



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:34 AM UTC

PDB ID : 2ZXC / pdb_00002zxc
Title : Ceramidase complexed with C2
Authors : Okano, H.; Inoue, T.; Okino, N.; Kakuta, Y.; Matsumura, H.; Ito, M.
Deposited on : 2008-12-22
Resolution : 2.20 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

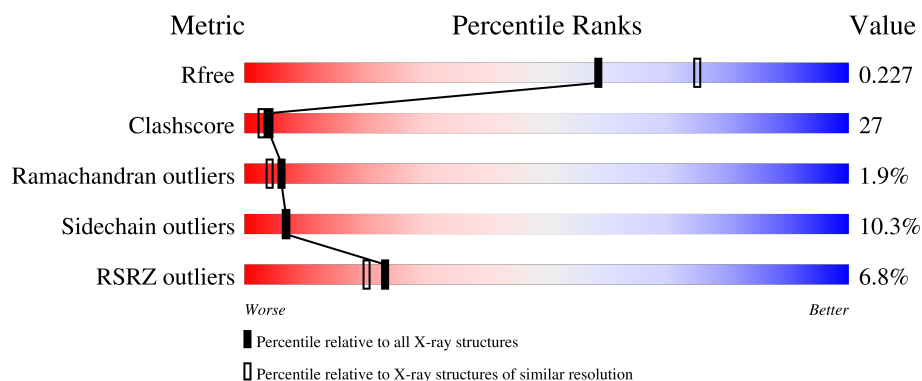
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	646	7% 61% 30% 8%
1	B	646	7% 61% 29% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2ED	A	701	-	-	X	-
3	2ED	B	702	X	-	-	-
6	DMS	B	652	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10943 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 Neutral ceramidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	643	Total	C	N	O	S	0	0	0
			4971	3139	870	946	16			
1	B	643	Total	C	N	O	S	0	0	0
			4971	3139	870	946	16			

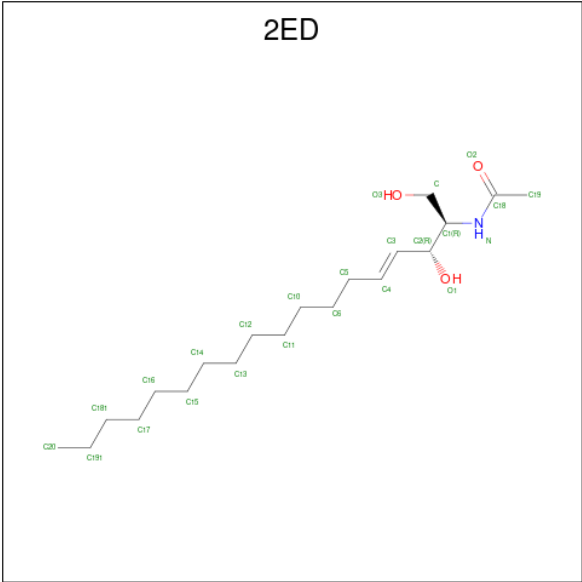
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	SER	ASN	SEE REMARK 999	UNP Q9I596
A	172	ALA	VAL	SEE REMARK 999	UNP Q9I596
A	574	VAL	GLU	SEE REMARK 999	UNP Q9I596
B	157	SER	ASN	SEE REMARK 999	UNP Q9I596
B	172	ALA	VAL	SEE REMARK 999	UNP Q9I596
B	574	VAL	GLU	SEE REMARK 999	UNP Q9I596

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

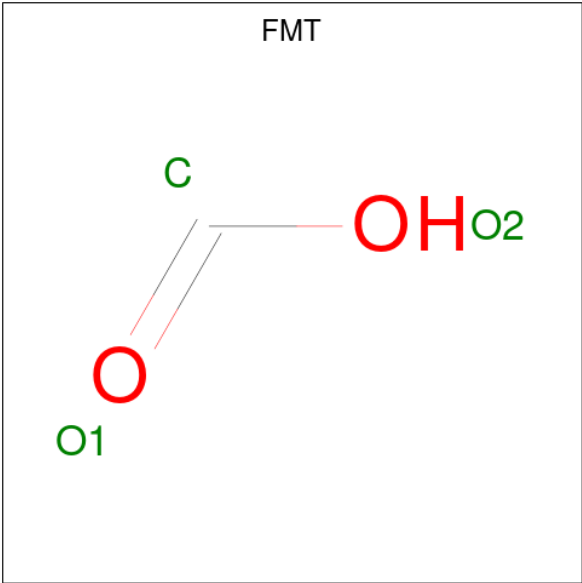
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N-[(1R,2R,3E)-2-hydroxy-1-(hydroxymethyl)heptadec-3-en-1-yl]acetamide (CCD ID: 2ED) (formula: C₂₀H₃₉NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	9	1	3		
3	B	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		

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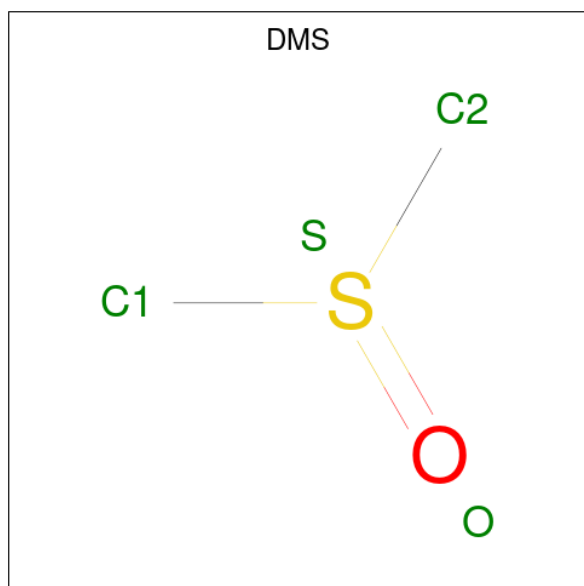
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	S	0	0
			4	2	1	1		

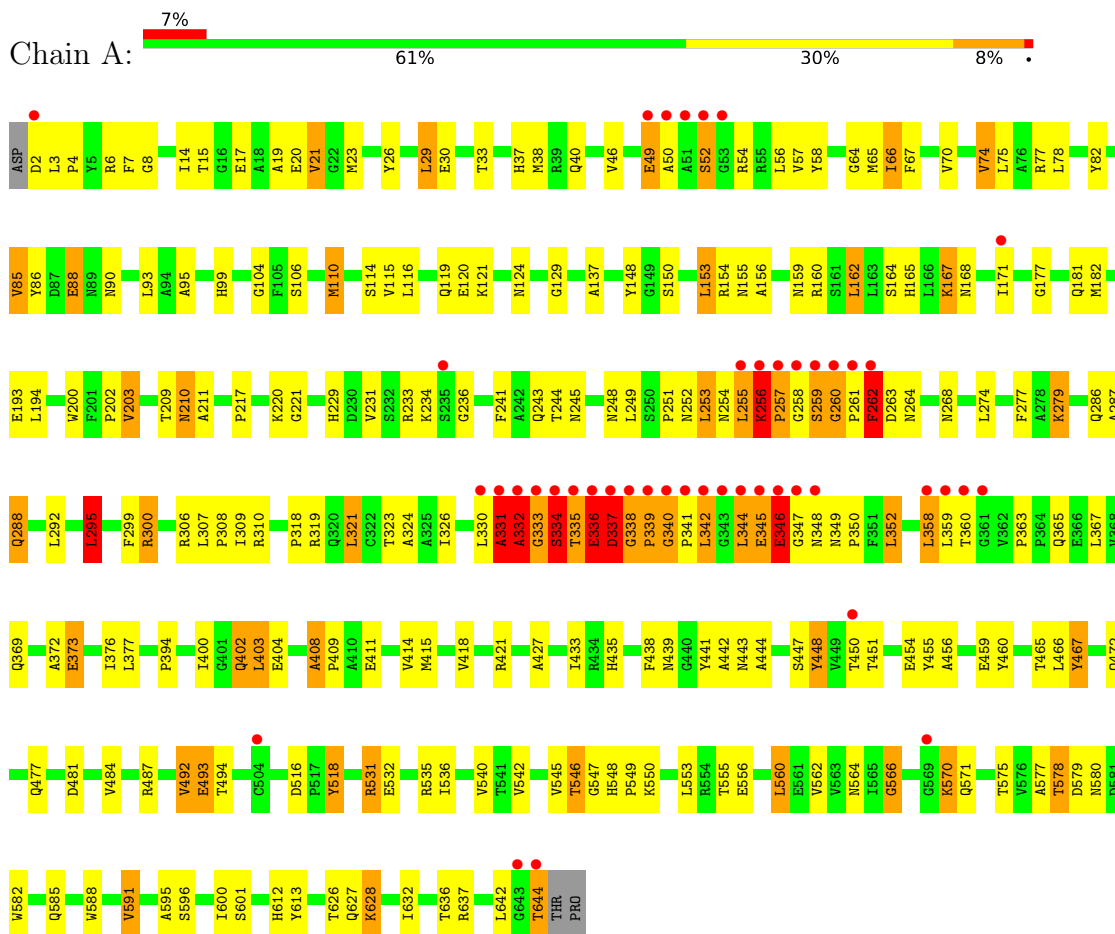
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	474	Total	O	0	0
			474	474		
7	B	465	Total	O	0	0
			465	465		

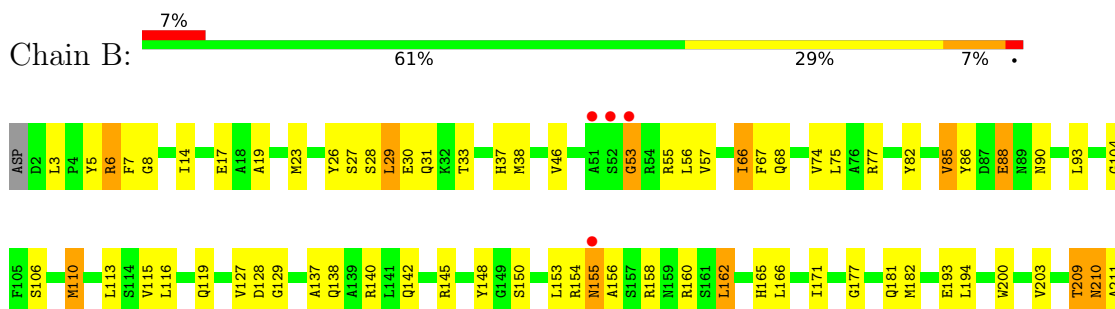
3 Residue-property plots

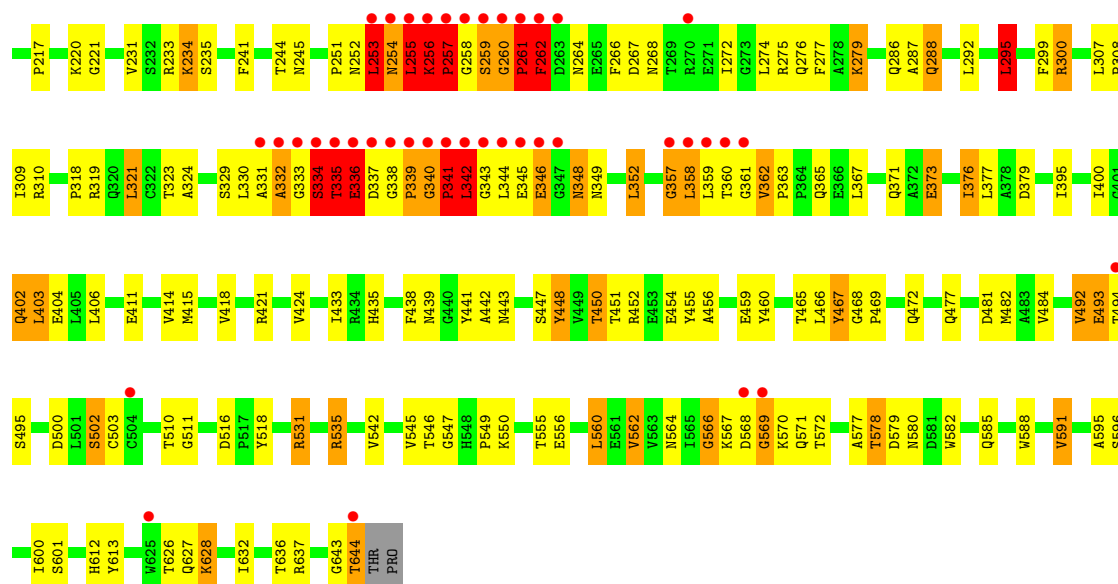
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Neutral ceramidase



• Molecule 1: Neutral ceramidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.74Å 65.80Å 340.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.97 – 2.20 35.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (35.97-2.20) 96.8 (35.97-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 1.97Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.228 0.194 , 0.227	Depositor DCC
R_{free} test set	3781 reflections (3.67%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.430 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10943	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FMT, 2ED, DMS, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	15/5091 (0.3%)	1.20	69/6915 (1.0%)
1	B	0.51	5/5091 (0.1%)	1.32	68/6915 (1.0%)
All	All	0.58	20/10182 (0.2%)	1.26	137/13830 (1.0%)

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	A	0	1
1	B	1	0
All	All	1	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	THR	CA-CB	13.86	1.76	1.53
1	A	262	PHE	N-CA	-10.10	1.33	1.45
1	B	335	THR	N-CA	-9.62	1.33	1.46
1	B	257	PRO	CA-C	-9.41	1.39	1.52
1	A	335	THR	CB-CG2	9.14	1.82	1.52
1	A	335	THR	N-CA	-8.04	1.35	1.46
1	A	337	ASP	CA-CB	7.91	1.66	1.53
1	A	334	SER	CA-C	-7.88	1.42	1.52
