Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2023 – 04:16 PM EST

PDB ID	:	2RS3
Title	:	STRUCTURAL ANALYSIS OF ANTIVIRAL AGENTS THAT INTERACT WITH THE CAPSID OF HUMAN RHINOVIRUSES
Authors	:	Badger, J.; Smith, T.J.; Rossmann, M.G.
Deposited on	:	1988-10-03
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

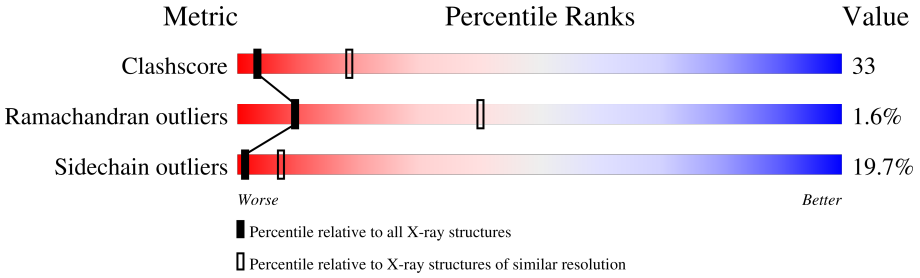
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	1	289	33% 41% 15% 6% 6%
2	2	262	43% 36% 13% 5% •
3	3	236	42% 35% 17% 6%
4	4	68	18% 16% 16% 9% 41%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6299 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1).

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

- Molecule 2 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2).

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

There is a discrepancy between the modelled and reference sequences:

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

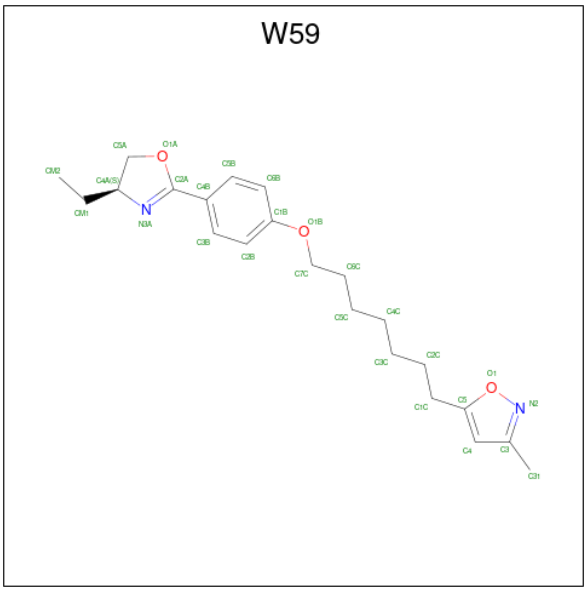
- Molecule 3 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3).

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

- Molecule 4 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP4).

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

- Molecule 5 is 5-(7-(5-HYDRO-4-ETHYL-2-OXAZOLYL)PHENOXY)HEPTYL)-3-METHYL ISOXAZOLE (three-letter code: W59) (formula: $C_{22}H_{30}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	1	1	27	22	2	3	0	0

- Molecule 6 is water.

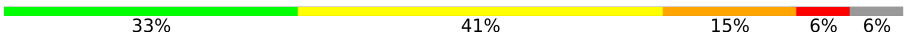
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	1	4	4	4	0	0

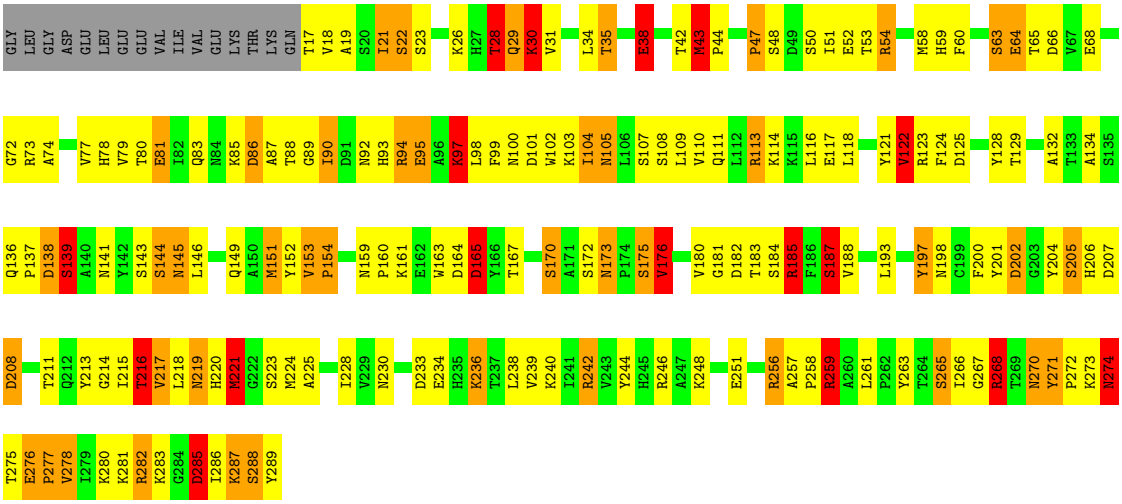
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1)

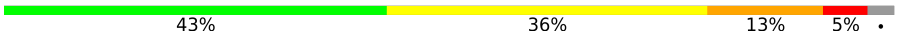
Chain 1:

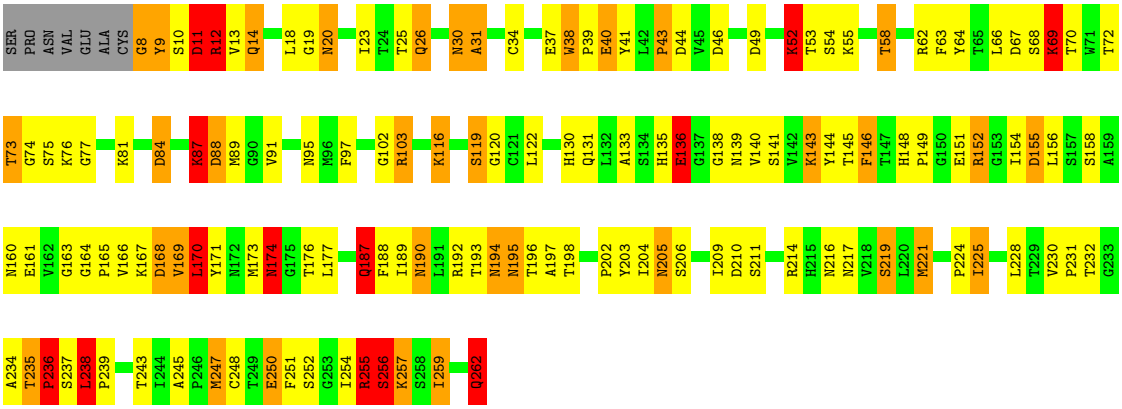




• Molecule 2: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2)

Chain 2:





• Molecule 3: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3)

Chain 3:

G1 T15 T16 D17 D18 R19 Q20 S21 P26 N27 Y28 E29 P30 T31 P32 R33 I34 H35 I36 P37 G38 N42 L43 L44 E45 I46 I47 D50 I53 P54 M55 N56 N57 T58 H59 T60 K61 D62 E63 V64 N65 S66 Y67 L68 N74 R75 Q76 N77 E78 Q79 V80 F81 N84

L85 F86 D89 G90 V91 F92 K93 T94 T95 G98 E99 I100 V101 Q102 Y103 Y104 S108 R112 F113 S114 L115 M116 Y117 T118 A121 A125 L129 A130 Y131 R137 G138 P139 Q140 D141 R142 R143 E144 A145 M146 L147 G148 T149 H150 V151 I155 G156 L157 Q158 S159 T160 I161

V162 M163 T164 I165 P166 W167 Q172 F173 R174 Y175 T176 D177 P178 D179 T180 Y181 T182 S183 F186 W190 Y191 Q192 T193 S194 L195 I196 L197 P198 P199 E200 T201 V205 L208 S209 F210 I211 S212 A213 C214 P215 D216 F217 K218 L219 R220 L221 M222 K223 D224 T225 Q226 T227 I228 S229 Q230

T231 T235 E236

- Molecule 4: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP4)

Chain 4: 18% 16% 16% 9% 41%

GLY ALA GLN VAL SER THR GLN LYS SER GLY SER HIS GLU ASN GLN ASN ILE LEU THR ASN GLY SER ASN GLN THR PHE THR VAL I29 N30 Y31 Y32 K33 A36 S37 T38 S39 S40 A41 G42 Q43 S44 L45 S46 M47 D48 P49 S50 K51 E54 K57 D58 L59 M60 L61 K62 G63

L67 N68

4 Data and refinement statistics (i)

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 39.19 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00) 15.1 (39.19-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.24 (at 3.01Å)	Xtriage
Refinement program	REAL-SPACE REFINEMENT	Depositor
R, R_{free}	(Not available) , (Not available) 0.226 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	15.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , -19.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	0.148 for l,-k,h	Xtriage
F_o,F_c correlation	0.71	EDS
Total number of atoms	6299	wwPDB-VP
Average B, all atoms (Å^2)	1.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: W59

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	1.88	41/2228 (1.8%)	2.38	119/3031 (3.9%)
2	2	1.85	32/2001 (1.6%)	2.17	78/2735 (2.9%)
3	3	1.77	21/1898 (1.1%)	2.18	76/2597 (2.9%)
4	4	2.30	13/302 (4.3%)	2.46	21/406 (5.2%)
All	All	1.86	107/6429 (1.7%)	2.26	294/8769 (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	2
2	2	0	2
All	All	0	4

