	6.30	123.97	118.30
1	1	95	GLU	CB-CG-CD	-6.28	97.25	114.20
4	4	44	SER	CA-C-N	-6.26	103.43	117.20
2	2	38	TRP	N-CA-CB	-6.24	99.36	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	63	GLU	CG-CD-OE1	-6.23	105.84	118.30
3	3	19	ARG	CA-CB-CG	6.23	127.11	113.40
3	3	27	ASN	CA-CB-CG	-6.23	99.70	113.40
1	1	145	ASN	CA-CB-CG	-6.21	99.74	113.40
1	1	224	MET	CG-SD-CE	6.20	110.12	100.20
2	2	203	TYR	CB-CG-CD1	-6.19	117.28	121.00
1	1	122	VAL	N-CA-CB	-6.18	97.91	111.50
1	1	271	TYR	CB-CG-CD1	6.17	124.70	121.00
2	2	136	GLU	CB-CG-CD	-6.13	97.64	114.20
1	1	221	MET	CG-SD-CE	6.13	110.01	100.20
1	1	153	VAL	O-C-N	6.12	132.73	121.10
2	2	69	LYS	CA-CB-CG	6.12	126.87	113.40
1	1	117	GLU	CG-CD-OE1	-6.09	106.11	118.30
3	3	222	MET	CG-SD-CE	-6.09	90.45	100.20
2	2	219	SER	CB-CA-C	6.09	121.66	110.10
1	1	151	MET	CG-SD-CE	6.08	109.94	100.20
1	1	118	LEU	CA-CB-CG	6.07	129.27	115.30
3	3	66	SER	CB-CA-C	6.05	121.61	110.10
2	2	119	SER	N-CA-CB	6.05	119.57	110.50
3	3	219	LEU	CA-CB-CG	6.05	129.22	115.30
1	1	164	ASP	C-N-CA	6.04	136.80	121.70
2	2	235	THR	CA-CB-CG2	-6.03	103.96	112.40
1	1	86	ASP	CB-CG-OD1	6.02	123.72	118.30
2	2	67	ASP	CA-CB-CG	-6.02	100.16	113.40
2	2	247	MET	CB-CA-C	6.00	122.39	110.40
4	4	48	ASP	CB-CG-OD2	-5.99	112.91	118.30
2	2	103	ARG	CA-CB-CG	5.97	126.53	113.40
2	2	12	ARG	NE-CZ-NH2	-5.97	117.32	120.30
3	3	1	GLY	N-CA-C	5.96	128.00	113.10
4	4	61	LEU	CB-CG-CD2	-5.95	100.88	111.00
3	3	58	THR	CA-CB-CG2	-5.95	104.07	112.40
1	1	35	THR	N-CA-CB	-5.92	99.06	110.30
1	1	257	ALA	N-CA-CB	-5.91	101.82	110.10
3	3	45	GLU	CG-CD-OE1	-5.90	106.50	118.30
1	1	256	ARG	CD-NE-CZ	-5.89	115.35	123.60
4	4	30	ASN	CA-CB-CG	-5.88	100.47	113.40
2	2	256	SER	CA-C-N	5.87	130.12	117.20
1	1	94	ARG	CG-CD-NE	-5.87	99.48	111.80
1	1	236	LYS	CD-CE-NZ	-5.85	98.24	111.70
1	1	268	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	2	214	ARG	NE-CZ-NH2	-5.83	117.38	120.30
2	2	238	LEU	N-CA-CB	-5.83	98.74	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	33	LYS	CD-CE-NZ	-5.82	98.31	111.70
2	2	31	ALA	N-CA-CB	5.82	118.24	110.10
3	3	27	ASN	O-C-N	5.81	132.00	122.70
1	1	28	THR	OG1-CB-CG2	5.78	123.29	110.00
3	3	77	ASN	CA-C-N	5.77	129.90	117.20
2	2	255	ARG	CB-CG-CD	5.77	126.61	111.60
2	2	73	THR	CA-CB-OG1	-5.76	96.91	109.00
1	1	233	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	1	274	ASN	N-CA-CB	5.73	120.91	110.60
1	1	95	GLU	CA-CB-CG	-5.72	100.81	113.40
1	1	246	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
2	2	68	SER	N-CA-CB	-5.71	101.94	110.50
2	2	161	GLU	CA-CB-CG	5.70	125.94	113.40
3	3	147	LEU	CA-CB-CG	5.70	128.40	115.30
1	1	48	SER	CA-C-O	-5.69	108.15	120.10
2	2	52	LYS	CD-CE-NZ	-5.69	98.61	111.70
3	3	1	GLY	O-C-N	-5.67	113.63	122.70
3	3	177	ASP	CB-CG-OD1	-5.66	113.21	118.30
1	1	198	ASN	O-C-N	-5.65	113.66	122.70
2	2	75	SER	N-CA-CB	-5.65	102.03	110.50
3	3	164	THR	N-CA-CB	-5.63	99.60	110.30
1	1	154	PRO	N-CA-CB	-5.60	96.44	102.60
4	4	44	SER	O-C-N	5.57	131.62	122.70
2	2	210	ASP	N-CA-CB	-5.57	100.58	110.60
3	3	94	THR	O-C-N	5.56	131.59	122.70
1	1	122	VAL	CB-CA-C	5.56	121.96	111.40
1	1	244	TYR	CB-CG-CD2	-5.56	117.67	121.00
1	1	202	ASP	CA-CB-CG	5.52	125.54	113.40
1	1	109	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	1	233	ASP	CB-CG-OD1	5.51	123.26	118.30
2	2	84	ASP	CB-CG-OD2	-5.50	113.34	118.30
2	2	9	TYR	CB-CA-C	5.50	121.40	110.40
4	4	44	SER	C-N-CA	-5.50	107.96	121.70
2	2	12	ARG	CD-NE-CZ	-5.49	115.92	123.60
1	1	81	GLU	CG-CD-OE1	-5.48	107.34	118.30