1	A	337	ASP	C-O	-7.58	1.14	1.24
1	A	332	ALA	CA-CB	7.03	1.65	1.53
1	A	335	THR	CA-C	6.96	1.62	1.52
1	A	335	THR	C-O	6.53	1.32	1.24
1	A	336	GLU	N-CA	-6.43	1.37	1.46
1	A	335	THR	CB-OG1	5.93	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	334	SER	C-N	-5.85	1.25	1.33
1	A	262	PHE	CA-CB	-5.66	1.45	1.53
1	A	261	PRO	C-O	-5.64	1.15	1.23
1	A	334	SER	CA-CB	-5.34	1.44	1.53
1	B	255	LEU	C-O	5.18	1.30	1.24
1	B	257	PRO	N-CD	-5.05	1.40	1.47

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	335	THR	N-CA-C	29.40	149.27	113.41
1	B	256	LYS	CA-C-N	25.58	151.82	119.84
1	B	256	LYS	C-N-CA	25.58	151.82	119.84
1	B	340	GLY	N-CA-C	13.86	140.62	112.34
1	B	257	PRO	CB-CA-C	13.63	134.06	111.56
1	B	335	THR	N-CA-CB	-13.04	91.43	110.47
1	B	335	THR	CA-C-N	-12.47	101.67	122.11
1	B	335	THR	C-N-CA	-12.47	101.67	122.11
1	A	260	GLY	N-CA-C	-12.45	86.95	112.34
1	B	334	SER	CA-C-N	-12.35	99.98	122.09
1	B	334	SER	C-N-CA	-12.35	99.98	122.09
1	A	331	ALA	N-CA-C	-11.14	87.08	110.80
1	A	333	GLY	CA-C-N	-11.07	100.40	121.54
1	A	333	GLY	C-N-CA	-11.07	100.40	121.54
1	A	334	SER	CA-CB-OG	-10.76	89.59	111.10
1	B	257	PRO	CA-CB-CG	-10.52	84.52	104.50
1	A	334	SER	CA-C-N	-10.50	101.49	121.54
1	A	334	SER	C-N-CA	-10.50	101.49	121.54
1	A	261	PRO	CA-C-N	-10.35	104.53	123.05
1	A	261	PRO	C-N-CA	-10.35	104.53	123.05
1	A	52	SER	N-CA-C	10.15	125.98	113.50
1	A	340	GLY	N-CA-C	9.91	132.56	112.34
1	A	335	THR	N-CA-C	9.64	131.33	110.80
1	B	357	GLY	N-CA-C	8.92	126.89	114.85
1	B	336	GLU	N-CA-CB	8.60	122.62	110.67
1	B	332	ALA	N-CA-C	-8.31	102.24	112.38
1	A	332	ALA	N-CA-C	-8.24	93.25	110.80
1	B	234	LYS	N-CA-C	8.20	122.27	109.07
1	A	339	PRO	N-CA-C	-8.19	99.12	111.57
1	B	342	LEU	N-CA-C	-8.09	103.61	113.97
1	B	569	GLY	N-CA-C	7.97	132.06	113.18
1	B	643	GLY	N-CA-C	-7.84	102.50	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	PRO	CA-N-CD	-7.82	101.06	112.00
1	B	257	PRO	O-C-N	7.79	133.16	122.64
1	A	340	GLY	CA-C-N	7.62	129.37	119.84
1	A	340	GLY	C-N-CA	7.62	129.37	119.84
1	A	337	ASP	N-CA-C	7.62	127.03	110.80
1	A	236	GLY	N-CA-C	-7.35	105.59	115.36
1	A	335	THR	CA-CB-CG2	-7.18	98.29	110.50
1	B	336	GLU	CB-CA-C	6.99	120.81	109.07
1	A	408	ALA	CA-C-N	6.84	128.39	119.84
1	A	408	ALA	C-N-CA	6.84	128.39	119.84
1	A	344	LEU	N-CA-C	-6.78	98.87	109.25
1	B	288	GLN	N-CA-C	6.76	119.22	111.11
1	A	288	GLN	N-CA-C	6.68	119.12	111.11
1	A	20	GLU	N-CA-C	6.62	120.79	111.92
1	A	336	GLU	CA-C-N	6.61	134.16	121.54
1	A	336	GLU	C-N-CA	6.61	134.16	121.54
1	B	467	TYR	N-CA-C	6.60	120.32	112.93
1	B	261	PRO	CA-C-N	6.59	134.12	121.54
1	B	261	PRO	C-N-CA	6.59	134.12	121.54
1	B	637	ARG	N-CA-C	-6.51	102.40	110.41
1	A	545	VAL	N-CA-C	-6.45	100.37	108.89
1	A	466	LEU	N-CA-C	6.44	122.00	111.37
1	A	37	HIS	N-CA-C	-6.44	104.11	112.68
1	A	338	GLY	N-CA-C	6.44	125.47	112.34
1	A	49	GLU	N-CA-C	6.42	119.35	107.99
1	B	341	PRO	N-CA-C	6.40	125.66	112.47
1	B	336	GLU	CA-C-N	-6.40	109.41	121.63
1	B	336	GLU	C-N-CA	-6.40	109.41	121.63
1	A	54	ARG	N-CA-C	-6.39	100.57	110.10
1	B	37	HIS	N-CA-C	-6.39	102.95	111.96
1	B	466	LEU	N-CA-C	6.34	121.84	111.37
1	A	337	ASP	N-CA-CB	6.34	121.20	110.49
1	A	467	TYR	N-CA-C	6.21	119.88	112.93
1	A	342	LEU	CA-CB-CG	-6.15	94.76	116.30
1	A	637	ARG	N-CA-C	-6.15	102.60	110.53
1	B	459	GLU	N-CA-C	-6.14	101.88	110.35
1	B	545	VAL	N-CA-C	-6.11	100.82	108.89