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	170	SER	CB-OG	-14.28	1.23	1.42
1	1	285	ASP	CA-CB	11.80	1.79	1.53
4	4	42	GLY	N-CA	11.71	1.63	1.46
4	4	40	SER	CB-OG	10.77	1.56	1.42
2	2	256	SER	CB-OG	10.18	1.55	1.42
1	1	95	GLU	CB-CG	10.15	1.71	1.52
4	4	44	SER	CB-OG	9.91	1.55	1.42
4	4	41	ALA	C-O	9.40	1.41	1.23
1	1	117	GLU	CD-OE2	9.38	1.35	1.25
1	1	175	SER	CB-OG	-9.13	1.30	1.42
1	1	38	GLU	CB-CG	-9.05	1.34	1.52
1	1	187	SER	CB-OG	-8.87	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	21	SER	CA-CB	8.74	1.66	1.52
1	1	63	SER	CB-OG	-8.73	1.30	1.42
2	2	248	CYS	CB-SG	-8.67	1.67	1.82
3	3	57	ASN	CA-CB	8.43	1.75	1.53
2	2	40	GLU	CD-OE2	8.22	1.34	1.25
1	1	288	SER	CA-CB	8.04	1.65	1.52
2	2	52	LYS	CE-NZ	7.92	1.68	1.49
3	3	1	GLY	N-CA	7.83	1.57	1.46
3	3	63	GLU	CD-OE2	7.73	1.34	1.25
2	2	219	SER	CA-CB	-7.70	1.41	1.52
1	1	283	LYS	N-CA	7.66	1.61	1.46
2	2	136	GLU	CB-CG	7.55	1.66	1.52
3	3	108	SER	CB-OG	7.47	1.51	1.42
4	4	33	LYS	CE-NZ	7.42	1.67	1.49
1	1	282	ARG	CD-NE	7.39	1.59	1.46
1	1	234	GLU	CD-OE2	7.38	1.33	1.25
1	1	139	SER	CB-OG	7.26	1.51	1.42
2	2	152	ARG	CD-NE	7.20	1.58	1.46
1	1	187	SER	N-CA	7.16	1.60	1.46
2	2	152	ARG	CZ-NH2	7.03	1.42	1.33
2	2	194	ASN	CA-CB	6.97	1.71	1.53
4	4	46	SER	CB-OG	6.93	1.51	1.42
3	3	164	THR	C-O	6.86	1.36	1.23
4	4	51	LYS	CE-NZ	6.78	1.66	1.49
1	1	143	SER	CB-OG	6.76	1.51	1.42
3	3	61	LYS	CE-NZ	6.73	1.65	1.49
2	2	256	SER	C-O	6.68	1.36	1.23
1	1	72	GLY	C-O	6.52	1.34	1.23
1	1	30	LYS	CE-NZ	6.48	1.65	1.49
1	1	81	GLU	CD-OE2	6.42	1.32	1.25
2	2	12	ARG	NE-CZ	6.42	1.41	1.33
2	2	8	GLY	N-CA	6.39	1.55	1.46
1	1	283	LYS	CE-NZ	6.37	1.65	1.49
1	1	52	GLU	C-O	6.34	1.35	1.23
2	2	87	LYS	CB-CG	-6.29	1.35	1.52
1	1	30	LYS	CD-CE	6.29	1.67	1.51
3	3	138	GLY	N-CA	6.26	1.55	1.46
3	3	194	SER	CB-OG	-6.19	1.34	1.42
4	4	33	LYS	CD-CE	6.11	1.66	1.51
3	3	50	ASP	CA-CB	-6.08	1.40	1.53
1	1	144	SER	N-CA	6.01	1.58	1.46
1	1	94	ARG	CD-NE	6.00	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	108	SER	CA-CB	-5.99	1.44	1.52
4	4	54	GLU	CD-OE2	5.94	1.32	1.25
3	3	99	GLU	CB-CG	-5.92	1.41	1.52
2	2	102	GLY	N-CA	5.89	1.54	1.46
1	1	285	ASP	N-CA	-5.79	1.34	1.46
2	2	11	ASP	CA-CB	5.69	1.66	1.53
2	2	168	ASP	C-O	5.66	1.34	1.23
1	1	175	SER	CA-CB	-5.65	1.44	1.52
4	4	37	SER	CB-OG	-5.64	1.34	1.42
3	3	172	GLN	CG-CD	-5.63	1.38	1.51
4	4	63	GLY	N-CA	5.63	1.54	1.46
1	1	97	LYS	CD-CE	5.62	1.65	1.51
2	2	187	GLN	N-CA	5.61	1.57	1.46
3	3	45	GLU	CD-OE2	5.59	1.31	1.25
2	2	235	THR	C-N	-5.58	1.23	1.34
3	3	222	MET	CG-SD	5.57	1.95	1.81
4	4	45	LEU	C-N	5.56	1.46	1.34
1	1	139	SER	CA-CB	5.56	1.61	1.52
2	2	219	SER	CB-OG	-5.49	1.35	1.42
1	1	73	ARG	C-O	5.43	1.33	1.23
2	2	236	PRO	C-O	5.43	1.34	1.23
1	1	276	GLU	CD-OE2	5.42	1.31	1.25
2	2	54	SER	CA-CB	-5.41	1.44	1.52
4	4	50	SER	CB-OG	5.40	1.49	1.42
2	2	262	GLN	CD-OE1	5.39	1.35	1.24
2	2	187	GLN	CB-CG	-5.38	1.38	1.52
1	1	267	GLY	C-O	5.36	1.32	1.23
1	1	94	ARG	NE-CZ	5.33	1.40	1.33
2	2	40	GLU	CB-CG	5.28	1.62	1.52
1	1	117	GLU	CD-OE1	-5.27	1.19	1.25
2	2	68	SER	CB-OG	-5.26	1.35	1.42
1	1	246	ARG	CZ-NH2	5.25	1.39	1.33
1	1	175	SER	N-CA	5.25	1.56	1.46
3	3	118	THR	CB-OG1	5.24	1.53	1.43
1	1	251	GLU	CA-CB	-5.24	1.42	1.53
3	3	33	ARG	CZ-NH2	5.22	1.39	1.33
2	2	120	GLY	N-CA	5.21	1.53	1.46
2	2	74	GLY	C-O	5.17	1.31	1.23
1	1	143	SER	C-O	5.16	1.33	1.23
2	2	161	GLU	CA-CB	-5.16	1.42	1.53
2	2	12	ARG	CZ-NH2	5.15	1.39	1.33
1	1	202	ASP	CA-CB	-5.12	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	38	GLY	CA-C	-5.12	1.43	1.51
1	1	283	LYS	CD-CE	5.11	1.64	1.51
1	1	68	GLU	CD-OE1	-5.10	1.20	1.25
1	1	26	LYS	CB-CG	-5.08	1.38	1.52
3	3	77	ASN	C-O	5.08	1.33	1.23
2	2	58	THR	C-O	5.06	1.32	1.23
3	3	86	PHE	CA-CB	-5.04	1.42	1.53
2	2	136	GLU	CD-OE2	5.04	1.31	1.25
2	2	38	TRP	CG-CD1	5.04	1.43	1.36
3	3	30	PRO	N-CD	-5.04	1.40	1.47
1	1	288	SER	C-O	5.03	1.32	1.23