3	3	186	PHE	CB-CG-CD1	-5.47	116.97	120.80
3	3	112	ARG	CA-CB-CG	5.47	125.44	113.40
1	1	43	MET	CG-SD-CE	5.47	108.95	100.20
1	1	26	LYS	CD-CE-NZ	-5.47	99.13	111.70
2	2	43	PRO	N-CD-CG	-5.46	95.01	103.20
1	1	270	ASN	O-C-N	5.43	131.39	122.70
3	3	60	THR	CA-CB-OG1	-5.43	97.61	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	115	LEU	CA-CB-CG	5.42	127.77	115.30
4	4	44	SER	N-CA-CB	5.42	118.63	110.50
3	3	161	ILE	CA-CB-CG1	-5.40	100.74	111.00
2	2	174	ASN	CA-C-N	5.40	127.00	116.20
2	2	44	ASP	CA-CB-CG	5.39	125.26	113.40
1	1	123	ARG	NH1-CZ-NH2	-5.38	113.48	119.40
3	3	231	THR	CA-CB-OG1	-5.37	97.72	109.00
2	2	262	GLN	CA-C-O	-5.36	108.84	120.10
3	3	65	ASN	N-CA-CB	-5.36	100.95	110.60
1	1	64	GLU	CA-CB-CG	5.36	125.18	113.40
2	2	169	VAL	CB-CA-C	-5.33	101.28	111.40
2	2	259	ILE	CB-CG1-CD1	-5.32	99.00	113.90
3	3	42	ASN	CB-CG-OD1	-5.32	110.96	121.60
1	1	202	ASP	CB-CA-C	5.31	121.03	110.40
2	2	88	ASP	CA-CB-CG	-5.29	101.76	113.40
2	2	143	LYS	CD-CE-NZ	-5.28	99.56	111.70
3	3	116	MET	CB-CG-SD	-5.26	96.61	112.40
1	1	205	SER	O-C-N	5.26	131.12	122.70
3	3	33	ARG	CB-CG-CD	-5.25	97.94	111.60
1	1	275	THR	CA-C-N	5.24	128.73	117.20
1	1	242	ARG	CD-NE-CZ	-5.23	116.28	123.60
1	1	149	GLN	CB-CA-C	-5.23	99.94	110.40
2	2	38	TRP	CA-CB-CG	-5.22	103.78	113.70
2	2	203	TYR	CZ-CE2-CD2	-5.22	115.10	119.80
3	3	74	ASN	OD1-CG-ND2	5.21	133.88	121.90
4	4	48	ASP	CA-CB-CG	-5.21	101.95	113.40
2	2	170	LEU	CB-CG-CD2	5.20	119.84	111.00
2	2	219	SER	N-CA-CB	5.20	118.30	110.50
1	1	275	THR	CA-C-O	-5.19	109.20	120.10
3	3	222	MET	CB-CG-SD	-5.19	96.83	112.40
4	4	36	ALA	C-N-CA	-5.19	108.73	121.70
3	3	78	GLU	CA-CB-CG	5.18	124.80	113.40
2	2	14	GLN	OE1-CD-NE2	5.18	133.81	121.90
1	1	282	ARG	CG-CD-NE	-5.17	100.93	111.80
1	1	21	ILE	CA-CB-CG1	-5.17	101.18	111.00
1	1	219	ASN	O-C-N	5.17	130.97	122.70
3	3	141	ASP	CB-CG-OD1	5.17	122.95	118.30
1	1	271	TYR	CB-CG-CD2	-5.16	117.91	121.00
2	2	11	ASP	CB-CG-OD2	-5.16	113.66	118.30
2	2	52	LYS	CA-C-N	5.15	128.52	117.20
1	1	50	SER	CA-C-N	5.14	128.50	117.20
4	4	31	TYR	CG-CD2-CE2	-5.14	117.19	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	203	TYR	CG-CD2-CE2	5.12	125.40	121.30
1	1	162	GLU	OE1-CD-OE2	5.12	129.44	123.30
4	4	58	ASP	O-C-N	5.12	130.88	122.70
2	2	221	MET	CA-CB-CG	-5.11	104.61	113.30
1	1	141	ASN	CA-CB-CG	-5.11	102.16	113.40
2	2	14	GLN	CA-CB-CG	-5.10	102.17	113.40
1	1	164	ASP	CB-CG-OD2	5.09	122.88	118.30
1	1	17	THR	CA-CB-CG2	-5.08	105.30	112.40
2	2	18	LEU	CB-CA-C	5.08	119.84	110.20
3	3	144	GLU	CA-CB-CG	5.08	124.56	113.40
1	1	282	ARG	CB-CA-C	-5.07	100.27	110.40
1	1	274	ASN	CA-C-N	-5.05	106.08	117.20
1	1	270	ASN	CB-CA-C	-5.05	100.31	110.40
3	3	172	GLN	CG-CD-NE2	5.04	128.80	116.70
3	3	175	TYR	N-CA-CB	-5.04	101.53	110.60
2	2	170	LEU	CB-CA-C	5.04	119.77	110.20
3	3	86	PHE	CB-CA-C	5.04	120.47	110.40
1	1	158	PRO	O-C-N	5.03	130.75	122.70
4	4	39	SER	O-C-N	5.03	130.75	122.70
3	3	187	LEU	N-CA-CB	-5.03	100.34	110.40
3	3	86	PHE	CG-CD1-CE1	5.01	126.31	120.80
1	1	22	SER	CA-C-O	-5.01	109.58	120.10
3	3	77	ASN	O-C-N	-5.01	114.69	122.70
3	3	57	ASN	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	259	ARG	Sidechain
1	1	265	SER	Mainchain
1	1	268	ARG	Sidechain
2	2	12	ARG	Sidechain
2	2	255	ARG	Sidechain

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	1	2170	0	2106	171	0
2	2	1952	0	1926	114	0
3	3	1849	0	1831	136	0
4	4	297	0	294	29	0
5	1	26	0	20	3	0
All	All	6294	0	6177	376	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 30.