1	B	31	GLN	N-CA-C	6.09	119.66	108.58
1	A	323	THR	N-CA-C	-6.09	102.33	110.55
1	B	566	GLY	N-CA-C	6.07	119.68	112.33
1	B	181	GLN	N-CA-C	6.02	118.99	109.96
1	A	336	GLU	CA-CB-CG	-6.00	102.09	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	TYR	N-CA-C	5.93	119.72	110.17
1	A	295	LEU	N-CA-C	-5.92	99.75	109.40
1	B	343	GLY	N-CA-C	5.90	127.17	113.18
1	A	331	ALA	CA-C-N	5.89	132.80	121.54
1	A	331	ALA	C-N-CA	5.89	132.80	121.54
1	A	459	GLU	N-CA-C	-5.89	102.22	110.35
1	A	264	ASN	N-CA-C	5.86	118.46	108.90
1	A	331	ALA	O-C-N	5.86	130.39	122.59
1	B	448	TYR	N-CA-C	5.86	119.61	110.17
1	A	333	GLY	N-CA-C	-5.84	99.33	113.18
1	A	324	ALA	N-CA-C	5.81	118.44	110.24
1	B	156	ALA	N-CA-C	5.74	119.86	112.41
1	A	263	ASP	N-CA-C	-5.73	106.16	114.12
1	B	253	LEU	N-CA-C	5.72	118.29	111.71
1	A	337	ASP	CA-C-O	-5.69	112.38	120.51
1	B	447	SER	N-CA-C	5.69	116.42	108.00
1	B	468	GLY	CA-C-N	5.66	125.33	119.56
1	B	468	GLY	C-N-CA	5.66	125.33	119.56
1	A	372	ALA	CB-CA-C	-5.64	110.06	116.54
1	A	337	ASP	CA-C-N	-5.62	113.05	121.87
1	A	337	ASP	C-N-CA	-5.62	113.05	121.87
1	A	229	HIS	N-CA-C	5.60	118.23	111.40
1	B	256	LYS	CA-C-O	5.59	127.82	120.16
1	B	3	LEU	CA-C-N	5.58	125.24	119.05
1	B	3	LEU	C-N-CA	5.58	125.24	119.05
1	B	518	TYR	N-CA-C	-5.55	102.80	110.35
1	B	376	ILE	N-CA-C	5.55	116.86	109.37
1	A	447	SER	N-CA-C	5.54	116.19	108.00
1	A	181	GLN	N-CA-C	5.50	118.51	109.76
1	B	260	GLY	CA-C-N	-5.46	113.89	127.00
1	B	260	GLY	C-N-CA	-5.46	113.89	127.00
1	B	324	ALA	N-CA-C	5.45	117.92	110.24
1	B	256	LYS	N-CA-CB	5.42	120.01	110.37
1	B	255	LEU	CA-C-N	5.40	134.97	121.80
1	B	255	LEU	C-N-CA	5.40	134.97	121.80
1	A	377	LEU	N-CA-C	-5.39	106.39	113.12
1	A	332	ALA	N-CA-CB	5.38	119.59	110.49
1	B	254	ASN	N-CA-C	-5.38	99.35	110.80
1	A	376	ILE	N-CA-C	5.35	116.31	109.30
1	A	335	THR	N-CA-CB	-5.34	101.47	110.49
1	B	155	ASN	N-CA-CB	-5.33	102.61	110.49
1	A	518	TYR	N-CA-C	-5.32	103.12	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	ALA	N-CA-C	5.28	116.33	108.31
1	A	566	GLY	N-CA-C	5.27	119.55	112.17
1	A	546	THR	N-CA-C	5.26	115.23	108.34
1	B	209	THR	N-CA-C	5.25	116.70	110.19
1	B	295	LEU	N-CA-C	-5.24	101.15	109.59
1	B	562	VAL	N-CA-C	-5.24	100.34	107.99
1	B	257	PRO	N-CA-CB	-5.24	97.75	103.25
1	B	257	PRO	CA-C-O	5.21	130.09	120.60
1	B	340	GLY	CA-C-N	5.18	126.32	119.84
1	B	340	GLY	C-N-CA	5.18	126.32	119.84
1	B	323	THR	N-CA-C	-5.17	102.83	110.48
1	B	503	CYS	N-CA-C	5.15	116.97	111.36
1	B	90	ASN	N-CA-C	5.15	119.13	111.87
1	B	53	GLY	N-CA-C	-5.14	101.00	113.18
1	A	90	ASN	N-CA-C	5.11	119.07	111.87
1	A	334	SER	N-CA-C	5.10	121.67	110.80
1	B	113	LEU	N-CA-C	5.09	117.23	111.02
1	A	349	ASN	CA-C-N	5.09	124.87	119.28
1	A	349	ASN	C-N-CA	5.09	124.87	119.28
1	A	262	PHE	CB-CA-C	5.01	119.28	110.36
1	A	363	PRO	N-CA-C	-5.01	104.59	110.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	335	THR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	262	PHE	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	A	4971	0	4820	263	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4971	0	4820	267	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	13	0	14	24	0
3	B	13	0	14	13	0
4	A	12	0	4	0	0
4	B	12	0	4	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	8	0	12	6	0
7	A	474	0	0	19	0
7	B	465	0	0	19	0
All	All	10943	0	9688	539	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 27.