All (294) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	246	ARG	NE-CZ-NH1	22.42	131.51	120.30
1	1	256	ARG	NE-CZ-NH2	20.42	130.51	120.30
1	1	123	ARG	NE-CZ-NH1	19.20	129.90	120.30
2	2	255	ARG	NE-CZ-NH2	-18.51	111.04	120.30
2	2	87	LYS	CA-CB-CG	17.64	152.21	113.40
1	1	285	ASP	CB-CG-OD2	-17.60	102.46	118.30
1	1	256	ARG	NE-CZ-NH1	-16.93	111.83	120.30
3	3	137	ARG	NE-CZ-NH1	-16.86	111.87	120.30
1	1	94	ARG	NE-CZ-NH2	-16.51	112.05	120.30
3	3	216	ASP	CB-CG-OD1	16.15	132.84	118.30
1	1	282	ARG	NE-CZ-NH2	-14.17	113.22	120.30
2	2	255	ARG	NE-CZ-NH1	13.98	127.29	120.30
1	1	165	ASP	CB-CG-OD1	13.05	130.04	118.30
1	1	197	TYR	N-CA-CB	-12.92	87.34	110.60
2	2	168	ASP	CB-CG-OD2	-12.82	106.76	118.30
1	1	185	ARG	NE-CZ-NH1	12.29	126.45	120.30
3	3	50	ASP	CA-CB-CG	12.24	140.33	113.40
1	1	94	ARG	CD-NE-CZ	-12.04	106.75	123.60
2	2	11	ASP	CB-CG-OD1	-11.72	107.75	118.30
2	2	194	ASN	N-CA-CB	-11.56	89.79	110.60
2	2	193	THR	C-N-CA	11.38	150.15	121.70
3	3	174	ARG	NE-CZ-NH2	-11.33	114.64	120.30
1	1	170	SER	CA-CB-OG	11.12	141.21	111.20
3	3	215	PRO	C-N-CA	11.00	149.20	121.70
2	2	152	ARG	NE-CZ-NH2	-10.99	114.81	120.30
4	4	41	ALA	CA-C-N	10.88	137.96	116.20
4	4	48	ASP	CB-CG-OD2	-10.87	108.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	19	ARG	NE-CZ-NH2	10.79	125.69	120.30
3	3	33	ARG	NE-CZ-NH2	-10.63	114.98	120.30
1	1	197	TYR	CA-CB-CG	10.60	133.55	113.40
1	1	285	ASP	CB-CG-OD1	10.59	127.83	118.30
1	1	285	ASP	CA-CB-CG	-10.46	90.39	113.40
3	3	50	ASP	CB-CG-OD1	10.43	127.69	118.30
2	2	151	GLU	CA-CB-CG	10.36	136.19	113.40
1	1	246	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	1	187	SER	CB-CA-C	10.07	129.24	110.10
1	1	282	ARG	CD-NE-CZ	-10.05	109.53	123.60
1	1	246	ARG	CD-NE-CZ	10.01	137.62	123.60
1	1	113	ARG	NE-CZ-NH2	-9.83	115.39	120.30
1	1	208	ASP	CB-CG-OD2	-9.83	109.45	118.30
3	3	57	ASN	N-CA-CB	-9.82	92.92	110.60
3	3	146	MET	CG-SD-CE	9.81	115.90	100.20
3	3	216	ASP	CB-CG-OD2	-9.77	109.51	118.30
2	2	88	ASP	CB-CG-OD2	-9.68	109.59	118.30
1	1	242	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	1	54	ARG	CD-NE-CZ	-9.39	110.45	123.60
1	1	66	ASP	CB-CG-OD2	-9.19	110.03	118.30
3	3	57	ASN	CB-CA-C	-9.02	92.36	110.40
2	2	11	ASP	CA-CB-CG	-8.98	93.64	113.40
1	1	38	GLU	CA-CB-CG	8.88	132.93	113.40
3	3	112	ARG	NE-CZ-NH2	-8.83	115.88	120.30
3	3	137	ARG	NE-CZ-NH2	8.76	124.68	120.30
3	3	182	THR	CA-CB-CG2	8.55	124.37	112.40
1	1	165	ASP	CB-CG-OD2	-8.54	110.62	118.30
1	1	285	ASP	N-CA-CB	-8.52	95.26	110.60
1	1	268	ARG	CD-NE-CZ	-8.46	111.76	123.60
1	1	175	SER	CB-CA-C	8.41	126.07	110.10
1	1	123	ARG	CD-NE-CZ	8.38	135.33	123.60
1	1	63	SER	CB-CA-C	-8.37	94.20	110.10
1	1	165	ASP	CB-CA-C	-8.35	93.70	110.40
2	2	250	GLU	CA-CB-CG	8.32	131.72	113.40
1	1	285	ASP	CB-CA-C	-8.29	93.81	110.40
3	3	172	GLN	CB-CG-CD	8.25	133.05	111.60
1	1	187	SER	N-CA-CB	-8.20	98.20	110.50
2	2	152	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	1	251	GLU	CA-CB-CG	8.18	131.38	113.40
4	4	45	LEU	N-CA-CB	-8.13	94.13	110.40
3	3	224	ASP	CB-CG-OD2	-8.11	111.00	118.30
2	2	255	ARG	CA-CB-CG	8.03	131.07	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	181	TYR	CB-CG-CD2	-8.03	116.18	121.00
2	2	11	ASP	OD1-CG-OD2	8.03	138.55	123.30
4	4	48	ASP	OD1-CG-OD2	8.02	138.54	123.30
1	1	95	GLU	OE1-CD-OE2	8.01	132.91	123.30
1	1	38	GLU	CB-CG-CD	7.99	135.78	114.20
4	4	47	MET	CA-CB-CG	-7.85	99.95	113.30
2	2	219	SER	CA-CB-OG	7.85	132.39	111.20
3	3	174	ARG	CD-NE-CZ	-7.84	112.62	123.60
1	1	145	ASN	OD1-CG-ND2	7.80	139.84	121.90
2	2	155	ASP	CB-CG-OD2	-7.70	111.37	118.30
3	3	21	SER	CB-CA-C	-7.69	95.50	110.10
1	1	121	TYR	CB-CG-CD1	-7.68	116.39	121.00
3	3	78	GLU	OE1-CD-OE2	7.63	132.46	123.30
2	2	187	GLN	CA-CB-CG	7.58	130.09	113.40
1	1	277	PRO	N-CD-CG	-7.54	91.88	103.20
2	2	11	ASP	C-N-CA	7.54	140.54	121.70
1	1	123	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	1	173	ASN	N-CA-CB	-7.51	97.08	110.60
2	2	170	LEU	CA-CB-CG	7.51	132.57	115.30
2	2	187	GLN	CB-CA-C	7.50	125.39	110.40
1	1	182	ASP	CB-CG-OD2	-7.49	111.56	118.30
3	3	112	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	1	259	ARG	CA-CB-CG	-7.36	97.22	113.40
1	1	282	ARG	NH1-CZ-NH2	7.26	127.38	119.40
1	1	117	GLU	CG-CD-OE1	7.25	132.81	118.30
2	2	214	ARG	NE-CZ-NH1	7.25	123.92	120.30
3	3	142	ARG	CA-CB-CG	7.21	129.25	113.40
2	2	194	ASN	CA-CB-CG	-7.13	97.71	113.40
2	2	190	ASN	CA-CB-CG	7.08	128.98	113.40
1	1	197	TYR	CB-CA-C	7.06	124.52	110.40
2	2	168	ASP	N-CA-CB	-7.06	97.90	110.60
3	3	137	ARG	CD-NE-CZ	-7.04	113.74	123.60
1	1	185	ARG	NH1-CZ-NH2	-7.04	111.66	119.40
1	1	113	ARG	NE-CZ-NH1	7.03	123.82	120.30
3	3	121	ALA	CB-CA-C	-7.03	99.55	110.10
3	3	28	TYR	CB-CG-CD1	-7.03	116.78	121.00
2	2	256	SER	CA-C-O	-7.01	105.38	120.10
1	1	68	GLU	CG-CD-OE1	6.99	132.29	118.30
3	3	174	ARG	NH1-CZ-NH2	6.98	127.07	119.40
4	4	41	ALA	CA-C-O	-6.97	105.46	120.10
1	1	28	THR	CB-CA-C	-6.93	92.89	111.60
1	1	42	THR	CA-CB-CG2	6.88	122.03	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	26	LYS	CA-CB-CG	6.88	128.53	113.40
1	1	125	ASP	CB-CG-OD2	-6.87	112.11	118.30
2	2	136	GLU	CG-CD-OE2	-6.78	104.75	118.30
4	4	37	SER	CB-CA-C	6.77	122.96	110.10
1	1	151	MET	CG-SD-CE	6.75	110.99	100.20
3	3	194	SER	N-CA-CB	-6.73	100.40	110.50
3	3	163	MET	CA-CB-CG	-6.72	101.87	113.30
2	2	146	PHE	CB-CG-CD1	-6.68	116.13	120.80
3	3	216	ASP	N-CA-CB	-6.65	98.63	110.60
2	2	103	ARG	CD-NE-CZ	-6.63	114.31	123.60
1	1	265	SER	N-CA-CB	-6.63	100.55	110.50
3	3	57	ASN	CA-CB-CG	-6.61	98.86	113.40
3	3	45	GLU	CG-CD-OE1	6.59	131.47	118.30
2	2	87	LYS	CB-CG-CD	6.58	128.70	111.60
3	3	27	ASN	CB-CA-C	-6.57	97.26	110.40
1	1	94	ARG	NH1-CZ-NH2	6.56	126.62	119.40
1	1	276	GLU	OE1-CD-OE2	6.56	131.17	123.30
1	1	68	GLU	CG-CD-OE2	-6.55	105.20	118.30
1	1	288	SER	CB-CA-C	-6.54	97.68	110.10
1	1	53	THR	CA-CB-OG1	-6.53	95.30	109.00
2	2	203	TYR	CB-CG-CD1	6.51	124.91	121.00
3	3	74	ASN	CA-CB-CG	-6.49	99.13	113.40
4	4	45	LEU	CB-CA-C	6.49	122.53	110.20
1	1	144	SER	N-CA-CB	-6.47	100.79	110.50
1	1	22	SER	N-CA-CB	-6.46	100.80	110.50
1	1	288	SER	N-CA-CB	-6.46	100.80	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
1	1	274	ASN	O-C-N	6.44	133.01	122.70
3	3	55	MET	CA-CB-CG	-6.42	102.39	113.30