All (376) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:4:33:LYS:NZ	4:4:33:LYS:CE	1.67	1.57
3:3:57:ASN:CB	3:3:57:ASN:CA	1.75	1.55
1:1:285:ASP:CB	1:1:285:ASP:CA	1.80	1.54
2:2:52:LYS:NZ	2:2:52:LYS:CE	1.68	1.53
1:1:266:ILE:HD12	3:3:235:THR:C	1.51	1.27
3:3:179:ASP:OD2	3:3:182:THR:HB	1.41	1.19
1:1:266:ILE:O	1:1:266:ILE:HG22	1.39	1.17
1:1:266:ILE:HD12	3:3:235:THR:CA	1.76	1.15
2:2:158:SER:OG	2:2:167:LYS:HE2	1.46	1.13
1:1:285:ASP:OD1	1:1:285:ASP:CA	2.00	1.09
1:1:47:PRO:HA	3:3:164:THR:HG21	1.34	1.07
1:1:258:PRO:HG2	3:3:99:GLU:HG2	1.36	1.07
3:3:21:SER:O	4:4:37:SER:HB2	1.54	1.06
2:2:12:ARG:HG3	2:2:12:ARG:NH1	1.69	1.04
2:2:255:ARG:HG2	2:2:256:SER:H	1.24	1.00
1:1:282:ARG:HG3	3:3:57:ASN:HB3	1.41	0.99
1:1:266:ILE:CD1	3:3:235:THR:HA	1.93	0.98
1:1:83:GLN:HG2	1:1:97:LYS:HB2	1.44	0.97
2:2:136:GLU:HB3	2:2:140:VAL:HG21	1.44	0.96
3:3:57:ASN:N	3:3:57:ASN:CB	2.28	0.95
1:1:83:GLN:HG3	1:1:85:LYS:HE2	1.47	0.94
3:3:57:ASN:C	3:3:57:ASN:CB	2.37	0.94
2:2:12:ARG:HH11	2:2:12:ARG:HG3	1.27	0.93
1:1:136:GLN:HE21	1:1:235:HIS:CD2	1.84	0.93
1:1:285:ASP:CG	1:1:285:ASP:CA	2.37	0.93
1:1:58:MET:HE1	3:3:216:ASP:HA	1.48	0.92
2:2:41:TYR:CE2	2:2:55:LYS:HD3	2.05	0.92
1:1:266:ILE:O	1:1:266:ILE:CG2	2.14	0.92

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:235:THR:HG23	2:2:236:PRO:HD2	1.53	0.91
3:3:175:TYR:HB2	3:3:182:THR:HG21	1.53	0.91
1:1:28:THR:HB	1:1:30:LYS:H	1.35	0.91
2:2:11:ASP:HB2	4:4:68:ASN:OD1	1.71	0.90
1:1:92:ASN:ND2	1:1:95:GLU:HB2	1.87	0.90
1:1:285:ASP:CB	1:1:285:ASP:C	2.40	0.90
1:1:285:ASP:CB	1:1:285:ASP:N	2.34	0.90
3:3:198:PRO:HD2	3:3:201:THR:HG21	1.55	0.89
1:1:47:PRO:HA	3:3:164:THR:CG2	2.03	0.88
1:1:266:ILE:CD1	3:3:235:THR:CA	2.50	0.88
2:2:20:ASN:ND2	2:2:62:ARG:HE	1.72	0.87
1:1:285:ASP:HA	1:1:285:ASP:OD1	1.73	0.87
1:1:158:PRO:HB2	1:1:167:THR:HG22	1.57	0.86
2:2:9:TYR:CD1	2:2:9:TYR:N	2.43	0.85
1:1:90:ILE:HD13	1:1:90:ILE:N	1.92	0.84
3:3:57:ASN:CG	3:3:57:ASN:CA	2.45	0.84
1:1:282:ARG:HD2	1:1:285:ASP:O	1.78	0.84
2:2:116:LYS:HB3	3:3:121:ALA:HB3	1.58	0.83
2:2:10:SER:OG	2:2:12:ARG:HB2	1.78	0.83
2:2:9:TYR:HD1	2:2:9:TYR:N	1.77	0.83
2:2:136:GLU:CB	2:2:140:VAL:HG21	2.09	0.82
2:2:52:LYS:NZ	2:2:52:LYS:CD	2.43	0.82
4:4:68:ASN:OD1	4:4:68:ASN:N	2.11	0.82
2:2:12:ARG:HH11	2:2:12:ARG:CG	1.89	0.81
1:1:107:SER:HB2	1:1:113:ARG:HD2	1.63	0.81
1:1:58:MET:CE	3:3:216:ASP:HA	2.11	0.81
4:4:59:LEU:HD21	4:4:61:LEU:HD13	1.61	0.80
1:1:248:LYS:HE3	4:4:38:THR:O	1.80	0.79
2:2:158:SER:OG	2:2:167:LYS:CE	2.27	0.79
1:1:208:ASP:HB3	1:1:211:THR:CG2	2.13	0.78
1:1:58:MET:HE1	3:3:216:ASP:CA	2.13	0.77
1:1:47:PRO:CA	3:3:164:THR:HG21	2.15	0.77
2:2:12:ARG:CG	2:2:12:ARG:NH1	2.44	0.77
1:1:282:ARG:HG3	3:3:57:ASN:CB	2.15	0.77
3:3:79:GLN:HB2	3:3:190:TRP:CZ3	2.19	0.77
1:1:153:VAL:HG12	1:1:153:VAL:O	1.85	0.76
1:1:266:ILE:HD11	3:3:235:THR:HA	1.64	0.76
2:2:255:ARG:HG2	2:2:256:SER:N	2.00	0.76
1:1:136:GLN:NE2	1:1:235:HIS:NE2	2.32	0.76
1:1:224:MET:HG2	1:1:226:PHE:CZ	2.20	0.76
1:1:266:ILE:HD12	3:3:236:GLU:N	2.01	0.76
1:1:94:ARG:NH1	1:1:94:ARG:HG2	2.00	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:208:ASP:HB3	1:1:211:THR:HG22	1.68	0.75
2:2:262:GLN:C	2:2:262:GLN:HE21	1.91	0.74
1:1:149:GLN:O	1:1:149:GLN:HG2	1.86	0.74
1:1:270:ASN:HA	2:2:133:ALA:HB1	1.68	0.74
3:3:197:LEU:HB3	3:3:201:THR:CG2	2.18	0.74
4:4:43:GLN:HG2	4:4:45:LEU:HB2	1.70	0.74
1:1:258:PRO:CG	3:3:99:GLU:HG2	2.16	0.73
2:2:188:PHE:O	2:2:194:ASN:ND2	2.22	0.73
3:3:26:PRO:O	3:3:27:ASN:HB2	1.89	0.73