All (539) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:THR:CB	1:A:335:THR:CA	1.76	1.60
1:A:335:THR:CB	1:A:335:THR:CG2	1.82	1.58
1:A:334:SER:O	1:A:335:THR:HB	1.23	1.32
1:B:26:TYR:CE2	1:B:337:ASP:HB3	1.68	1.29
1:A:334:SER:O	1:A:335:THR:CB	1.84	1.25
1:A:262:PHE:HB2	1:A:268:ASN:HD21	1.06	1.11
1:A:334:SER:C	1:A:335:THR:CB	2.23	1.11
1:B:256:LYS:HG2	1:B:257:PRO:HD2	1.16	1.10
3:B:702:2ED:H	3:B:702:2ED:O2	1.46	1.09
1:A:536:ILE:H	1:A:644:THR:HG21	1.13	1.09
1:A:334:SER:CB	3:A:701:2ED:H4	1.82	1.08
1:A:262:PHE:HB2	1:A:268:ASN:ND2	1.69	1.07
1:A:256:LYS:CG	1:A:257:PRO:HD3	1.83	1.06
1:B:546:THR:HG22	1:B:547:GLY:H	1.21	1.06
1:A:202:PRO:HG3	1:A:244:THR:OG1	1.57	1.05
1:A:546:THR:HG22	1:A:547:GLY:H	1.22	1.05
1:A:336:GLU:O	1:A:337:ASP:OD1	1.76	1.03
1:B:253:LEU:HB2	1:B:259:SER:O	1.57	1.03
1:A:310:ARG:H	1:A:477:GLN:HE22	1.06	1.01
1:B:256:LYS:CG	1:B:257:PRO:HD2	1.89	1.01
1:B:402:GLN:HE21	1:B:402:GLN:H	1.00	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASN:HB2	1:A:258:GLY:O	1.66	0.96
1:B:55:ARG:HH12	6:B:652:DMS:H11	1.29	0.96
1:B:160:ARG:HH11	1:B:336:GLU:CG	1.78	0.96
1:A:402:GLN:HE21	1:A:402:GLN:N	1.64	0.95
1:B:26:TYR:CE2	1:B:337:ASP:CB	2.49	0.95
1:A:256:LYS:CB	1:A:257:PRO:HD3	1.96	0.95
1:B:310:ARG:H	1:B:477:GLN:HE22	1.09	0.95
1:B:411:GLU:HG2	1:B:441:TYR:CE1	2.02	0.94
1:A:335:THR:H	3:A:701:2ED:C3	1.81	0.94
1:A:402:GLN:H	1:A:402:GLN:NE2	1.67	0.93
3:B:702:2ED:H19A	7:B:678:HOH:O	1.69	0.92
1:B:160:ARG:HH11	1:B:336:GLU:HG2	1.34	0.92
1:A:402:GLN:HE21	1:A:402:GLN:H	0.91	0.91
1:A:334:SER:OG	3:A:701:2ED:H4	1.70	0.91
1:A:334:SER:HB3	3:A:701:2ED:H4	1.52	0.91
1:A:256:LYS:HB3	1:A:257:PRO:CD	2.00	0.90
1:B:27:SER:HB2	1:B:340:GLY:HA2	1.54	0.90
1:A:217:PRO:HB2	1:A:221:GLY:HA3	1.55	0.89
1:A:334:SER:HB3	3:A:701:2ED:C4	2.03	0.88
1:B:256:LYS:HG2	1:B:257:PRO:CD	2.03	0.88
1:A:536:ILE:N	1:A:644:THR:HG21	1.88	0.87
1:B:402:GLN:HE21	1:B:402:GLN:N	1.72	0.87
1:A:411:GLU:HG2	1:A:441:TYR:CE1	2.09	0.86
1:A:335:THR:H	3:A:701:2ED:C4	1.90	0.85
1:B:155:ASN:ND2	1:B:275:ARG:HD3	1.92	0.84
1:B:74:VAL:HG21	1:B:93:LEU:HD11	1.57	0.84
1:A:256:LYS:CB	1:A:257:PRO:CD	2.56	0.83
1:B:262:PHE:HB3	7:B:742:HOH:O	1.79	0.83
1:B:402:GLN:H	1:B:402:GLN:NE2	1.75	0.83
1:A:160:ARG:HH12	3:A:701:2ED:H19B	1.44	0.83
1:A:309:ILE:HD11	1:A:321:LEU:HD13	1.61	0.82
1:A:536:ILE:H	1:A:644:THR:CG2	1.90	0.82
1:A:335:THR:CB	1:A:335:THR:N	2.43	0.82
1:A:310:ARG:H	1:A:477:GLN:NE2	1.76	0.81
1:B:310:ARG:H	1:B:477:GLN:NE2	1.78	0.81
1:A:256:LYS:HG3	1:A:257:PRO:HD3	1.62	0.81
1:B:546:THR:HG22	1:B:547:GLY:N	1.94	0.80
1:A:450:THR:OG1	1:A:454:GLU:HB2	1.80	0.80
1:B:345:GLU:H	1:B:345:GLU:CD	1.88	0.80
1:B:259:SER:OG	1:B:268:ASN:HB3	1.81	0.80
1:A:110:MET:SD	1:A:342:LEU:HD13	2.22	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ASN:HD22	1:B:267:ASP:H	1.30	0.79
1:A:326:ILE:HD11	7:A:785:HOH:O	1.84	0.78
3:A:701:2ED:H5A	3:A:701:2ED:O1	1.83	0.78
1:A:546:THR:HG22	1:A:547:GLY:N	1.95	0.78
1:A:358:LEU:HB3	1:A:359:LEU:HD12	1.65	0.77
1:B:345:GLU:O	1:B:346:GLU:HG3	1.82	0.77
1:B:259:SER:HB3	1:B:272:ILE:CD1	2.15	0.77
1:A:253:LEU:HB2	1:A:259:SER:C	2.10	0.77
1:B:26:TYR:HB3	1:B:338:GLY:O	1.84	0.76
3:A:701:2ED:H19A	7:A:686:HOH:O	1.83	0.76
1:B:256:LYS:HZ3	1:B:256:LYS:CB	1.98	0.76
1:A:642:LEU:O	1:A:644:THR:HG22	1.84	0.75
1:A:70:VAL:O	1:A:74:VAL:HG13	1.85	0.75
1:B:262:PHE:HD1	1:B:267:ASP:HB3	1.51	0.75
1:A:66:ILE:HG12	1:A:66:ILE:O	1.85	0.74
1:B:55:ARG:NH1	6:B:652:DMS:H11	2.02	0.74
1:B:160:ARG:HD2	1:B:336:GLU:HG2	1.69	0.74
1:A:334:SER:HB3	3:A:701:2ED:C3	2.18	0.74
1:A:210:ASN:OD1	1:A:338:GLY:HA2	1.88	0.73
1:A:373:GLU:HG3	1:A:456:ALA:HA	1.70	0.73
1:B:66:ILE:HG12	1:B:66:ILE:O	1.86	0.73
1:A:560:LEU:HD13	1:A:579:ASP:HB3	1.69	0.73
1:B:560:LEU:HD13	1:B:579:ASP:HB3	1.69	0.73
3:B:702:2ED:O2	3:B:702:2ED:C	2.30	0.73
1:B:264:ASN:HD21	1:B:266:PHE:HB2	1.54	0.72
1:A:253:LEU:HB2	1:A:259:SER:O	1.90	0.72
1:B:542:VAL:HG11	1:B:636:THR:HG21	1.72	0.71