2	2	168	ASP	OD1-CG-OD2	6.41	135.49	123.30
3	3	29	GLU	CB-CG-CD	6.41	131.52	114.20
1	1	138	ASP	CB-CG-OD1	6.35	124.01	118.30
2	2	97	PHE	CB-CG-CD1	-6.33	116.37	120.80
3	3	16	THR	N-CA-CB	-6.32	98.30	110.30
3	3	65	ASN	CA-CB-CG	-6.32	99.51	113.40
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	-6.25	99.34	110.60
3	3	27	ASN	CA-CB-CG	-6.25	99.66	113.40
3	3	19	ARG	CA-CB-CG	6.24	127.13	113.40
3	3	63	GLU	CG-CD-OE2	-6.24	105.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	145	ASN	CA-CB-CG	-6.22	99.71	113.40
1	1	271	TYR	CB-CG-CD2	6.22	124.73	121.00
2	2	203	TYR	CB-CG-CD2	-6.21	117.27	121.00
1	1	122	VAL	N-CA-CB	-6.18	97.90	111.50
2	2	136	GLU	CB-CG-CD	-6.16	97.57	114.20
2	2	69	LYS	CA-CB-CG	6.14	126.91	113.40
1	1	97	LYS	CD-CE-NZ	-6.11	97.65	111.70
1	1	117	GLU	CG-CD-OE2	-6.11	106.09	118.30
2	2	219	SER	CB-CA-C	6.10	121.69	110.10
3	3	222	MET	CG-SD-CE	-6.09	90.46	100.20
3	3	66	SER	CB-CA-C	6.07	121.63	110.10
1	1	86	ASP	CB-CG-OD2	6.06	123.75	118.30
3	3	219	LEU	CA-CB-CG	6.05	129.22	115.30
2	2	235	THR	CA-CB-CG2	-6.05	103.93	112.40
1	1	118	LEU	CA-CB-CG	6.05	129.21	115.30
1	1	164	ASP	C-N-CA	6.05	136.82	121.70
2	2	119	SER	N-CA-CB	6.05	119.57	110.50
2	2	12	ARG	NE-CZ-NH2	-6.03	117.28	120.30
2	2	67	ASP	CA-CB-CG	-6.02	100.15	113.40
2	2	103	ARG	CA-CB-CG	6.01	126.62	113.40
2	2	247	MET	CB-CA-C	6.01	122.41	110.40
4	4	48	ASP	CB-CG-OD1	-5.98	112.92	118.30
4	4	61	LEU	CB-CG-CD2	-5.98	100.84	111.00
3	3	1	GLY	N-CA-C	5.96	128.01	113.10
3	3	58	THR	CA-CB-CG2	-5.91	104.12	112.40
1	1	35	THR	N-CA-CB	-5.89	99.11	110.30
1	1	94	ARG	CG-CD-NE	-5.89	99.43	111.80
1	1	257	ALA	N-CA-CB	-5.89	101.86	110.10
1	1	256	ARG	CD-NE-CZ	-5.88	115.37	123.60
3	3	45	GLU	CG-CD-OE2	-5.87	106.55	118.30
2	2	256	SER	CA-C-N	5.86	130.10	117.20
4	4	30	ASN	CA-CB-CG	-5.86	100.50	113.40
2	2	214	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	1	236	LYS	CD-CE-NZ	-5.84	98.26	111.70
1	1	268	ARG	NE-CZ-NH2	-5.83	117.39	120.30
2	2	238	LEU	N-CA-CB	-5.81	98.78	110.40
2	2	31	ALA	N-CA-CB	5.81	118.23	110.10
4	4	33	LYS	CD-CE-NZ	-5.81	98.35	111.70
3	3	27	ASN	O-C-N	5.78	131.95	122.70
1	1	233	ASP	CB-CG-OD2	-5.78	113.10	118.30
2	2	255	ARG	CB-CG-CD	5.78	126.61	111.60
2	2	73	THR	CA-CB-OG1	-5.77	96.89	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	28	THR	OG1-CB-CG2	5.76	123.25	110.00
3	3	77	ASN	CA-C-N	5.75	129.85	117.20
2	2	68	SER	N-CA-CB	-5.75	101.88	110.50
1	1	274	ASN	N-CA-CB	5.74	120.92	110.60
1	1	95	GLU	CA-CB-CG	-5.72	100.82	113.40
3	3	1	GLY	O-C-N	-5.71	113.57	122.70
3	3	147	LEU	CA-CB-CG	5.71	128.43	115.30
2	2	52	LYS	CD-CE-NZ	-5.70	98.59	111.70
2	2	75	SER	N-CA-CB	-5.70	101.95	110.50
2	2	161	GLU	CA-CB-CG	5.68	125.90	113.40
1	1	224	MET	CG-SD-CE	5.68	109.29	100.20
1	1	48	SER	CA-C-O	-5.67	108.19	120.10
1	1	246	ARG	NH1-CZ-NH2	-5.66	113.17	119.40
3	3	177	ASP	CB-CG-OD2	-5.66	113.21	118.30
3	3	164	THR	N-CA-CB	-5.63	99.61	110.30
4	4	44	SER	O-C-N	5.62	131.70	122.70
3	3	94	THR	O-C-N	5.59	131.65	122.70
2	2	210	ASP	N-CA-CB	-5.58	100.56	110.60
3	3	186	PHE	CB-CG-CD1	-5.54	116.92	120.80
1	1	202	ASP	CA-CB-CG	5.53	125.56	113.40
1	1	122	VAL	CB-CA-C	5.53	121.90	111.40
2	2	9	TYR	CB-CA-C	5.50	121.41	110.40
2	2	12	ARG	CD-NE-CZ	-5.50	115.89	123.60
4	4	44	SER	C-N-CA	-5.50	107.96	121.70
1	1	81	GLU	CG-CD-OE2	-5.49	107.33	118.30
1	1	233	ASP	CB-CG-OD1	5.49	123.24	118.30
3	3	112	ARG	CA-CB-CG	5.48	125.45	113.40
1	1	43	MET	CG-SD-CE	5.47	108.96	100.20
1	1	244	TYR	CB-CG-CD2	-5.47	117.72	121.00
2	2	84	ASP	CB-CG-OD2	-5.47	113.38	118.30
2	2	43	PRO	N-CD-CG	-5.46	95.01	103.20
1	1	26	LYS	CD-CE-NZ	-5.46	99.15	111.70
1	1	270	ASN	O-C-N	5.43	131.39	122.70
1	1	193	LEU	CA-CB-CG	5.43	127.78	115.30
3	3	60	THR	CA-CB-OG1	-5.42	97.61	109.00
1	1	221	MET	CG-SD-CE	5.42	108.86	100.20
2	2	174	ASN	CA-C-N	5.41	127.02	116.20
4	4	44	SER	N-CA-CB	5.40	118.60	110.50
3	3	115	LEU	CA-CB-CG	5.40	127.71	115.30
1	1	123	ARG	NH1-CZ-NH2	-5.38	113.48	119.40
2	2	44	ASP	CA-CB-CG	5.38	125.24	113.40
3	3	161	ILE	CA-CB-CG1	-5.38	100.79	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	65	ASN	N-CA-CB	-5.37	100.94	110.60
3	3	231	THR	CA-CB-OG1	-5.36	97.74	109.00
1	1	202	ASP	CB-CA-C	5.35	121.11	110.40
2	2	262	GLN	CA-C-O	-5.35	108.86	120.10
2	2	169	VAL	CB-CA-C	-5.34	101.25	111.40
1	1	64	GLU	CA-CB-CG	5.33	125.12	113.40
1	1	205	SER	O-C-N	5.32	131.22	122.70
2	2	259	ILE	CB-CG1-CD1	-5.31	99.03	113.90
3	3	42	ASN	CB-CG-OD1	-5.30	111.00	121.60
2	2	88	ASP	CA-CB-CG	-5.29	101.77	113.40
1	1	128	TYR	CB-CG-CD2	5.29	124.17	121.00
2	2	143	LYS	CD-CE-NZ	-5.26	99.59	111.70
3	3	116	MET	CB-CG-SD	-5.26	96.63	112.40
1	1	242	ARG	CD-NE-CZ	-5.25	116.25	123.60
3	3	33	ARG	CB-CG-CD	-5.25	97.96	111.60
3	3	78	GLU	CA-CB-CG	5.23	124.91	113.40
2	2	38	TRP	CA-CB-CG	-5.23	103.77	113.70
3	3	74	ASN	OD1-CG-ND2	5.22	133.90	121.90
2	2	170	LEU	CB-CG-CD2	5.21	119.87	111.00
1	1	275	THR	CA-C-O	-5.21	109.17	120.10
3	3	222	MET	CB-CG-SD	-5.20	96.80	112.40
1	1	271	TYR	CB-CG-CD1	-5.20	117.88	121.00
2	2	203	TYR	CD1-CE1-CZ	-5.19	115.13	119.80
1	1	275	THR	CA-C-N	5.19	128.61	117.20
1	1	21	ILE	CA-CB-CG1	-5.18	101.15	111.00
2	2	219	SER	N-CA-CB	5.18	118.28	110.50
4	4	48	ASP	CA-CB-CG	-5.18	102.00	113.40
2	2	11	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	1	282	ARG	CG-CD-NE	-5.17	100.95	111.80
2	2	14	GLN	OE1-CD-NE2	5.17	133.78	121.90
4	4	36	ALA	C-N-CA	-5.16	108.80	121.70
1	1	219	ASN	O-C-N	5.16	130.95	122.70
1	1	164	ASP	CB-CG-OD1	5.15	122.94	118.30
1	1	50	SER	CA-C-N	5.14	128.52	117.20
2	2	52	LYS	CA-C-N	5.14	128.51	117.20
4	4	31	TYR	CG-CD2-CE2	-5.13	117.20	121.30
2	2	14	GLN	CA-CB-CG	-5.11	102.15	113.40
4	4	58	ASP	O-C-N	5.11	130.88	122.70
1	1	141	ASN	CA-CB-CG	-5.11	102.15	113.40
2	2	203	TYR	CG-CD1-CE1	5.10	125.38	121.30
2	2	221	MET	CA-CB-CG	-5.10	104.63	113.30
1	1	274	ASN	CA-C-N	-5.08	106.03	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	18	LEU	CB-CA-C	5.07	119.84	110.20
3	3	144	GLU	CA-CB-CG	5.07	124.54	113.40
4	4	39	SER	O-C-N	5.07	130.80	122.70
3	3	175	TYR	N-CA-CB	-5.06	101.49	110.60
3	3	141	ASP	CB-CG-OD2	5.06	122.85	118.30
1	1	270	ASN	CB-CA-C	-5.05	100.29	110.40
3	3	86	PHE	CB-CA-C	5.05	120.49	110.40
1	1	282	ARG	CB-CA-C	-5.04	100.31	110.40