4:4:33:LYS:NZ	4:4:33:LYS:CD	2.52	0.72
1:1:19:ALA:HB2	1:1:58:MET:HG2	1.72	0.72
2:2:230:VAL:CG2	2:2:234:ALA:HB3	2.20	0.72
2:2:53:THR:HG22	2:2:252:SER:HB2	1.71	0.71
2:2:136:GLU:HB3	2:2:140:VAL:CG2	2.21	0.71
3:3:57:ASN:OD1	3:3:57:ASN:CA	2.38	0.71
2:2:174:ASN:C	2:2:174:ASN:HD22	1.93	0.71
1:1:282:ARG:CG	3:3:57:ASN:HB3	2.18	0.70
2:2:20:ASN:HD21	2:2:62:ARG:HE	1.39	0.70
2:2:235:THR:CG2	2:2:236:PRO:HD2	2.21	0.70
1:1:89:GLY:C	1:1:90:ILE:HD13	2.13	0.69
1:1:191:VAL:O	1:1:191:VAL:HG23	1.90	0.69
3:3:98:GLY:O	3:3:102:GLN:HG3	1.92	0.69
1:1:266:ILE:CD1	3:3:235:THR:C	2.47	0.68
2:2:195:ASN:OD1	2:2:196:THR:HG23	1.93	0.68
4:4:29:ILE:O	4:4:29:ILE:HG22	1.93	0.68
2:2:230:VAL:HG23	2:2:234:ALA:HB3	1.74	0.68
1:1:146:LEU:HD13	1:1:228:ILE:HD13	1.77	0.67
2:2:84:ASP:OD1	2:2:87:LYS:HE2	1.94	0.66
1:1:285:ASP:CB	1:1:285:ASP:H	2.09	0.66
3:3:197:LEU:HB3	3:3:201:THR:HG22	1.77	0.66
1:1:278:VAL:HG12	3:3:62:ASP:OD2	1.95	0.66
3:3:89:ASP:HA	3:3:93:LYS:HD2	1.78	0.65
3:3:179:ASP:OD2	3:3:182:THR:CB	2.31	0.65
2:2:256:SER:O	2:2:257:LYS:HB3	1.96	0.65
1:1:158:PRO:HB2	1:1:167:THR:CG2	2.26	0.65
3:3:61:LYS:HD3	3:3:63:GLU:OE2	1.95	0.65
2:2:149:PRO:HG3	2:2:154:ILE:HG13	1.78	0.64
2:2:12:ARG:HH21	3:3:157:LEU:HD21	1.63	0.64
2:2:12:ARG:NH1	4:4:68:ASN:O	2.31	0.64
1:1:94:ARG:CG	1:1:94:ARG:NH1	2.60	0.63
3:3:79:GLN:HB2	3:3:190:TRP:CE3	2.32	0.63
2:2:23:ILE:HD11	2:2:243:THR:HG21	1.79	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:83:GLN:CG	1:1:85:LYS:HE2	2.24	0.63
2:2:13:VAL:O	2:2:14:GLN:HG2	1.99	0.63
1:1:60:PHE:CE2	3:3:218:LYS:HB3	2.33	0.62
2:2:40:GLU:HG3	2:2:41:TYR:O	2.00	0.62
1:1:104:ILE:HG13	1:1:222:GLY:O	1.99	0.62
1:1:90:ILE:N	1:1:90:ILE:CD1	2.62	0.62
3:3:55:MET:O	3:3:55:MET:HG3	1.99	0.61
1:1:153:VAL:CG1	1:1:153:VAL:O	2.32	0.61
1:1:38:GLU:CD	3:3:116:MET:HE1	2.20	0.61
1:1:87:ALA:HA	1:1:90:ILE:HG12	1.80	0.61
1:1:87:ALA:HB2	1:1:98:LEU:CD1	2.30	0.61
3:3:75:ARG:O	3:3:194:SER:HB2	2.00	0.61
3:3:57:ASN:ND2	3:3:91:VAL:HG13	2.15	0.61
2:2:133:ALA:O	2:2:166:VAL:HG12	2.01	0.61
3:3:56:ASN:HB3	3:3:66:SER:HA	1.83	0.61
1:1:87:ALA:HB2	1:1:98:LEU:HD11	1.82	0.61
1:1:51:ILE:HD13	3:3:166:PRO:HG3	1.82	0.61
1:1:281:LYS:HD2	3:3:59:HIS:O	2.01	0.61
3:3:131:TYR:HB3	3:3:149:THR:HB	1.82	0.60
3:3:175:TYR:H	3:3:182:THR:HG21	1.66	0.60
2:2:155:ASP:OD1	2:2:155:ASP:C	2.37	0.60
2:2:38:TRP:CZ3	4:4:57:LYS:HD2	2.36	0.60
1:1:265:SER:HB3	1:1:268:ARG:HG2	1.84	0.60
3:3:76:GLN:O	3:3:78:GLU:N	2.34	0.60
1:1:149:GLN:O	1:1:149:GLN:CG	2.45	0.60
2:2:11:ASP:H	4:4:68:ASN:CG	2.06	0.59
1:1:259:ARG:HD2	1:1:263:TYR:CE1	2.38	0.58
1:1:285:ASP:HB3	1:1:287:LYS:N	2.18	0.58
1:1:83:GLN:NE2	1:1:97:LYS:HG3	2.18	0.58
3:3:180:THR:O	3:3:183:SER:HB3	2.02	0.58
1:1:58:MET:HE1	3:3:216:ASP:C	2.24	0.58
2:2:177:LEU:HD11	3:3:94:THR:HG21	1.86	0.58
2:2:256:SER:O	2:2:257:LYS:CB	2.50	0.58
2:2:52:LYS:NZ	2:2:52:LYS:HD3	2.20	0.57
3:3:199:PRO:O	3:3:200:GLU:HB2	2.04	0.57
1:1:107:SER:HB2	1:1:113:ARG:CD	2.34	0.57
1:1:205:SER:HB3	1:1:217:VAL:HG13	1.86	0.57
3:3:53:ILE:HD11	3:3:211:ILE:HB	1.87	0.57
1:1:85:LYS:HB3	1:1:236:LYS:HG3	1.87	0.56
2:2:230:VAL:HG23	2:2:231:PRO:O	2.05	0.56
3:3:31:THR:CG2	3:3:32:PRO:HD2	2.34	0.56
2:2:10:SER:OG	2:2:12:ARG:CB	2.53	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:3:175:TYR:H	3:3:182:THR:CG2	2.19	0.56
2:2:64:TYR:CD1	2:2:89:MET:HB3	2.39	0.56
1:1:187:SER:O	3:3:23:SER:HA	2.05	0.56
2:2:38:TRP:HZ3	4:4:57:LYS:HD2	1.70	0.56
3:3:179:ASP:OD2	3:3:182:THR:CG2	2.53	0.56
1:1:96:ALA:C	1:1:97:LYS:HG2	2.26	0.56