1:B:345:GLU:O	1:B:346:GLU:CG	2.38	0.71
3:A:701:2ED:O1	3:A:701:2ED:C5	2.37	0.71
1:B:338:GLY:N	3:B:702:2ED:O1	2.21	0.71
1:B:546:THR:CG2	1:B:547:GLY:H	2.01	0.71
1:A:292:LEU:H	1:A:402:GLN:HE22	1.38	0.70
1:B:29:LEU:HD13	7:B:1031:HOH:O	1.91	0.70
1:B:160:ARG:CD	1:B:336:GLU:HG2	2.21	0.70
1:B:341:PRO:CG	1:B:460:TYR:HE1	2.04	0.70
3:B:702:2ED:C18	7:B:678:HOH:O	2.38	0.70
1:B:318:PRO:O	1:B:319:ARG:HD3	1.91	0.70
1:A:336:GLU:C	1:A:337:ASP:OD1	2.35	0.70
1:B:373:GLU:HG3	1:B:456:ALA:HA	1.74	0.70
1:B:309:ILE:HD11	1:B:321:LEU:HD13	1.72	0.69
1:B:342:LEU:C	1:B:342:LEU:HD13	2.17	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:SER:C	1:A:260:GLY:O	2.27	0.69
1:A:334:SER:CB	3:A:701:2ED:C4	2.61	0.69
1:B:217:PRO:HB2	1:B:221:GLY:HA3	1.75	0.68
1:A:258:GLY:HA2	1:A:262:PHE:O	1.93	0.68
1:A:335:THR:CA	1:A:335:THR:CG2	2.71	0.68
1:B:6:ARG:HG3	1:B:6:ARG:HH11	1.59	0.68
1:B:66:ILE:HD13	1:B:66:ILE:H	1.58	0.68
1:B:292:LEU:H	1:B:402:GLN:HE22	1.40	0.68
1:A:217:PRO:CB	1:A:221:GLY:HA3	2.24	0.68
1:A:338:GLY:H	3:A:701:2ED:HA	1.59	0.67
1:A:66:ILE:HD13	1:A:66:ILE:H	1.58	0.67
1:B:253:LEU:HD22	1:B:260:GLY:HA3	1.75	0.67
1:A:29:LEU:HD13	7:A:989:HOH:O	1.93	0.67
1:A:256:LYS:HB3	1:A:257:PRO:HD3	1.64	0.67
1:A:256:LYS:CD	1:A:257:PRO:HD3	2.25	0.67
1:A:340:GLY:O	1:A:342:LEU:N	2.27	0.67
1:B:160:ARG:NH1	1:B:336:GLU:CG	2.57	0.67
1:A:560:LEU:HB3	1:A:600:ILE:HD13	1.78	0.66
1:A:26:TYR:CE2	1:A:337:ASP:HB2	2.30	0.66
1:A:244:THR:HA	1:A:438:PHE:O	1.95	0.66
1:B:335:THR:H	3:B:702:2ED:H5A	1.60	0.66
1:A:29:LEU:HD11	1:A:348:ASN:ND2	2.10	0.66
1:B:261:PRO:HG2	1:B:262:PHE:HD2	1.60	0.66
1:B:262:PHE:CD1	1:B:267:ASP:HB3	2.29	0.66
1:A:254:ASN:O	1:A:255:LEU:CB	2.44	0.65
1:B:256:LYS:C	1:B:256:LYS:HD2	2.20	0.65
1:A:346:GLU:HB3	1:A:352:LEU:HD13	1.77	0.65
1:A:460:TYR:CD1	3:A:701:2ED:H5A	2.31	0.65
1:A:88:GLU:CD	1:A:88:GLU:H	2.03	0.64
1:A:335:THR:O	1:A:336:GLU:HB2	1.97	0.64
1:B:256:LYS:CB	1:B:256:LYS:NZ	2.57	0.64
1:A:421:ARG:HD3	7:A:858:HOH:O	1.96	0.64
1:B:244:THR:HA	1:B:438:PHE:O	1.97	0.64
1:B:259:SER:HB3	1:B:272:ILE:HD11	1.78	0.64
1:B:341:PRO:HG2	1:B:460:TYR:HE1	1.61	0.64
1:B:160:ARG:HH12	3:B:702:2ED:C19	2.11	0.63
1:B:560:LEU:HB3	1:B:600:ILE:HD13	1.80	0.63
1:B:500:ASP:OD1	1:B:502:SER:HB2	1.99	0.63
1:A:254:ASN:CB	1:A:258:GLY:O	2.44	0.63
1:B:331:ALA:C	1:B:333:GLY:N	2.52	0.62
1:A:546:THR:CG2	1:A:547:GLY:H	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:SER:HG	3:A:701:2ED:H4	1.64	0.62
1:B:421:ARG:HD3	7:B:938:HOH:O	1.99	0.62
1:B:363:PRO:HG3	1:B:379:ASP:HB2	1.82	0.62
1:B:260:GLY:O	1:B:275:ARG:NH2	2.32	0.62
1:A:154:ARG:NH1	1:A:154:ARG:HG2	2.15	0.62
1:B:67:PHE:CD1	1:B:106:SER:HB2	2.35	0.61
1:B:253:LEU:CB	1:B:259:SER:O	2.43	0.61
1:B:542:VAL:HG11	1:B:636:THR:CG2	2.30	0.61
1:B:88:GLU:H	1:B:88:GLU:CD	2.06	0.61
1:B:66:ILE:HD11	1:B:442:ALA:HA	1.83	0.61
1:B:330:LEU:HG	1:B:331:ALA:N	2.15	0.61
1:B:335:THR:H	3:B:702:2ED:C5	2.14	0.61
1:A:542:VAL:HG11	1:A:636:THR:HG21	1.83	0.61
1:B:55:ARG:HH12	6:B:652:DMS:C1	2.09	0.61
1:A:256:LYS:HB3	1:A:257:PRO:HD2	1.81	0.61
1:A:310:ARG:N	1:A:477:GLN:HE22	1.89	0.60
6:B:652:DMS:H13	7:B:856:HOH:O	2.01	0.60
1:A:335:THR:N	3:A:701:2ED:C4	2.64	0.59
1:B:66:ILE:HD13	7:B:989:HOH:O	2.01	0.59
1:A:251:PRO:O	1:A:253:LEU:HD13	2.01	0.59
1:B:67:PHE:CG	1:B:106:SER:HB2	2.37	0.59
1:B:6:ARG:HG3	1:B:6:ARG:NH1	2.15	0.59
1:B:160:ARG:NH1	1:B:336:GLU:HG3	2.17	0.59
1:B:210:ASN:C	1:B:210:ASN:HD22	2.11	0.59
1:A:546:THR:HG21	7:A:736:HOH:O	2.02	0.59
1:A:66:ILE:HD13	7:A:947:HOH:O	2.01	0.58
1:A:532:GLU:HB3	7:A:977:HOH:O	2.01	0.58
1:B:154:ARG:NH1	1:B:154:ARG:HG2	2.17	0.58
1:A:334:SER:HB3	3:A:701:2ED:H3	1.84	0.58
1:A:548:HIS:ND1	1:A:550:LYS:HB2	2.19	0.58
1:B:160:ARG:HH11	1:B:336:GLU:HG3	1.62	0.58
1:B:450:THR:CG2	1:B:455:TYR:HB2	2.34	0.58
1:A:154:ARG:HG2	1:A:154:ARG:HH11	1.68	0.58
1:A:578:THR:HG23	7:A:674:HOH:O	2.04	0.57
1:B:254:ASN:O	1:B:255:LEU:CB	2.51	0.57
1:A:252:ASN:CG	1:A:256:LYS:O	2.47	0.57
1:B:321:LEU:HG	1:B:467:TYR:HB3	1.86	0.57