1	1	17	THR	CA-CB-CG2	-5.04	105.34	112.40
2	2	170	LEU	CB-CA-C	5.04	119.77	110.20
3	3	172	GLN	CG-CD-NE2	5.03	128.77	116.70
1	1	121	TYR	CB-CG-CD2	5.03	124.02	121.00
3	3	224	ASP	CB-CG-OD1	5.02	122.82	118.30
3	3	146	MET	CB-CA-C	5.02	120.43	110.40
3	3	178	PRO	O-C-N	5.01	130.72	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2170	0	2106	180	0
2	2	1952	0	1926	125	0
3	3	1849	0	1831	152	0
4	4	297	0	294	36	0
5	1	27	0	30	6	0
6	1	4	0	0	2	0
All	All	6299	0	6187	412	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (412) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:57:ASN:CB	3:3:57:ASN:CA	1.75	1.58
4:4:33:LYS:CE	4:4:33:LYS:NZ	1.67	1.55
2:2:52:LYS:NZ	2:2:52:LYS:CE	1.68	1.54
1:1:285:ASP:CB	1:1:285:ASP:CA	1.79	1.54
2:2:158:SER:OG	2:2:167:LYS:HE2	1.46	1.14
3:3:21:SER:O	4:4:37:SER:HB2	1.54	1.07
1:1:285:ASP:CA	1:1:285:ASP:OD2	2.00	1.07
1:1:258:PRO:HG2	3:3:99:GLU:HG2	1.36	1.06
1:1:47:PRO:HA	3:3:164:THR:HG21	1.34	1.05
2:2:12:ARG:NH1	2:2:12:ARG:HG3	1.69	1.05
1:1:215:ILE:HD11	1:1:219:ASN:ND2	1.71	1.04
2:2:255:ARG:HG2	2:2:256:SER:H	1.24	1.03
1:1:282:ARG:HG3	3:3:57:ASN:HB3	1.41	1.02
2:2:136:GLU:HB3	2:2:140:VAL:HG21	1.44	0.97
3:3:57:ASN:CB	3:3:57:ASN:N	2.28	0.97
1:1:215:ILE:HD11	1:1:219:ASN:HD22	1.30	0.95
1:1:58:MET:HE1	3:3:216:ASP:HA	1.49	0.95
1:1:83:GLN:HG3	1:1:85:LYS:HE2	1.47	0.94
1:1:152:TYR:O	1:1:154:PRO:HD2	1.67	0.93
2:2:41:TYR:CE2	2:2:55:LYS:HD3	2.05	0.92
3:3:57:ASN:CB	3:3:57:ASN:C	2.37	0.92
1:1:285:ASP:CB	1:1:285:ASP:N	2.34	0.91
1:1:285:ASP:CA	1:1:285:ASP:CG	2.37	0.91
2:2:235:THR:HG23	2:2:236:PRO:HD2	1.53	0.91
2:2:12:ARG:HG3	2:2:12:ARG:HH11	1.27	0.91
1:1:28:THR:HB	1:1:30:LYS:H	1.35	0.90
2:2:11:ASP:HB2	4:4:68:ASN:OD1	1.71	0.90
1:1:285:ASP:CB	1:1:285:ASP:C	2.40	0.89
1:1:285:ASP:OD2	1:1:285:ASP:HA	1.73	0.88
3:3:198:PRO:HD2	3:3:201:THR:HG21	1.55	0.88
2:2:20:ASN:ND2	2:2:62:ARG:HE	1.72	0.87
1:1:47:PRO:HA	3:3:164:THR:CG2	2.03	0.87
2:2:195:ASN:ND2	2:2:196:THR:HG23	1.91	0.86
2:2:12:ARG:HH11	2:2:12:ARG:CG	1.89	0.85
2:2:116:LYS:HB3	3:3:121:ALA:HB3	1.57	0.85
1:1:90:ILE:HD13	1:1:90:ILE:N	1.92	0.84
3:3:57:ASN:CA	3:3:57:ASN:CG	2.45	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:188:VAL:HG11	5:1:900:W59:H3C1	1.57	0.84
1:1:282:ARG:HD2	1:1:285:ASP:O	1.78	0.84
2:2:158:SER:OG	2:2:167:LYS:CE	2.27	0.82
2:2:10:SER:OG	2:2:12:ARG:HB2	1.78	0.82
2:2:30:ASN:HD22	2:2:31:ALA:H	1.27	0.82
2:2:52:LYS:NZ	2:2:52:LYS:CD	2.43	0.82
1:1:248:LYS:HE3	4:4:38:THR:O	1.80	0.82
2:2:136:GLU:CB	2:2:140:VAL:HG21	2.09	0.82
3:3:175:TYR:HB2	3:3:182:THR:HG21	1.60	0.81
4:4:59:LEU:HD21	4:4:61:LEU:HD13	1.61	0.81
2:2:9:TYR:HD1	2:2:9:TYR:N	1.77	0.80
1:1:58:MET:CE	3:3:216:ASP:HA	2.11	0.80
1:1:220:HIS:C	1:1:221:MET:HG2	2.03	0.79
1:1:110:VAL:HG22	3:3:230:GLN:OE1	1.81	0.79
4:4:68:ASN:OD1	4:4:68:ASN:N	2.11	0.79
2:2:195:ASN:HD22	2:2:196:THR:HG23	1.48	0.79
2:2:9:TYR:N	2:2:9:TYR:CD1	2.43	0.79
1:1:58:MET:HE1	3:3:216:ASP:CA	2.13	0.78
1:1:208:ASP:HB3	1:1:211:THR:CG2	2.13	0.77
1:1:282:ARG:HG3	3:3:57:ASN:CB	2.15	0.77
2:2:255:ARG:HG2	2:2:256:SER:N	2.00	0.77
3:3:79:GLN:HB2	3:3:190:TRP:CZ3	2.19	0.76
1:1:94:ARG:NH1	1:1:94:ARG:HG2	2.00	0.76
1:1:77:VAL:O	1:1:109:LEU:HD12	1.87	0.75
1:1:270:ASN:HA	2:2:133:ALA:HB1	1.68	0.75
1:1:208:ASP:HB3	1:1:211:THR:HG22	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	0.73
1:1:152:TYR:O	1:1:154:PRO:CD	2.36	0.73
3:3:26:PRO:O	3:3:27:ASN:HB2	1.89	0.73
2:2:188:PHE:O	2:2:194:ASN:ND2	2.22	0.73
1:1:282:ARG:CG	3:3:57:ASN:HB3	2.18	0.73
2:2:262:GLN:HE21	2:2:262:GLN:C	1.91	0.73
1:1:92:ASN:OD1	1:1:95:GLU:HB2	1.87	0.73
1:1:107:SER:CB	6:1:502:HOH:O	2.36	0.72
1:1:198:ASN:O	1:1:215:ILE:HD11	1.89	0.72
1:1:47:PRO:CA	3:3:164:THR:HG21	2.15	0.72
1:1:258:PRO:CG	3:3:99:GLU:HG2	2.16	0.71
2:2:53:THR:HG22	2:2:252:SER:HB2	1.71	0.71
2:2:20:ASN:HD21	2:2:62:ARG:HE	1.39	0.71
4:4:33:LYS:NZ	4:4:33:LYS:CD	2.52	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:19:ALA:HB2	1:1:58:MET:HG2	1.72	0.71
2:2:230:VAL:CG2	2:2:234:ALA:HB3	2.20	0.71
3:3:57:ASN:CA	3:3:57:ASN:OD1	2.38	0.70
2:2:174:ASN:C	2:2:174:ASN:HD22	1.93	0.70
1:1:104:ILE:HG13	1:1:223:SER:HA	1.74	0.70
2:2:235:THR:CG2	2:2:236:PRO:HD2	2.21	0.70
3:3:98:GLY:O	3:3:102:GLN:HG3	1.92	0.69
1:1:77:VAL:C	1:1:109:LEU:HD12	2.12	0.69
2:2:136:GLU:HB3	2:2:140:VAL:CG2	2.21	0.69
2:2:230:VAL:HG23	2:2:234:ALA:HB3	1.74	0.69
1:1:89:GLY:C	1:1:90:ILE:HD13	2.13	0.68
4:4:29:ILE:HG22	4:4:29:ILE:O	1.94	0.68
3:3:20:GLN:HE22	4:4:31:TYR:H	1.42	0.68
1:1:83:GLN:CG	1:1:85:LYS:HE2	2.24	0.67
1:1:188:VAL:HG21	5:1:900:W59:H3C1	1.75	0.67
1:1:278:VAL:HG12	3:3:62:ASP:OD1	1.95	0.67
2:2:84:ASP:OD1	2:2:87:LYS:HE2	1.94	0.67
3:3:61:LYS:HD3	3:3:63:GLU:OE1	1.95	0.67
1:1:101:ASP:OD2	1:1:101:ASP:N	2.25	0.67
2:2:195:ASN:HD22	2:2:195:ASN:C	1.99	0.66
1:1:146:LEU:HD13	1:1:228:ILE:HD13	1.77	0.66
3:3:89:ASP:HA	3:3:93:LYS:HD2	1.78	0.66
1:1:198:ASN:O	1:1:215:ILE:CD1	2.43	0.66
3:3:42:ASN:HD22	3:3:44:LEU:H	1.43	0.66
3:3:197:LEU:HB3	3:3:201:THR:HG22	1.77	0.66
1:1:285:ASP:CB	1:1:285:ASP:H	2.09	0.65
2:2:190:ASN:HD21	3:3:118:THR:HA	1.62	0.65
2:2:256:SER:O	2:2:257:LYS:HB3	1.96	0.65
2:2:149:PRO:HG3	2:2:154:ILE:HG13	1.78	0.64
2:2:205:ASN:HD22	2:2:206:SER:H	1.45	0.64
3:3:79:GLN:HB2	3:3:190:TRP:CE3	2.32	0.64
2:2:12:ARG:HH21	3:3:157:LEU:HD21	1.63	0.64
2:2:30:ASN:HD22	2:2:31:ALA:N	1.94	0.64
2:2:23:ILE:HD11	2:2:243:THR:HG21	1.79	0.64
2:2:12:ARG:NH1	4:4:68:ASN:O	2.31	0.64
1:1:60:PHE:CE2	3:3:218:LYS:HB3	2.33	0.64
1:1:205:SER:HB3	1:1:217:VAL:HG21	1.78	0.63
2:2:205:ASN:ND2	2:2:206:SER:H	1.96	0.63
2:2:187:GLN:HE21	2:2:197:ALA:HA	1.63	0.63
1:1:103:LYS:HA	1:1:223:SER:HB3	1.80	0.63
1:1:87:ALA:HA	1:1:90:ILE:HG12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:220:HIS:O	1:1:221:MET:CE	2.47	0.63
2:2:155:ASP:OD2	2:2:155:ASP:C	2.37	0.62
3:3:75:ARG:O	3:3:194:SER:HB2	1.99	0.62
2:2:40:GLU:HG3	2:2:41:TYR:O	2.00	0.62
3:3:179:ASP:HB3	3:3:182:THR:HG22	1.82	0.62
3:3:84:ASN:ND2	3:3:86:PHE:H	1.98	0.62
2:2:13:VAL:O	2:2:14:GLN:HG2	1.99	0.61
1:1:101:ASP:HA	1:1:225:ALA:HA	1.82	0.61
2:2:38:TRP:CZ3	4:4:57:LYS:HD2	2.36	0.61
1:1:205:SER:HB3	1:1:217:VAL:CG2	2.30	0.61
2:2:133:ALA:O	2:2:166:VAL:HG12	2.01	0.61
3:3:57:ASN:ND2	3:3:91:VAL:HG13	2.15	0.61