4:4:43:GLN:O	4:4:45:LEU:HB3	2.05	0.56
2:2:204:ILE:HG12	3:3:37:PRO:HG2	1.87	0.56
3:3:197:LEU:HB3	3:3:201:THR:HG21	1.87	0.55
1:1:87:ALA:CB	1:1:98:LEU:HD11	2.36	0.55
1:1:117:GLU:HB3	1:1:200:PHE:HZ	1.70	0.55
1:1:43:MET:HG3	1:1:44:PRO:HD2	1.87	0.55
1:1:97:LYS:C	1:1:99:PHE:N	2.59	0.55
3:3:198:PRO:O	3:3:201:THR:HB	2.07	0.55
2:2:230:VAL:HB	2:2:231:PRO:HD2	1.89	0.55
1:1:271:TYR:HB2	1:1:272:PRO:HD2	1.89	0.55
2:2:189:ILE:HA	2:2:194:ASN:ND2	2.21	0.55
3:3:31:THR:HG23	3:3:32:PRO:HD2	1.88	0.55
3:3:193:THR:O	3:3:194:SER:CB	2.55	0.54
1:1:228:ILE:HD11	1:1:239:VAL:HG21	1.88	0.54
1:1:236:LYS:HE3	1:1:238:LEU:HD13	1.88	0.54
1:1:79:VAL:HG22	1:1:242:ARG:HG2	1.89	0.54
2:2:77:GLY:O	2:2:156:LEU:HB2	2.07	0.54
2:2:170:LEU:CD2	3:3:64:VAL:HA	2.38	0.54
1:1:81:GLU:HG2	1:1:97:LYS:HZ2	1.72	0.54
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.42	0.53
1:1:192:GLY:HA2	1:1:221:MET:HE1	1.91	0.53
3:3:55:MET:HA	3:3:91:VAL:HG11	1.90	0.53
3:3:57:ASN:C	3:3:57:ASN:HB3	2.27	0.53
3:3:117:TYR:CD1	3:3:155:ILE:HD13	2.44	0.53
1:1:35:THR:HG23	3:3:160:THR:HB	1.90	0.53
2:2:12:ARG:NH2	3:3:157:LEU:HD21	2.24	0.53
3:3:216:ASP:O	3:3:218:LYS:HE3	2.09	0.53
3:3:86:PHE:CD1	3:3:178:PRO:HB3	2.44	0.53
1:1:276:GLU:HB3	1:1:277:PRO:CD	2.39	0.53
2:2:235:THR:CG2	2:2:236:PRO:CD	2.86	0.53
3:3:61:LYS:HG2	3:3:61:LYS:O	2.07	0.53
3:3:193:THR:O	3:3:194:SER:HB3	2.08	0.52
1:1:88:THR:O	1:1:90:ILE:CD1	2.58	0.52
2:2:174:ASN:C	2:2:174:ASN:ND2	2.63	0.52
3:3:18:ASP:OD2	4:4:40:SER:HB2	2.09	0.52
1:1:88:THR:O	1:1:90:ILE:HD13	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:3:75:ARG:NH1	3:3:78:GLU:OE2	2.41	0.52
3:3:210:PHE:N	3:3:210:PHE:CD1	2.78	0.52
4:4:59:LEU:HD21	4:4:61:LEU:CD1	2.34	0.52
4:4:44:SER:O	4:4:45:LEU:C	2.48	0.52
1:1:273:LYS:O	1:1:274:ASN:O	2.28	0.52
1:1:236:LYS:HE3	1:1:238:LEU:CD1	2.40	0.52
2:2:235:THR:HG22	2:2:236:PRO:N	2.22	0.52
1:1:152:TYR:O	1:1:154:PRO:HD3	2.09	0.52
1:1:81:GLU:HG2	1:1:97:LYS:NZ	2.25	0.52
2:2:177:LEU:CD1	3:3:94:THR:HG21	2.40	0.52
3:3:214:CYS:HB3	3:3:215:PRO:HD2	1.92	0.51
1:1:236:LYS:NZ	1:1:238:LEU:HD11	2.25	0.51
1:1:65:THR:HG22	3:3:104:TYR:CZ	2.46	0.51
2:2:34:CYS:HB2	2:2:202:PRO:CD	2.41	0.51
1:1:122:VAL:HG13	1:1:124:PHE:CE2	2.45	0.51
1:1:266:ILE:CD1	3:3:236:GLU:N	2.72	0.51
3:3:63:GLU:C	3:3:65:ASN:H	2.14	0.51
2:2:171:TYR:HA	2:2:176:THR:O	2.11	0.51
1:1:265:SER:HB2	2:2:138:GLY:O	2.11	0.51
1:1:60:PHE:CD2	3:3:218:LYS:HB3	2.46	0.50
1:1:117:GLU:HB3	1:1:200:PHE:CZ	2.46	0.50
3:3:57:ASN:N	3:3:57:ASN:HB2	2.25	0.50
1:1:114:LYS:NZ	3:3:99:GLU:OE2	2.44	0.50
1:1:96:ALA:O	1:1:97:LYS:HG2	2.12	0.50
1:1:94:ARG:CG	1:1:94:ARG:HH11	2.24	0.50
2:2:139:ASN:N	2:2:139:ASN:OD1	2.44	0.50
1:1:151:MET:HA	1:1:175:SER:HB2	1.93	0.50
3:3:54:PRO:O	3:3:91:VAL:HG12	2.12	0.49
2:2:8:GLY:C	2:2:9:TYR:HD1	2.14	0.49
2:2:170:LEU:HD21	3:3:64:VAL:HA	1.94	0.49
2:2:19:GLY:HA2	2:2:58:THR:HG22	1.94	0.49
4:4:59:LEU:HG	4:4:60:MET:N	2.27	0.49
1:1:58:MET:CE	3:3:216:ASP:O	2.60	0.49
1:1:168:TRP:CH2	1:1:225:ALA:HB1	2.47	0.49
1:1:83:GLN:HG3	1:1:85:LYS:CE	2.31	0.49
1:1:280:LYS:HE3	3:3:89:ASP:OD1	2.13	0.49
2:2:143:LYS:HG2	2:2:163:GLY:O	2.12	0.49
3:3:112:ARG:HG2	3:3:112:ARG:NH1	2.27	0.49
1:1:152:TYR:C	1:1:154:PRO:HD3	2.33	0.49
3:3:125:ALA:HB3	3:3:155:ILE:HD12	1.95	0.48
2:2:34:CYS:HB2	2:2:202:PRO:HD2	1.95	0.48
3:3:112:ARG:HD3	3:3:162:VAL:CG1	2.43	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:3:129:LEU:O	3:3:150:HIS:HA	2.13	0.48
2:2:10:SER:CB	4:4:68:ASN:OXT	2.61	0.48
1:1:58:MET:HE1	3:3:216:ASP:O	2.13	0.48