1:A:253:LEU:N	1:A:259:SER:HA	2.20	0.57
1:B:26:TYR:CD2	1:B:337:ASP:HB3	2.32	0.56
1:A:29:LEU:HD11	1:A:348:ASN:HD22	1.69	0.56
1:A:110:MET:HG2	7:A:785:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:HD12	1:A:359:LEU:N	2.21	0.56
1:B:155:ASN:HD21	1:B:275:ARG:HD3	1.70	0.56
1:A:6:ARG:HG2	1:A:6:ARG:HH11	1.71	0.56
1:B:77:ARG:HD2	7:B:1069:HOH:O	2.06	0.56
1:B:251:PRO:O	1:B:253:LEU:HD13	2.04	0.56
1:B:331:ALA:C	1:B:333:GLY:H	2.13	0.56
1:B:155:ASN:HD21	1:B:275:ARG:CD	2.19	0.55
1:A:548:HIS:CE1	1:A:550:LYS:HB2	2.42	0.55
1:A:66:ILE:HD11	1:A:442:ALA:HA	1.89	0.55
1:B:612:HIS:HD2	7:B:1072:HOH:O	1.90	0.55
1:A:256:LYS:HD2	1:A:257:PRO:HD3	1.88	0.55
1:B:193:GLU:OE1	1:B:234:LYS:HD2	2.07	0.55
1:A:334:SER:C	1:A:335:THR:CG2	2.80	0.55
1:B:155:ASN:ND2	1:B:275:ARG:CD	2.67	0.55
1:B:256:LYS:HZ3	1:B:256:LYS:HB3	1.72	0.55
1:B:272:ILE:HG22	1:B:276:GLN:HE21	1.71	0.55
1:B:209:THR:HG22	1:B:257:PRO:HG2	1.87	0.55
1:A:348:ASN:O	1:A:350:PRO:HD3	2.07	0.55
1:B:231:VAL:HG21	1:B:277:PHE:CZ	2.42	0.55
1:B:341:PRO:HG3	1:B:460:TYR:HE1	1.72	0.55
1:A:318:PRO:O	1:A:319:ARG:HD3	2.07	0.54
1:B:27:SER:CB	1:B:340:GLY:HA2	2.32	0.54
1:B:307:LEU:HD23	1:B:308:PRO:N	2.23	0.54
1:B:535:ARG:NH1	1:B:644:THR:OG1	2.40	0.54
1:A:345:GLU:C	1:A:347:GLY:H	2.15	0.54
1:A:373:GLU:CG	1:A:456:ALA:HA	2.38	0.54
1:B:165:HIS:CD2	1:B:177:GLY:HA2	2.43	0.54
1:B:578:THR:HG23	7:B:743:HOH:O	2.08	0.54
1:A:66:ILE:HD11	1:A:443:ASN:N	2.22	0.54
1:B:531:ARG:CB	1:B:531:ARG:HH21	2.19	0.54
1:A:321:LEU:HG	1:A:467:TYR:HB3	1.88	0.54
1:B:28:SER:HB2	1:B:339:PRO:CD	2.38	0.54
1:B:345:GLU:C	1:B:346:GLU:CG	2.81	0.54
1:A:460:TYR:CE1	3:A:701:2ED:H5A	2.42	0.54
1:B:259:SER:H	1:B:268:ASN:CG	2.15	0.54
1:A:345:GLU:O	1:A:347:GLY:N	2.41	0.54
1:B:258:GLY:HA3	7:B:935:HOH:O	2.07	0.54
1:A:150:SER:H	1:A:288:GLN:NE2	2.05	0.54
1:A:560:LEU:CB	1:A:600:ILE:HD13	2.38	0.54
1:B:66:ILE:HD11	1:B:443:ASN:N	2.23	0.54
1:B:104:GLY:HA3	1:B:119:GLN:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:THR:HG22	1:B:556:GLU:HG2	1.90	0.54
1:A:49:GLU:HB2	1:A:295:LEU:HD22	1.89	0.53
1:A:104:GLY:HA3	1:A:119:GLN:HG2	1.90	0.53
1:B:7:PHE:HA	1:B:46:VAL:O	2.08	0.53
1:B:331:ALA:HA	7:B:684:HOH:O	2.09	0.53
1:B:341:PRO:HG2	1:B:460:TYR:CE1	2.42	0.53
1:B:546:THR:HG21	7:B:824:HOH:O	2.08	0.53
1:B:546:THR:HG23	1:B:632:ILE:HD11	1.90	0.53
1:B:26:TYR:HE2	1:B:337:ASP:CB	2.13	0.53
1:A:566:GLY:HA3	1:A:571:GLN:HG2	1.91	0.53
1:B:261:PRO:C	1:B:262:PHE:CD2	2.87	0.53
1:A:30:GLU:OE1	1:A:30:GLU:HA	2.08	0.53
1:A:150:SER:H	1:A:288:GLN:HE22	1.57	0.53
1:A:414:VAL:O	1:A:418:VAL:HG23	2.09	0.53
1:B:342:LEU:C	1:B:342:LEU:CD1	2.82	0.53
1:A:231:VAL:HG21	1:A:277:PHE:CZ	2.44	0.53
1:A:332:ALA:HB2	7:A:754:HOH:O	2.08	0.53
1:A:450:THR:HG23	1:A:455:TYR:HB2	1.91	0.53
1:A:200:TRP:HE1	1:A:439:ASN:ND2	2.06	0.53
1:A:210:ASN:C	1:A:210:ASN:HD22	2.16	0.53
1:B:74:VAL:HG21	1:B:93:LEU:CD1	2.34	0.53
1:A:17:GLU:HB2	1:A:21:VAL:HG11	1.91	0.52
1:A:256:LYS:HD2	1:A:257:PRO:CD	2.39	0.52
1:A:373:GLU:H	1:A:373:GLU:CD	2.17	0.52
1:B:110:MET:HA	1:B:110:MET:HE2	1.91	0.52
1:B:373:GLU:CD	1:B:373:GLU:H	2.17	0.52
1:B:414:VAL:O	1:B:418:VAL:HG23	2.09	0.52
1:A:67:PHE:CD1	1:A:106:SER:HB2	2.44	0.52
1:A:555:THR:HG22	1:A:556:GLU:HG2	1.90	0.52
1:B:154:ARG:HG2	1:B:154:ARG:HH11	1.74	0.52
1:B:357:GLY:O	1:B:358:LEU:CB	2.57	0.52
1:B:19:ALA:HA	1:B:33:THR:O	2.10	0.52
1:B:373:GLU:CG	1:B:456:ALA:HA	2.39	0.52
1:B:562:VAL:HB	1:B:577:ALA:HB3	1.91	0.52
1:B:403:LEU:HD12	1:B:435:HIS:HB2	1.90	0.52
1:A:300:ARG:HG3	1:A:492:VAL:HG13	1.91	0.52
1:B:262:PHE:CB	7:B:742:HOH:O	2.48	0.52
1:B:591:VAL:HG22	1:B:595:ALA:HB3	1.91	0.52
1:B:158:ARG:HD3	1:B:252:ASN:O	2.09	0.52
1:A:331:ALA:HA	1:A:335:THR:HG21	1.92	0.52
1:B:256:LYS:HD2	1:B:256:LYS:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ARG:HB3	1:B:492:VAL:HG11	1.91	0.52
1:B:330:LEU:HG	1:B:331:ALA:H	1.75	0.52
1:B:260:GLY:N	1:B:261:PRO:HA	2.24	0.52
1:B:492:VAL:HG22	7:B:1042:HOH:O	2.09	0.52
1:A:67:PHE:CG	1:A:106:SER:HB2	2.44	0.51