1:1:187:SER:HB3	3:3:21:SER:CB	2.31	0.61
1:1:188:VAL:HG21	5:1:900:W59:C3C	2.30	0.61
1:1:281:LYS:HD2	3:3:59:HIS:O	2.01	0.61
3:3:55:MET:HG3	3:3:55:MET:O	1.99	0.61
1:1:90:ILE:N	1:1:90:ILE:CD1	2.62	0.61
3:3:175:TYR:H	3:3:182:THR:HG21	1.66	0.60
3:3:56:ASN:HB3	3:3:66:SER:HA	1.83	0.60
3:3:76:GLN:O	3:3:78:GLU:N	2.34	0.60
1:1:265:SER:HB3	1:1:268:ARG:HG2	1.83	0.60
1:1:51:ILE:HD13	3:3:166:PRO:HG3	1.82	0.59
3:3:131:TYR:HB3	3:3:149:THR:HB	1.82	0.59
1:1:58:MET:HE1	3:3:216:ASP:C	2.23	0.59
1:1:215:ILE:CD1	1:1:219:ASN:HD22	2.10	0.59
1:1:102:TRP:O	1:1:104:ILE:N	2.35	0.59
2:2:256:SER:O	2:2:257:LYS:CB	2.50	0.59
1:1:94:ARG:NH1	1:1:94:ARG:CG	2.60	0.59
1:1:152:TYR:CG	1:1:154:PRO:HD3	2.37	0.59
1:1:259:ARG:HD2	1:1:263:TYR:CE2	2.38	0.59
3:3:84:ASN:HD22	3:3:86:PHE:H	1.49	0.59
2:2:30:ASN:HD21	4:4:58:ASP:H	1.51	0.59
1:1:110:VAL:O	1:1:111:GLN:C	2.40	0.58
2:2:11:ASP:H	4:4:68:ASN:CG	2.06	0.58
3:3:180:THR:O	3:3:183:SER:HB3	2.02	0.58
1:1:151:MET:CB	1:1:175:SER:HB2	2.32	0.58
1:1:201:TYR:HD2	1:1:214:GLY:O	1.87	0.57
2:2:177:LEU:HD11	3:3:94:THR:HG21	1.86	0.57
2:2:204:ILE:HG12	3:3:37:PRO:HG2	1.87	0.57
2:2:64:TYR:CD2	2:2:89:MET:HB3	2.39	0.57
1:1:285:ASP:HB3	1:1:287:LYS:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:52:LYS:NZ	2:2:52:LYS:HD3	2.20	0.57
1:1:43:MET:HG3	1:1:44:PRO:HD2	1.87	0.56
3:3:175:TYR:H	3:3:182:THR:CG2	2.19	0.56
1:1:85:LYS:HB3	1:1:236:LYS:HG3	1.87	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
3:3:53:ILE:HD11	3:3:211:ILE:HB	1.87	0.56
1:1:236:LYS:HE3	1:1:238:LEU:HD13	1.88	0.56
2:2:189:ILE:HA	2:2:194:ASN:ND2	2.21	0.55
4:4:43:GLN:O	4:4:45:LEU:HB3	2.05	0.55
1:1:38:GLU:CD	3:3:116:MET:HE1	2.27	0.55
1:1:77:VAL:C	1:1:109:LEU:CD1	2.75	0.55
2:2:77:GLY:O	2:2:156:LEU:HB2	2.07	0.55
2:2:235:THR:HG22	2:2:236:PRO:N	2.22	0.55
2:2:230:VAL:HG23	2:2:231:PRO:O	2.05	0.55
1:1:228:ILE:HD11	1:1:239:VAL:HG21	1.88	0.55
3:3:199:PRO:O	3:3:200:GLU:HB2	2.05	0.55
1:1:215:ILE:CD1	1:1:219:ASN:ND2	2.59	0.55
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.42	0.55
1:1:79:VAL:HG22	1:1:242:ARG:HG2	1.89	0.54
1:1:266:ILE:HD12	3:3:235:THR:HA	1.88	0.54
3:3:31:THR:HG23	3:3:32:PRO:HD2	1.87	0.54
3:3:198:PRO:O	3:3:201:THR:HB	2.07	0.54
4:4:59:LEU:HD21	4:4:61:LEU:CD1	2.34	0.54
2:2:230:VAL:HB	2:2:231:PRO:HD2	1.89	0.54
3:3:20:GLN:HE22	4:4:31:TYR:N	2.04	0.54
2:2:38:TRP:HZ3	4:4:57:LYS:HD2	1.70	0.54
1:1:35:THR:HG23	3:3:160:THR:HB	1.90	0.54
2:2:170:LEU:CD2	3:3:64:VAL:HA	2.38	0.54
3:3:193:THR:O	3:3:194:SER:CB	2.55	0.54
3:3:197:LEU:HB3	3:3:201:THR:HG21	1.87	0.54
3:3:55:MET:HA	3:3:91:VAL:HG11	1.90	0.54
1:1:204:TYR:CE2	1:1:213:TYR:HB2	2.42	0.53
3:3:117:TYR:CD2	3:3:155:ILE:HD13	2.44	0.53
1:1:271:TYR:HB2	1:1:272:PRO:HD2	1.89	0.53
1:1:160:PRO:HB3	1:1:167:THR:OG1	2.08	0.53
2:2:235:THR:CG2	2:2:236:PRO:CD	2.86	0.53
3:3:18:ASP:OD1	4:4:40:SER:HB2	2.09	0.53
3:3:86:PHE:CD1	3:3:178:PRO:HB3	2.44	0.53
2:2:12:ARG:NH2	3:3:157:LEU:HD21	2.24	0.52
3:3:57:ASN:HB3	3:3:57:ASN:C	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:88:THR:O	1:1:90:ILE:HD13	2.10	0.52
1:1:83:GLN:HG3	1:1:85:LYS:CE	2.31	0.52
1:1:88:THR:O	1:1:90:ILE:CD1	2.58	0.52
1:1:105:ASN:ND2	1:1:266:ILE:HD13	2.25	0.52
1:1:276:GLU:HB3	1:1:277:PRO:CD	2.39	0.52
1:1:187:SER:HB3	3:3:21:SER:HB2	1.92	0.52
1:1:236:LYS:NZ	1:1:238:LEU:HD11	2.25	0.52
2:2:174:ASN:C	2:2:174:ASN:ND2	2.63	0.52
3:3:216:ASP:O	3:3:218:LYS:HE3	2.09	0.52
1:1:110:VAL:HG22	3:3:230:GLN:CD	2.31	0.52
1:1:217:VAL:CG2	1:1:217:VAL:O	2.57	0.52
1:1:122:VAL:HG13	1:1:124:PHE:CE2	2.45	0.51
1:1:176:VAL:HG22	5:1:900:W59:H312	1.90	0.51
1:1:236:LYS:HE3	1:1:238:LEU:CD1	2.40	0.51
2:2:177:LEU:CD1	3:3:94:THR:HG21	2.40	0.51
3:3:75:ARG:NH1	3:3:78:GLU:OE1	2.41	0.51
1:1:43:MET:HE3	1:1:43:MET:HA	1.92	0.51
1:1:217:VAL:O	1:1:217:VAL:HG22	2.09	0.51
1:1:273:LYS:O	1:1:274:ASN:O	2.28	0.51
3:3:193:THR:O	3:3:194:SER:HB3	2.08	0.51
3:3:214:CYS:HB3	3:3:215:PRO:HD2	1.92	0.51
1:1:94:ARG:CZ	1:1:101:ASP:OD2	2.58	0.51
2:2:34:CYS:HB2	2:2:202:PRO:CD	2.41	0.51
4:4:44:SER:O	4:4:45:LEU:C	2.48	0.51
1:1:265:SER:HB2	2:2:138:GLY:O	2.11	0.51
3:3:210:PHE:N	3:3:210:PHE:CD1	2.77	0.51
1:1:94:ARG:CG	1:1:94:ARG:HH11	2.24	0.51
3:3:84:ASN:HD22	3:3:86:PHE:N	2.08	0.51
2:2:171:TYR:HA	2:2:176:THR:O	2.11	0.50
1:1:65:THR:HG22	3:3:104:TYR:CZ	2.46	0.50
2:2:139:ASN:N	2:2:139:ASN:OD1	2.44	0.50
2:2:255:ARG:CG	2:2:256:SER:H	2.00	0.50
1:1:58:MET:CE	3:3:216:ASP:O	2.60	0.50
1:1:97:LYS:C	1:1:99:PHE:H	2.13	0.50
1:1:114:LYS:NZ	3:3:99:GLU:OE1	2.44	0.50
1:1:216:THR:CG2	3:3:236:GLU:CG	2.89	0.50
1:1:58:MET:HE1	3:3:216:ASP:O	2.12	0.50
1:1:60:PHE:CD2	3:3:218:LYS:HB3	2.46	0.50
1:1:159:ASN:C	1:1:160:PRO:O	2.46	0.50
2:2:8:GLY:C	2:2:9:TYR:HD1	2.14	0.49
2:2:143:LYS:HG2	2:2:163:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:63:GLU:C	3:3:65:ASN:H	2.14	0.49
1:1:58:MET:O	1:1:59:HIS:HB2	2.13	0.49
2:2:205:ASN:HD22	2:2:206:SER:N	2.09	0.49
1:1:116:LEU:HD13	5:1:900:W59:HM22	1.94	0.49
2:2:19:GLY:HA2	2:2:58:THR:HG22	1.94	0.49
3:3:95:THR:O	3:3:99:GLU:HB2	2.13	0.49
2:2:34:CYS:HB2	2:2:202:PRO:HD2	1.94	0.49
3:3:20:GLN:NE2	4:4:31:TYR:H	2.11	0.49
1:1:273:LYS:O	1:1:274:ASN:C	2.52	0.49
2:2:30:ASN:ND2	2:2:31:ALA:H	2.05	0.48
1:1:220:HIS:O	1:1:221:MET:HE2	2.12	0.48
3:3:54:PRO:O	3:3:91:VAL:HG12	2.12	0.48
3:3:125:ALA:HB3	3:3:155:ILE:HD12	1.95	0.48
4:4:59:LEU:HG	4:4:60:MET:N	2.27	0.48
3:3:129:LEU:O	3:3:150:HIS:HA	2.13	0.48
1:1:105:ASN:OD1	1:1:105:ASN:C	2.51	0.48
1:1:153:VAL:C	1:1:154:PRO:O	2.49	0.48
2:2:10:SER:CB	4:4:68:ASN:OXT	2.61	0.48
2:2:170:LEU:HD21	3:3:64:VAL:HA	1.94	0.48
1:1:280:LYS:HE3	3:3:89:ASP:OD2	2.13	0.48
2:2:135:HIS:CD2	2:2:160:ASN:HB3	2.49	0.48
3:3:115:LEU:HD22	3:3:129:LEU:HD21	1.96	0.48
1:1:122:VAL:O	1:1:197:TYR:HB2	2.13	0.48
1:1:220:HIS:C	1:1:221:MET:CG	2.79	0.48
3:3:61:LYS:O	3:3:61:LYS:HG2	2.07	0.48
3:3:190:TRP:CD1	3:3:190:TRP:N	2.81	0.48
3:3:112:ARG:NH1	3:3:112:ARG:HG2	2.28	0.48
1:1:134:ALA:HB2	1:1:180:VAL:HG11	1.96	0.48
1:1:204:TYR:HE2	1:1:213:TYR:HB2	1.79	0.48
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.79	0.48
1:1:87:ALA:CA	1:1:90:ILE:HG12	2.44	0.47
3:3:112:ARG:HD3	3:3:162:VAL:CG1	2.43	0.47
1:1:165:ASP:HB3	1:1:167:THR:H	1.79	0.47
1:1:201:TYR:CG	1:1:218:LEU:HD22	2.49	0.47