2:2:40:GLU:CG	2:2:40:GLU:O	2.61	0.48
1:1:268:ARG:HH11	1:1:268:ARG:HD3	1.50	0.48
3:3:95:THR:O	3:3:99:GLU:HB2	2.13	0.48
1:1:58:MET:O	1:1:59:HIS:HB2	2.13	0.48
1:1:157:ALA:HB1	1:1:158:PRO:HD2	1.94	0.48
1:1:268:ARG:NH1	3:3:236:GLU:O	2.46	0.48
1:1:134:ALA:HB2	1:1:180:VAL:HG11	1.96	0.48
2:2:130:HIS:ND1	2:2:219:SER:OG	2.47	0.48
1:1:273:LYS:O	1:1:274:ASN:C	2.52	0.47
1:1:268:ARG:CZ	2:2:139:ASN:HB2	2.44	0.47
2:2:187:GLN:HE21	2:2:187:GLN:HB2	1.57	0.47
1:1:97:LYS:C	1:1:99:PHE:H	2.18	0.47
3:3:190:TRP:CD1	3:3:190:TRP:N	2.81	0.47
2:2:13:VAL:HA	2:2:25:THR:O	2.15	0.47
2:2:177:LEU:CD1	3:3:94:THR:CG2	2.93	0.47
3:3:115:LEU:HD22	3:3:129:LEU:HD21	1.95	0.47
1:1:83:GLN:OE1	1:1:236:LYS:HD2	2.15	0.47
1:1:87:ALA:CB	1:1:98:LEU:CD1	2.92	0.47
1:1:204:TYR:HD1	1:1:212:GLN:O	1.97	0.47
1:1:165:ASP:HB3	1:1:167:THR:H	1.79	0.47
1:1:107:SER:CB	1:1:113:ARG:HD2	2.38	0.47
1:1:74:ALA:HB3	3:3:15:THR:HB	1.97	0.47
2:2:170:LEU:HD23	3:3:64:VAL:CG2	2.45	0.47
1:1:43:MET:HE3	1:1:43:MET:HA	1.97	0.46
2:2:135:HIS:CD2	2:2:160:ASN:HB3	2.49	0.46
3:3:101:VAL:HG22	3:3:219:LEU:HD11	1.98	0.46
1:1:92:ASN:CG	1:1:95:GLU:HB2	2.36	0.46
4:4:61:LEU:HD12	4:4:61:LEU:HA	1.63	0.46
1:1:204:TYR:CZ	1:1:213:TYR:HD1	2.34	0.46
2:2:63:PHE:CD1	2:2:245:ALA:HB2	2.50	0.46
1:1:206:HIS:ND1	1:1:206:HIS:N	2.62	0.46
1:1:87:ALA:CA	1:1:90:ILE:HG12	2.44	0.46
1:1:218:LEU:HD23	1:1:218:LEU:HA	1.81	0.45
1:1:82:ILE:HG22	1:1:100:ASN:HB2	1.97	0.45
1:1:43:MET:CE	1:1:43:MET:HA	2.46	0.45
3:3:192:GLN:HA	3:3:192:GLN:HE21	1.81	0.45
1:1:78:HIS:CE1	1:1:102:TRP:CD1	3.03	0.45
3:3:55:MET:CE	3:3:91:VAL:HG21	2.46	0.45
2:2:190:ASN:H	2:2:194:ASN:CB	2.30	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:3:197:LEU:HD21	3:3:205:VAL:HG11	1.99	0.45
1:1:106:LEU:HG	5:1:290:SD8:H111	1.98	0.45
2:2:156:LEU:HD11	2:2:173:MET:SD	2.56	0.45
2:2:91:VAL:HG12	2:2:95:ASN:HD22	1.82	0.45
4:4:44:SER:C	4:4:46:SER:N	2.68	0.45
2:2:13:VAL:C	2:2:14:GLN:CG	2.85	0.45
3:3:55:MET:HE2	3:3:91:VAL:HG21	1.99	0.45
1:1:191:VAL:O	1:1:191:VAL:CG2	2.61	0.45
4:4:43:GLN:HG3	4:4:45:LEU:H	1.82	0.45
2:2:170:LEU:HD23	3:3:64:VAL:HG22	1.99	0.45
3:3:50:ASP:HA	3:3:212:SER:HB3	1.98	0.45
3:3:174:ARG:HH11	3:3:174:ARG:HD3	1.47	0.45
1:1:28:THR:HG22	1:1:29:GLN:H	1.82	0.45
1:1:207:ASP:HA	2:2:144:TYR:CE2	2.52	0.45
3:3:116:MET:HG3	3:3:159:SER:OG	2.17	0.44
1:1:64:GLU:HG2	1:1:64:GLU:O	2.17	0.44
3:3:181:TYR:CD1	3:3:181:TYR:C	2.91	0.44
2:2:146:PHE:CG	2:2:164:GLY:HA2	2.52	0.44
2:2:10:SER:OG	4:4:68:ASN:OXT	2.35	0.44
1:1:31:VAL:HG11	1:1:34:LEU:HD12	1.98	0.44
1:1:285:ASP:HB3	1:1:288:SER:H	1.82	0.44
2:2:148:HIS:N	2:2:149:PRO:CD	2.79	0.44
2:2:228:LEU:CD1	2:2:238:LEU:HD22	2.47	0.44
3:3:61:LYS:O	3:3:63:GLU:HG3	2.16	0.44
1:1:289:TYR:CE2	3:3:138:GLY:HA3	2.53	0.44
1:1:132:ALA:O	1:1:181:GLY:N	2.41	0.44
1:1:47:PRO:HB3	3:3:166:PRO:HB3	1.99	0.44
1:1:94:ARG:HD3	1:1:99:PHE:CE1	2.53	0.44
1:1:289:TYR:CD2	3:3:138:GLY:HA3	2.52	0.44
2:2:37:GLU:CD	3:3:35:HIS:HE2	2.19	0.44
3:3:57:ASN:H	3:3:57:ASN:CB	2.26	0.44
1:1:265:SER:OG	2:2:139:ASN:HB3	2.18	0.43
1:1:282:ARG:CG	3:3:57:ASN:CB	2.89	0.43
4:4:59:LEU:CD2	4:4:61:LEU:HD13	2.41	0.43
2:2:190:ASN:H	2:2:194:ASN:HB3	1.82	0.43
2:2:13:VAL:C	2:2:14:GLN:HG2	2.39	0.43
2:2:95:ASN:HB3	2:2:251:PHE:CE2	2.53	0.43
2:2:143:LYS:HG2	2:2:143:LYS:H	1.56	0.43
1:1:120:THR:O	1:1:199:CYS:HB2	2.18	0.43
3:3:61:LYS:HG2	3:3:63:GLU:HG3	2.00	0.43
2:2:91:VAL:HG12	2:2:95:ASN:ND2	2.34	0.43