1:A:193:GLU:OE1	1:A:234:LYS:HD2	2.10	0.51
1:A:338:GLY:H	3:A:701:2ED:C	2.23	0.51
1:A:546:THR:HG23	1:A:632:ILE:HD11	1.92	0.51
1:A:578:THR:HG22	1:A:580:ASN:H	1.75	0.51
1:A:200:TRP:HE1	1:A:439:ASN:HD22	1.58	0.51
1:B:286:GLN:O	1:B:287:ALA:C	2.53	0.51
1:A:531:ARG:CB	1:A:531:ARG:HH21	2.22	0.51
1:A:562:VAL:HB	1:A:577:ALA:HB3	1.93	0.51
1:B:57:VAL:HG21	1:B:86:TYR:CE2	2.45	0.51
1:A:77:ARG:HD2	7:A:1026:HOH:O	2.09	0.51
1:A:394:PRO:HG2	1:A:409:PRO:HG3	1.92	0.51
1:A:110:MET:HE2	1:A:110:MET:HA	1.93	0.51
1:A:542:VAL:HG11	1:A:636:THR:CG2	2.40	0.51
1:B:531:ARG:HH21	1:B:531:ARG:HB2	1.75	0.51
1:A:162:LEU:HD12	1:B:332:ALA:HA	1.93	0.51
1:A:306:ARG:HD3	7:A:719:HOH:O	2.10	0.51
1:A:404:GLU:HG3	1:A:433:ILE:HD12	1.92	0.51
1:B:252:ASN:CG	1:B:257:PRO:HD3	2.35	0.51
1:A:160:ARG:HD2	1:A:336:GLU:HG3	1.93	0.51
1:A:591:VAL:HG13	1:A:596:SER:HA	1.93	0.51
1:B:56:LEU:CD1	1:B:295:LEU:HG	2.41	0.51
1:A:210:ASN:HD22	1:A:211:ALA:N	2.09	0.51
1:B:264:ASN:ND2	1:B:266:PHE:HB2	2.22	0.51
1:B:591:VAL:HG13	1:B:596:SER:HA	1.93	0.51
1:A:448:TYR:O	1:A:465:THR:HA	2.10	0.51
1:B:259:SER:HB3	1:B:272:ILE:HD13	1.92	0.51
1:A:29:LEU:CD1	1:A:348:ASN:ND2	2.75	0.50
1:A:56:LEU:HD12	1:A:295:LEU:HG	1.91	0.50
1:A:307:LEU:HD23	1:A:308:PRO:N	2.26	0.50
1:A:342:LEU:HA	1:A:344:LEU:HD13	1.92	0.50
1:B:261:PRO:HG2	1:B:262:PHE:CD2	2.43	0.50
1:B:38:MET:HE2	1:B:582:TRP:HE3	1.76	0.50
1:B:451:THR:OG1	1:B:454:GLU:HG3	2.12	0.50
1:A:26:TYR:CZ	1:A:337:ASP:HB2	2.46	0.50
1:A:56:LEU:CD1	1:A:295:LEU:HG	2.41	0.50
1:A:82:TYR:HB3	1:A:85:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ILE:HD11	1:B:442:ALA:CA	2.42	0.50
1:A:578:THR:CG2	1:A:580:ASN:H	2.25	0.50
1:B:82:TYR:HB3	1:B:85:VAL:HG13	1.94	0.49
1:A:536:ILE:HB	1:A:644:THR:HG23	1.94	0.49
1:B:259:SER:CB	1:B:272:ILE:HD13	2.42	0.49
1:A:286:GLN:O	1:A:287:ALA:C	2.55	0.49
1:A:8:GLY:HA3	1:A:137:ALA:O	2.12	0.49
1:B:404:GLU:HG3	1:B:433:ILE:HD12	1.94	0.49
1:A:57:VAL:HG21	1:A:86:TYR:CE2	2.48	0.49
1:B:259:SER:CB	1:B:272:ILE:CD1	2.89	0.49
1:B:362:VAL:HG22	1:B:362:VAL:O	2.12	0.49
1:B:560:LEU:CB	1:B:600:ILE:HD13	2.41	0.49
1:A:338:GLY:N	3:A:701:2ED:C	2.76	0.49
1:B:259:SER:HB2	1:B:268:ASN:ND2	2.28	0.49
1:B:261:PRO:O	1:B:262:PHE:CG	2.66	0.49
1:A:153:LEU:HD13	1:A:156:ALA:HB3	1.95	0.48
1:B:115:VAL:O	1:B:116:LEU:HB2	2.11	0.48
1:B:345:GLU:C	1:B:346:GLU:HG2	2.37	0.48
1:B:566:GLY:HA3	1:B:571:GLN:CG	2.43	0.48
1:B:448:TYR:O	1:B:465:THR:HA	2.13	0.48
1:B:210:ASN:HD22	1:B:211:ALA:N	2.10	0.48
1:B:346:GLU:HA	1:B:352:LEU:HD13	1.95	0.48
1:B:562:VAL:CG2	1:B:577:ALA:HB3	2.43	0.48
1:A:93:LEU:H	1:A:443:ASN:ND2	2.11	0.48
1:A:82:TYR:O	1:A:85:VAL:HG13	2.13	0.48
1:A:450:THR:O	1:A:472:GLN:HB2	2.12	0.48
1:B:259:SER:HB2	1:B:268:ASN:CG	2.38	0.48
1:B:331:ALA:HB1	1:B:334:SER:HA	1.96	0.48
1:A:29:LEU:CD1	1:A:348:ASN:HD22	2.26	0.48
1:A:493:GLU:CD	1:A:493:GLU:H	2.20	0.48
1:A:531:ARG:HH21	1:A:531:ARG:HB2	1.78	0.48
1:B:411:GLU:HG2	1:B:441:TYR:HE1	1.70	0.48
1:A:202:PRO:HB2	1:A:249:LEU:CD1	2.44	0.48
1:A:403:LEU:HD12	1:A:435:HIS:HB2	1.96	0.48
1:A:400:ILE:O	1:A:403:LEU:HB2	2.14	0.47
1:B:8:GLY:HA3	1:B:137:ALA:O	2.13	0.47
1:A:333:GLY:O	1:A:334:SER:CB	2.58	0.47
1:A:165:HIS:CD2	1:A:177:GLY:HA2	2.49	0.47
1:A:93:LEU:H	1:A:443:ASN:HD21	1.63	0.47
1:A:450:THR:HG22	1:A:465:THR:OG1	2.14	0.47
1:A:570:LYS:HD2	1:A:570:LYS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ARG:N	1:B:477:GLN:HE22	1.93	0.47
1:B:626:THR:O	1:B:627:GLN:HB2	2.14	0.47
1:A:64:GLY:O	1:A:65:MET:HE3	2.14	0.47
1:B:93:LEU:H	1:B:443:ASN:ND2	2.12	0.47
1:B:200:TRP:HE1	1:B:439:ASN:HD22	1.63	0.47
1:B:253:LEU:CD2	1:B:260:GLY:HA3	2.44	0.47
1:B:335:THR:H	3:B:702:2ED:C6	2.27	0.47
1:B:578:THR:CG2	1:B:580:ASN:H	2.27	0.47
1:A:330:LEU:HD11	1:B:162:LEU:HD13	1.96	0.47
1:A:279:LYS:HE3	1:A:279:LYS:HA	1.97	0.47
1:B:279:LYS:HE3	1:B:279:LYS:HA	1.97	0.47
1:B:342:LEU:HD13	1:B:342:LEU:O	2.14	0.47
1:A:335:THR:CG2	1:A:335:THR:N	2.78	0.47
1:B:549:PRO:HD3	1:B:588:TRP:CD1	2.49	0.47