4:4:29:ILE:O	4:4:29:ILE:CG2	2.62	0.47
1:1:83:GLN:OE1	1:1:236:LYS:HD2	2.15	0.47
1:1:268:ARG:CZ	2:2:139:ASN:HB2	2.44	0.47
2:2:13:VAL:HA	2:2:25:THR:O	2.14	0.47
2:2:177:LEU:CD1	3:3:94:THR:CG2	2.93	0.47
1:1:206:HIS:ND1	1:1:206:HIS:N	2.62	0.47
2:2:63:PHE:CD2	2:2:245:ALA:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:44:SER:C	4:4:46:SER:N	2.68	0.47
2:2:195:ASN:ND2	2:2:195:ASN:C	2.66	0.47
1:1:268:ARG:HH11	1:1:268:ARG:HD3	1.50	0.47
1:1:101:ASP:HB3	1:1:225:ALA:HB2	1.97	0.46
1:1:129:THR:OG1	1:1:185:ARG:NH1	2.43	0.46
3:3:84:ASN:ND2	3:3:84:ASN:C	2.69	0.46
2:2:130:HIS:ND1	2:2:219:SER:OG	2.47	0.46
1:1:74:ALA:HB3	3:3:15:THR:HB	1.97	0.46
1:1:92:ASN:C	1:1:92:ASN:ND2	2.67	0.46
1:1:216:THR:HG21	3:3:236:GLU:HG2	1.97	0.46
2:2:170:LEU:HD23	3:3:64:VAL:CG2	2.45	0.46
4:4:61:LEU:HD12	4:4:61:LEU:HA	1.62	0.46
2:2:156:LEU:HD11	2:2:173:MET:SD	2.56	0.46
1:1:92:ASN:CG	1:1:95:GLU:HB2	2.36	0.46
1:1:236:LYS:HE2	1:1:236:LYS:HB3	1.83	0.46
3:3:101:VAL:HG22	3:3:219:LEU:HD11	1.98	0.46
3:3:55:MET:CE	3:3:91:VAL:HG21	2.46	0.46
1:1:151:MET:HB3	1:1:175:SER:HB2	1.98	0.45
2:2:148:HIS:N	2:2:149:PRO:CD	2.79	0.45
2:2:158:SER:HG	2:2:167:LYS:CE	2.27	0.45
3:3:57:ASN:CB	3:3:57:ASN:H	2.26	0.45
2:2:190:ASN:H	2:2:194:ASN:CB	2.30	0.45
2:2:228:LEU:CD1	2:2:238:LEU:HD22	2.47	0.45
4:4:30:ASN:HA	4:4:30:ASN:HD22	1.40	0.45
1:1:31:VAL:HG11	1:1:34:LEU:HD12	1.98	0.45
2:2:187:GLN:NE2	2:2:198:THR:H	2.14	0.45
3:3:50:ASP:HA	3:3:212:SER:HB3	1.97	0.45
2:2:170:LEU:HD23	3:3:64:VAL:HG22	1.99	0.45
1:1:159:ASN:O	1:1:160:PRO:C	2.52	0.45
3:3:84:ASN:HD22	3:3:84:ASN:C	2.20	0.45
1:1:64:GLU:O	1:1:64:GLU:HG2	2.17	0.45
1:1:107:SER:HB3	6:1:502:HOH:O	2.11	0.45
1:1:216:THR:CG2	3:3:236:GLU:HG2	2.46	0.45
2:2:91:VAL:HG12	2:2:95:ASN:HD22	1.82	0.45
1:1:28:THR:HG22	1:1:29:GLN:H	1.81	0.45
1:1:105:ASN:HD21	1:1:266:ILE:CD1	2.29	0.45
2:2:13:VAL:C	2:2:14:GLN:CG	2.85	0.45
2:2:37:GLU:CD	3:3:35:HIS:HE2	2.19	0.45
2:2:190:ASN:H	2:2:194:ASN:HB3	1.82	0.45
2:2:235:THR:CG2	2:2:236:PRO:N	2.79	0.45
3:3:192:GLN:HE21	3:3:192:GLN:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:285:ASP:HB3	1:1:288:SER:H	1.82	0.44
2:2:259:ILE:HG21	2:2:259:ILE:HD13	1.74	0.44
1:1:43:MET:HA	1:1:43:MET:CE	2.46	0.44
1:1:198:ASN:HB3	1:1:200:PHE:O	2.17	0.44
1:1:207:ASP:HA	2:2:144:TYR:CE1	2.52	0.44
1:1:268:ARG:NH1	3:3:236:GLU:O	2.46	0.44
3:3:57:ASN:N	3:3:57:ASN:HB2	2.25	0.44
3:3:61:LYS:O	3:3:63:GLU:HG3	2.17	0.44
1:1:289:TYR:CE1	3:3:138:GLY:HA3	2.53	0.44
3:3:116:MET:HG3	3:3:159:SER:OG	2.17	0.44
4:4:43:GLN:O	4:4:45:LEU:CB	2.65	0.44
4:4:59:LEU:CD2	4:4:61:LEU:HD13	2.41	0.44
3:3:197:LEU:HD21	3:3:205:VAL:HG11	1.99	0.44
3:3:55:MET:HE2	3:3:91:VAL:HG21	1.99	0.44
3:3:181:TYR:CD1	3:3:181:TYR:C	2.91	0.44
1:1:282:ARG:CG	3:3:57:ASN:CB	2.89	0.44
2:2:146:PHE:CG	2:2:164:GLY:HA2	2.52	0.44
1:1:289:TYR:CD1	3:3:138:GLY:HA3	2.53	0.44
4:4:43:GLN:HG3	4:4:45:LEU:H	1.82	0.44
1:1:47:PRO:HB3	3:3:166:PRO:HB3	1.99	0.43
1:1:87:ALA:HB2	1:1:98:LEU:CD1	2.48	0.43
1:1:286:ILE:HG23	3:3:81:PHE:HA	2.00	0.43
3:3:208:LEU:HA	3:3:208:LEU:HD12	1.73	0.43
1:1:132:ALA:O	1:1:181:GLY:N	2.41	0.43
1:1:110:VAL:O	1:1:113:ARG:N	2.51	0.43
2:2:262:GLN:C	2:2:262:GLN:NE2	2.66	0.43
3:3:57:ASN:HD21	3:3:91:VAL:HG13	1.84	0.43
1:1:97:LYS:C	1:1:99:PHE:N	2.71	0.43
3:3:179:ASP:HB3	3:3:182:THR:CG2	2.48	0.43
2:2:91:VAL:HG12	2:2:95:ASN:ND2	2.34	0.43
3:3:61:LYS:HG2	3:3:63:GLU:HG3	2.00	0.43
2:2:10:SER:CB	2:2:12:ARG:HB2	2.48	0.43
3:3:112:ARG:HG2	3:3:112:ARG:HH11	1.83	0.43
2:2:70:THR:HG22	2:2:72:THR:HG22	2.01	0.43
3:3:151:VAL:HG11	3:3:161:ILE:HD11	2.01	0.43
1:1:188:VAL:CG1	5:1:900:W59:H3C1	2.39	0.43
2:2:95:ASN:HB3	2:2:251:PHE:CE2	2.53	0.43
2:2:205:ASN:ND2	2:2:206:SER:N	2.66	0.43
3:3:195:LEU:C	3:3:196:ILE:HG12	2.40	0.43
1:1:78:HIS:HA	1:1:109:LEU:HD11	2.01	0.42
2:2:13:VAL:C	2:2:14:GLN:HG2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:149:GLN:O	1:1:149:GLN:HG2	2.18	0.42
1:1:87:ALA:HB2	1:1:98:LEU:HD11	2.02	0.42
1:1:187:SER:HB3	3:3:21:SER:HB3	2.01	0.42
1:1:206:HIS:NE2	1:1:208:ASP:HB2	2.34	0.42
2:2:10:SER:OG	4:4:68:ASN:OXT	2.35	0.42
3:3:174:ARG:HD2	3:3:182:THR:O	2.19	0.42
1:1:216:THR:HG22	3:3:236:GLU:CD	2.40	0.42
2:2:122:LEU:HD23	2:2:224:PRO:HA	2.02	0.42
2:2:225:ILE:O	3:3:68:LEU:HD21	2.19	0.42
3:3:226:GLN:HE21	3:3:226:GLN:HB2	1.21	0.42
4:4:43:GLN:O	4:4:44:SER:C	2.58	0.42
1:1:98:LEU:HD23	1:1:98:LEU:HA	1.80	0.42
2:2:40:GLU:O	2:2:40:GLU:CG	2.61	0.42
2:2:228:LEU:HD11	2:2:238:LEU:HD22	2.02	0.42
1:1:93:HIS:CE1	1:1:163:TRP:HD1	2.38	0.42
1:1:152:TYR:CD1	1:1:154:PRO:HD3	2.53	0.42
1:1:201:TYR:H	2:2:131:GLN:HE21	1.68	0.42
1:1:285:ASP:HB3	1:1:288:SER:N	2.34	0.42
3:3:44:LEU:HA	3:3:44:LEU:HD23	1.79	0.42
1:1:289:TYR:CZ	3:3:139:PRO:HD2	2.55	0.42
4:4:43:GLN:HG2	4:4:43:GLN:O	2.18	0.42
1:1:261:LEU:HD11	2:2:171:TYR:CD1	2.55	0.41
1:1:286:ILE:HD13	1:1:286:ILE:HG21	1.77	0.41
2:2:69:LYS:O	2:2:239:PRO:HA	2.20	0.41
3:3:47:ILE:HG21	3:3:47:ILE:HD13	1.51	0.41
3:3:113:PHE:CE1	3:3:115:LEU:HD13	2.55	0.41
1:1:86:ASP:OD2	1:1:88:THR:HB	2.21	0.41
2:2:235:THR:HG22	2:2:237:SER:N	2.35	0.41
3:3:167:TRP:HZ2	3:3:172:GLN:HA	1.86	0.41
2:2:43:PRO:HG2	2:2:46:ASP:HB2	2.02	0.41
3:3:18:ASP:CG	4:4:40:SER:HB2	2.41	0.41
3:3:137:ARG:HH11	3:3:137:ARG:HD3	1.22	0.41
1:1:38:GLU:CD	3:3:116:MET:CE	2.88	0.41
1:1:146:LEU:HA	1:1:230:ASN:OD1	2.20	0.41
1:1:165:ASP:CB	1:1:167:THR:OG1	2.69	0.41
1:1:54:ARG:HH11	1:1:54:ARG:HD2	1.55	0.41
2:2:84:ASP:HB2	2:2:216:ASN:HD21	1.86	0.41
3:3:64:VAL:HG12	3:3:64:VAL:O	2.21	0.41
1:1:78:HIS:NE2	1:1:80:THR:HB	2.36	0.41
3:3:157:LEU:HD23	3:3:157:LEU:O	2.21	0.41
3:3:175:TYR:CB	3:3:182:THR:HG21	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:13:VAL:HG22	2:2:26:GLN:HA	2.03	0.40
3:3:214:CYS:HB3	3:3:215:PRO:CD	2.51	0.40
3:3:20:GLN:NE2	4:4:30:ASN:HA	2.36	0.40
1:1:208:ASP:HB3	1:1:211:THR:HB	2.04	0.40
1:1:265:SER:OG	2:2:139:ASN:HB3	2.21	0.40
3:3:101:VAL:HG13	3:3:176:THR:HB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	271/289 (94%)	242 (89%)	21 (8%)	8 (3%)	4 24
2	2	253/262 (97%)	233 (92%)	18 (7%)	2 (1%)	19 57
3	3	234/236 (99%)	217 (93%)	15 (6%)	2 (1%)	17 55
4	4	38/68 (56%)	34 (90%)	3 (8%)	1 (3%)	5 27
All	All	796/855 (93%)	726 (91%)	57 (7%)	13 (2%)	9 40