2:2:262:GLN:C	2:2:262:GLN:NE2	2.66	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:286:ILE:HG21	1:1:286:ILE:HD13	1.77	0.43
1:1:83:GLN:HE21	1:1:97:LYS:HG3	1.82	0.43
3:3:47:ILE:HG21	3:3:47:ILE:HD13	1.51	0.43
4:4:43:GLN:O	4:4:45:LEU:CB	2.65	0.43
3:3:151:VAL:HG11	3:3:161:ILE:HD11	2.01	0.43
2:2:70:THR:HG22	2:2:72:THR:HG22	2.01	0.43
2:2:259:ILE:HG21	2:2:259:ILE:HD13	1.74	0.42
2:2:235:THR:CG2	2:2:236:PRO:N	2.79	0.42
1:1:261:LEU:HD11	2:2:171:TYR:CD2	2.55	0.42
2:2:225:ILE:O	3:3:68:LEU:HD21	2.19	0.42
2:2:228:LEU:HD11	2:2:238:LEU:HD22	2.02	0.42
1:1:206:HIS:NE2	1:1:208:ASP:HB2	2.34	0.42
1:1:197:TYR:HE1	1:1:221:MET:CE	2.33	0.42
1:1:136:GLN:NE2	1:1:235:HIS:CD2	2.64	0.42
2:2:10:SER:CB	2:2:12:ARG:HB2	2.49	0.42
1:1:286:ILE:HG23	3:3:81:PHE:HA	2.00	0.42
1:1:285:ASP:HB3	1:1:288:SER:N	2.34	0.41
1:1:93:HIS:CE1	1:1:163:TRP:HD1	2.38	0.41
1:1:146:LEU:HA	1:1:230:ASN:OD1	2.20	0.41
3:3:18:ASP:CG	4:4:40:SER:HB2	2.41	0.41
3:3:44:LEU:HD23	3:3:44:LEU:HA	1.79	0.41
3:3:174:ARG:HD2	3:3:182:THR:O	2.20	0.41
2:2:235:THR:HG22	2:2:237:SER:N	2.35	0.41
1:1:86:ASP:OD1	1:1:88:THR:HB	2.20	0.41
3:3:112:ARG:HG2	3:3:112:ARG:HH11	1.83	0.41
3:3:113:PHE:CE2	3:3:115:LEU:HD13	2.55	0.41
3:3:195:LEU:C	3:3:196:ILE:HG12	2.40	0.41
1:1:107:SER:HB3	5:1:290:SD8:H172	2.02	0.41
1:1:38:GLU:CD	3:3:116:MET:CE	2.88	0.41
3:3:208:LEU:HA	3:3:208:LEU:HD12	1.73	0.41
1:1:128:TYR:CZ	5:1:290:SD8:H7	2.55	0.41
1:1:98:LEU:HA	1:1:98:LEU:HD23	1.74	0.41
2:2:43:PRO:HG2	2:2:46:ASP:HB2	2.03	0.41
2:2:255:ARG:CG	2:2:256:SER:H	1.99	0.41
1:1:165:ASP:CB	1:1:167:THR:OG1	2.69	0.41
2:2:195:ASN:OD1	2:2:195:ASN:C	2.59	0.41
1:1:78:HIS:NE2	1:1:80:THR:HB	2.36	0.41
1:1:289:TYR:CZ	3:3:139:PRO:HD2	2.55	0.41
2:2:69:LYS:O	2:2:239:PRO:HA	2.20	0.41
2:2:122:LEU:HD23	2:2:224:PRO:HA	2.02	0.41
1:1:153:VAL:N	1:1:154:PRO:HD3	2.28	0.40
3:3:214:CYS:HB3	3:3:215:PRO:CD	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:285:ASP:H	1:1:285:ASP:HB2	1.85	0.40
4:4:43:GLN:HG2	4:4:43:GLN:O	2.18	0.40
1:1:38:GLU:N	3:3:116:MET:HE3	2.37	0.40
1:1:215:ILE:HG12	1:1:215:ILE:H	1.34	0.40
3:3:167:TRP:HZ2	3:3:172:GLN:HA	1.86	0.40
4:4:43:GLN:O	4:4:44:SER:C	2.58	0.40
2:2:13:VAL:HG22	2:2:26:GLN:HA	2.03	0.40
1:1:261:LEU:HD11	2:2:171:TYR:CE2	2.57	0.40
3:3:57:ASN:HD21	3:3:91:VAL:HG13	1.84	0.40
1:1:208:ASP:HB3	1:1:211:THR:HB	2.04	0.40
4:4:43:GLN:C	4:4:45:LEU:N	2.74	0.40
2:2:53:THR:OG1	2:2:250:GLU:HG2	2.22	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	1	271/289 (94%)	246 (91%)	18 (7%)	7 (3%)	8	39
2	2	253/262 (97%)	233 (92%)	18 (7%)	2 (1%)	27	76
3	3	234/236 (99%)	217 (93%)	15 (6%)	2 (1%)	25	73
4	4	38/68 (56%)	34 (90%)	3 (8%)	1 (3%)	8	39
All	All	796/855 (93%)	730 (92%)	54 (7%)	12 (2%)	15	58

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	139	SER
1	1	218	LEU
1	1	266	ILE
3	3	57	ASN
3	3	77	ASN
1	1	104	ILE

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Mol	Chain	Res	Type
1	1	165	ASP
2	2	255	ARG
2	2	257	LYS
1	1	223	SER
4	4	47	MET
1	1	224	MET

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	1	239/253 (94%)	196 (82%)	43 (18%)	2	13
2	2	223/229 (97%)	181 (81%)	42 (19%)	2	12
3	3	209/209 (100%)	172 (82%)	37 (18%)	3	14
4	4	33/57 (58%)	20 (61%)	13 (39%)	0	0
All	All	704/748 (94%)	569 (81%)	135 (19%)	2	12

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	18	VAL
1	1	21	ILE
1	1	22	SER
1	1	23	SER
1	1	28	THR
1	1	29	GLN
1	1	30	LYS
1	1	38	GLU
1	1	43	MET
1	1	47	PRO
1	1	63	SER
1	1	81	GLU
1	1	90	ILE
1	1	97	LYS
1	1	106	LEU
1	1	122	VAL

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Mol	Chain	Res	Type