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	139	SER
3	3	57	ASN
3	3	77	ASN
1	1	108	SER
1	1	165	ASP
1	1	221	MET
2	2	255	ARG
2	2	257	LYS
1	1	216	THR

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Mol	Chain	Res	Type
1	1	153	VAL
4	4	47	MET
1	1	104	ILE
1	1	154	PRO

5.3.2 Protein sidechains (i)

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%)	195 (82%)	44 (18%)	1	9
2	2	223/229 (97%)	179 (80%)	44 (20%)	1	7
3	3	209/209 (100%)	171 (82%)	38 (18%)	1	9
4	4	33/57 (58%)	20 (61%)	13 (39%)	0	0
All	All	704/748 (94%)	565 (80%)	139 (20%)	1	7

All (139) 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	100	ASN
1	1	105	ASN
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	187	SER
1	1	202	ASP
1	1	216	THR
1	1	217	VAL
1	1	221	MET
1	1	240	LYS
1	1	256	ARG
1	1	268	ARG
1	1	274	ASN
1	1	278	VAL
1	1	285	ASP
1	1	287	LYS
2	2	11	ASP
2	2	12	ARG
2	2	20	ASN
2	2	26	GLN
2	2	30	ASN
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

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Mol	Chain	Res	Type
2	2	116	LYS
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	205	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	56	ASN
3	3	60	THR
3	3	61	LYS
3	3	65	ASN
3	3	84	ASN
3	3	91	VAL
3	3	94	THR
3	3	101	VAL
3	3	112	ARG

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Mol	Chain	Res	Type
3	3	114	SER
3	3	115	LEU
3	3	137	ARG
3	3	146	MET
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	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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	ASN
1	1	92	ASN
1	1	100	ASN
1	1	136	GLN
1	1	173	ASN
1	1	198	ASN
1	1	219	ASN
2	2	15	GLN
2	2	20	ASN
2	2	30	ASN
2	2	131	GLN
2	2	174	ASN
2	2	187	GLN
2	2	190	ASN
2	2	195	ASN
2	2	205	ASN
2	2	216	ASN
2	2	217	ASN
2	2	262	GLN
3	3	20	GLN
3	3	41	HIS
3	3	42	ASN
3	3	56	ASN
3	3	84	ASN
3	3	102	GLN
3	3	140	GLN
3	3	192	GLN
3	3	226	GLN
4	4	30	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	W59	1	900	-	26,29,29	2.94	5 (19%)	32,37,37	2.85	8 (25%)

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	W59	1	900	-	-	9/16/26/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	900	W59	C2A-N3A	11.08	1.43	1.27
5	1	900	W59	C4A-N3A	-8.02	1.36	1.48
5	1	900	W59	O1A-C5A	-3.84	1.38	1.45
5	1	900	W59	C4-C5	-3.54	1.34	1.39
5	1	900	W59	O1A-C2A	-2.15	1.32	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	1	900	W59	O1A-C2A-N3A	-9.02	108.81	118.17
5	1	900	W59	CM1-C4A-N3A	7.63	132.39	111.61
5	1	900	W59	O1A-C5A-C4A	6.79	112.24	104.43
5	1	900	W59	O1A-C2A-C4B	5.91	123.67	115.85
5	1	900	W59	C5A-C4A-N3A	-2.97	98.49	103.55
5	1	900	W59	C4A-N3A-C2A	2.77	113.67	107.31
5	1	900	W59	C1C-C5-C4	2.67	135.51	128.60
5	1	900	W59	CM1-C4A-C5A	-2.20	102.93	114.12

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1	900	W59	C2C-C1C-C5-C4
5	1	900	W59	C5-C1C-C2C-C3C
5	1	900	W59	C1C-C2C-C3C-C4C
5	1	900	W59	C3C-C4C-C5C-C6C
5	1	900	W59	C2B-C1B-O1B-C7C
5	1	900	W59	C5C-C6C-C7C-O1B
5	1	900	W59	C6B-C1B-O1B-C7C
5	1	900	W59	C2C-C3C-C4C-C5C
5	1	900	W59	N3A-C4A-CM1-CM2

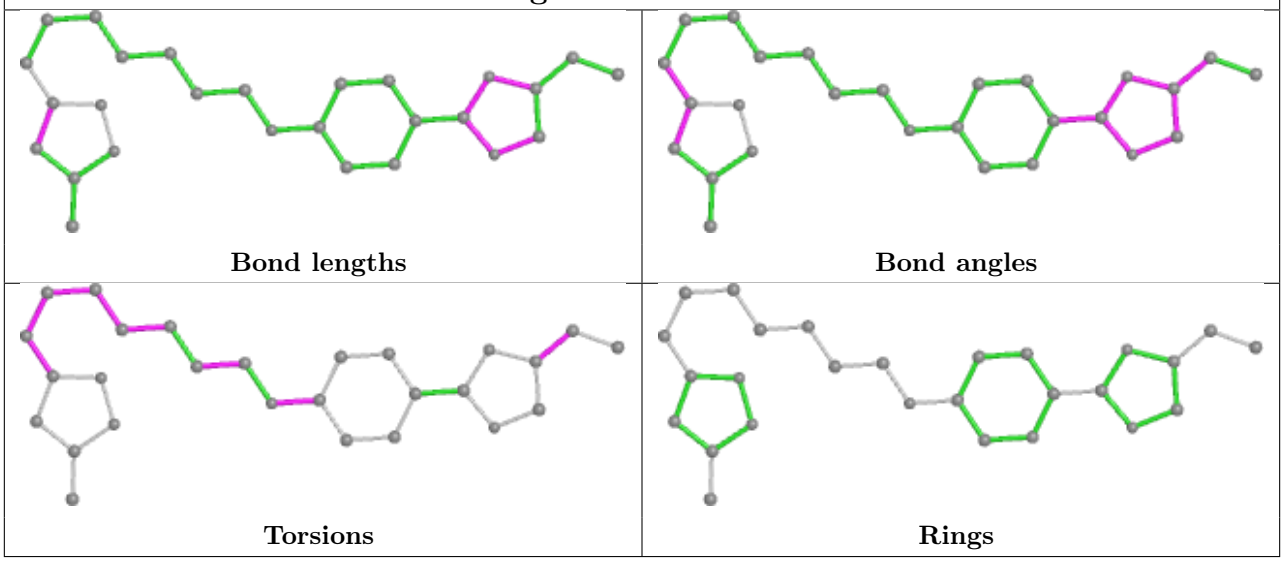
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	900	W59	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand W59 1 900



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

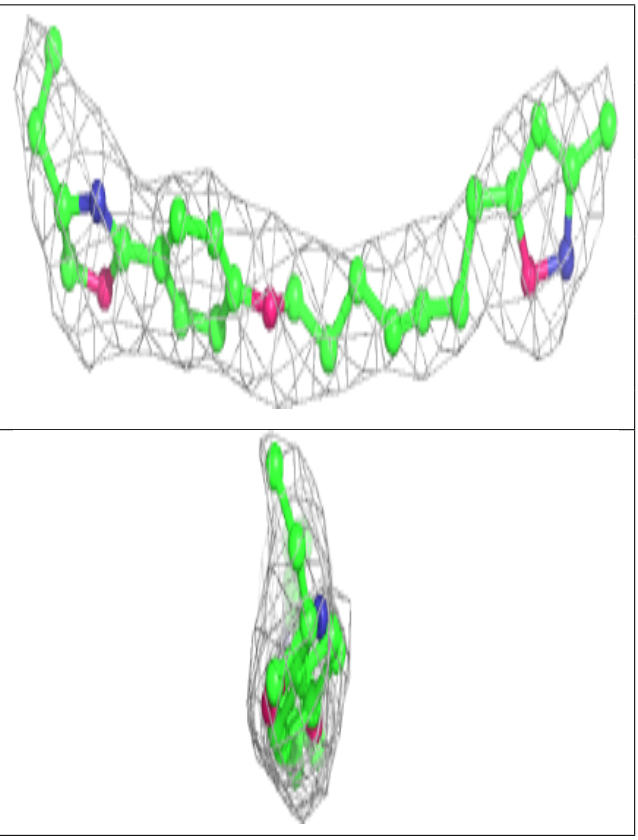
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around W59 1 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.