1	1	136	GLN
1	1	137	PRO
1	1	138	ASP
1	1	139	SER
1	1	144	SER
1	1	145	ASN
1	1	161	LYS
1	1	165	ASP
1	1	170	SER
1	1	172	SER
1	1	173	ASN
1	1	176	VAL
1	1	183	THR
1	1	184	SER
1	1	185	ARG
1	1	191	VAL
1	1	202	ASP
1	1	215	ILE
1	1	216	THR
1	1	223	SER
1	1	224	MET
1	1	240	LYS
1	1	256	ARG
1	1	268	ARG
1	1	274	ASN
1	1	278	VAL
1	1	287	LYS
2	2	11	ASP
2	2	12	ARG
2	2	20	ASN
2	2	26	GLN
2	2	49	ASP
2	2	52	LYS
2	2	66	LEU
2	2	69	LYS
2	2	73	THR
2	2	76	LYS
2	2	81	LYS
2	2	87	LYS
2	2	88	ASP
2	2	103	ARG
2	2	116	LYS

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Mol	Chain	Res	Type
2	2	119	SER
2	2	136	GLU
2	2	141	SER
2	2	145	THR
2	2	152	ARG
2	2	165	PRO
2	2	168	ASP
2	2	169	VAL
2	2	170	LEU
2	2	174	ASN
2	2	187	GLN
2	2	192	ARG
2	2	195	ASN
2	2	209	ILE
2	2	211	SER
2	2	217	ASN
2	2	221	MET
2	2	225	ILE
2	2	232	THR
2	2	236	PRO
2	2	238	LEU
2	2	247	MET
2	2	250	GLU
2	2	254	ILE
2	2	255	ARG
2	2	256	SER
2	2	262	GLN
3	3	16	THR
3	3	33	ARG
3	3	46	ILE
3	3	55	MET
3	3	60	THR
3	3	61	LYS
3	3	65	ASN
3	3	91	VAL
3	3	94	THR
3	3	101	VAL
3	3	112	ARG
3	3	114	SER
3	3	115	LEU
3	3	137	ARG
3	3	146	MET

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Mol	Chain	Res	Type
3	3	157	LEU
3	3	158	GLN
3	3	159	SER
3	3	164	THR
3	3	172	GLN
3	3	174	ARG
3	3	179	ASP
3	3	182	THR
3	3	192	GLN
3	3	194	SER
3	3	196	ILE
3	3	201	THR
3	3	208	LEU
3	3	211	ILE
3	3	217	PHE
3	3	218	LYS
3	3	219	LEU
3	3	220	ARG
3	3	223	LYS
3	3	226	GLN
3	3	228	ILE
3	3	230	GLN
4	4	29	ILE
4	4	33	LYS
4	4	40	SER
4	4	43	GLN
4	4	45	LEU
4	4	46	SER
4	4	47	MET
4	4	50	SER
4	4	51	LYS
4	4	59	LEU
4	4	61	LEU
4	4	67	LEU
4	4	68	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	ASN
1	1	136	GLN
1	1	173	ASN

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Mol	Chain	Res	Type
2	2	20	ASN
2	2	174	ASN
2	2	187	GLN
2	2	217	ASN
2	2	262	GLN
3	3	102	GLN
3	3	140	GLN
3	3	192	GLN
3	3	226	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\# Z > 2$
5	SD8	1	290	-	29,29,29	3.44	13 (44%)	39,40,40	1.87	7 (17%)

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
5	SD8	1	290	-	-	0/13/34/34	0/2/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	290	SD8	C8-C3	10.41	1.55	1.41
5	1	290	SD8	C1-N2	7.83	1.48	1.35
5	1	290	SD8	C4-C3	7.81	1.54	1.40
5	1	290	SD8	C2-S1	-5.35	1.76	1.80
5	1	290	SD8	C13-S2	-3.85	1.62	1.74
5	1	290	SD8	C8-N1	-3.44	1.32	1.39
5	1	290	SD8	C11-N3	2.94	1.51	1.46
5	1	290	SD8	O2-C16	2.66	1.40	1.33
5	1	290	SD8	C14-S2	2.57	1.74	1.70
5	1	290	SD8	C15-N4	2.49	1.43	1.38
5	1	290	SD8	C10-N3	2.24	1.50	1.46
5	1	290	SD8	C12-N2	2.20	1.51	1.47
5	1	290	SD8	C9-N2	2.02	1.50	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	290	SD8	C1-C2-S1	7.23	125.50	110.39
5	1	290	SD8	C8-N1-C1	3.81	129.32	116.79
5	1	290	SD8	C4-C3-C8	-3.42	114.13	119.16
5	1	290	SD8	C4-C3-S1	2.45	123.09	117.12
5	1	290	SD8	C15-C14-S2	-2.35	109.22	111.97
5	1	290	SD8	C2-S1-C3	2.23	99.46	96.51
5	1	290	SD8	C3-C8-N1	-2.11	121.96	125.08

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, 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	1	273/289 (94%)	-0.06	0 100 100	8, 14, 30, 42	0
2	2	255/262 (97%)	-0.05	0 100 100	7, 12, 24, 42	0
3	3	236/236 (100%)	-0.07	0 100 100	8, 12, 23, 31	0
4	4	40/68 (58%)	-0.03	0 100 100	13, 24, 37, 39	0
All	All	804/855 (94%)	-0.06	0 100 100	7, 13, 28, 42	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SD8	1	290	26/26	0.26	0.30	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.