1:A:19:ALA:HA	1:A:33:THR:O	2.15	0.46
1:A:14:ILE:HG22	1:A:129:GLY:HA3	1.97	0.46
1:A:159:ASN:HD21	1:A:248:ASN:ND2	2.13	0.46
1:A:516:ASP:O	1:A:595:ALA:HA	2.15	0.46
1:A:450:THR:OG1	1:A:454:GLU:CB	2.60	0.46
1:B:209:THR:CG2	1:B:257:PRO:HG2	2.45	0.46
1:B:259:SER:OG	1:B:272:ILE:HD13	2.15	0.46
1:B:626:THR:OG1	1:B:628:LYS:HB2	2.15	0.46
1:B:400:ILE:O	1:B:403:LEU:HB2	2.16	0.46
1:A:256:LYS:CD	1:A:256:LYS:C	2.89	0.46
1:B:335:THR:HG22	3:B:702:2ED:C6	2.46	0.46
1:B:28:SER:HB2	1:B:339:PRO:HD2	1.97	0.46
1:B:217:PRO:CB	1:B:221:GLY:HA3	2.46	0.46
1:A:451:THR:OG1	1:A:454:GLU:HG3	2.16	0.46
1:B:26:TYR:CZ	1:B:337:ASP:HB3	2.38	0.46
1:A:342:LEU:H	1:A:342:LEU:HG	1.58	0.46
1:A:255:LEU:O	1:A:256:LYS:HB2	2.16	0.46
1:B:220:LYS:HD3	1:B:241:PHE:O	2.16	0.46
1:A:334:SER:C	1:A:335:THR:HG22	2.41	0.45
1:A:334:SER:OG	3:A:701:2ED:C4	2.54	0.45
1:A:481:ASP:O	1:A:484:VAL:HG22	2.15	0.45
1:B:182:MET:HA	1:B:200:TRP:O	2.16	0.45
1:B:371:GLN:HG3	1:B:376:ILE:HD11	1.97	0.45
1:B:578:THR:HG23	1:B:579:ASP:N	2.31	0.45
1:B:28:SER:HB2	1:B:339:PRO:HD3	1.98	0.45
1:B:300:ARG:CZ	1:B:493:GLU:CG	2.94	0.45
1:B:148:TYR:C	1:B:148:TYR:CD1	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:GLN:O	1:B:572:THR:C	2.59	0.45
1:A:66:ILE:O	1:A:66:ILE:CG1	2.60	0.45
1:A:115:VAL:O	1:A:116:LEU:HB2	2.17	0.45
1:A:148:TYR:CD1	1:A:148:TYR:C	2.94	0.45
1:B:93:LEU:H	1:B:443:ASN:HD21	1.64	0.45
1:A:348:ASN:O	1:A:348:ASN:CG	2.59	0.45
1:B:38:MET:HE2	1:B:582:TRP:CE3	2.52	0.45
3:A:701:2ED:C19	7:A:686:HOH:O	2.54	0.45
1:B:14:ILE:HG22	1:B:129:GLY:HA3	1.99	0.45
1:B:421:ARG:HD2	7:B:725:HOH:O	2.17	0.45
1:A:65:MET:HA	1:A:95:ALA:HB3	1.98	0.45
1:B:88:GLU:HG3	6:B:653:DMS:O	2.17	0.45
1:A:182:MET:HA	1:A:200:TRP:O	2.17	0.45
1:B:150:SER:H	1:B:288:GLN:NE2	2.15	0.45
1:B:160:ARG:HH12	3:B:702:2ED:H19	1.82	0.45
1:B:264:ASN:ND2	1:B:266:PHE:H	2.14	0.45
1:B:329:SER:OG	1:B:460:TYR:HA	2.16	0.45
3:B:702:2ED:HA	3:B:702:2ED:H3	1.56	0.45
1:A:19:ALA:HB3	1:A:549:PRO:HG2	1.99	0.45
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.82	0.44
1:A:110:MET:HA	1:A:110:MET:CE	2.47	0.44
1:B:342:LEU:HB2	1:B:377:LEU:CD2	2.48	0.44
1:B:481:ASP:O	1:B:484:VAL:HG22	2.16	0.44
1:A:342:LEU:C	1:A:344:LEU:H	2.25	0.44
1:A:65:MET:HA	1:A:95:ALA:CB	2.48	0.44
1:B:200:TRP:HE1	1:B:439:ASN:ND2	2.14	0.44
1:B:564:ASN:HB2	1:B:613:TYR:CE1	2.52	0.44
1:B:256:LYS:HA	1:B:257:PRO:HD3	1.56	0.44
1:A:421:ARG:HD2	7:A:748:HOH:O	2.16	0.44
1:B:55:ARG:HH22	6:B:652:DMS:H11	1.82	0.44
1:A:15:THR:HA	1:A:40:GLN:HE21	1.83	0.44
1:A:319:ARG:NH1	7:A:702:HOH:O	2.49	0.44
1:A:612:HIS:HD2	7:A:1030:HOH:O	2.01	0.44
1:B:17:GLU:OE2	1:B:550:LYS:HD2	2.17	0.44
1:A:3:LEU:HD23	1:A:4:PRO:HD2	2.00	0.44
1:B:110:MET:HA	1:B:110:MET:CE	2.48	0.44
1:B:256:LYS:NZ	1:B:256:LYS:HB3	2.31	0.44
1:B:300:ARG:HA	1:B:495:SER:OG	2.18	0.44
1:A:253:LEU:CB	1:A:259:SER:O	2.64	0.44
1:A:66:ILE:HD11	1:A:442:ALA:CA	2.48	0.44
1:A:220:LYS:HD3	1:A:241:PHE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:PRO:O	1:A:409:PRO:HG2	2.17	0.44
1:A:409:PRO:HB3	1:A:444:ALA:HB3	2.00	0.44
1:B:5:TYR:C	1:B:6:ARG:HG2	2.40	0.44
1:B:450:THR:HG23	1:B:455:TYR:HB2	1.99	0.44
1:B:516:ASP:O	1:B:595:ALA:HA	2.17	0.44
1:A:300:ARG:CZ	1:A:493:GLU:CG	2.96	0.43
1:A:591:VAL:HG22	1:A:595:ALA:HB3	2.00	0.43
1:B:450:THR:O	1:B:472:GLN:HB2	2.17	0.43
1:A:121:LYS:HD2	7:A:1106:HOH:O	2.18	0.43
1:B:66:ILE:HD13	1:B:66:ILE:N	2.31	0.43
1:A:626:THR:OG1	1:A:628:LYS:HB2	2.17	0.43
1:A:88:GLU:HB2	1:A:299:PHE:CD2	2.52	0.43
1:A:560:LEU:HD22	1:A:560:LEU:O	2.18	0.43
1:A:578:THR:HG23	1:A:579:ASP:N	2.33	0.43
1:A:560:LEU:HG	1:A:600:ILE:HG23	2.00	0.43
1:B:57:VAL:CG2	1:B:86:TYR:CE2	3.01	0.43
1:B:233:ARG:HA	1:B:233:ARG:HD3	1.41	0.43
1:B:261:PRO:HB2	1:B:262:PHE:H	1.38	0.43
1:B:307:LEU:HD23	1:B:307:LEU:C	2.44	0.43
1:B:568:ASP:OD1	1:B:568:ASP:O	2.37	0.43
1:A:560:LEU:HD22	1:A:560:LEU:C	2.43	0.43
1:B:261:PRO:O	1:B:262:PHE:CD2	2.71	0.43
1:A:518:TYR:CZ	1:A:591:VAL:HG21	2.54	0.43
1:A:564:ASN:HB2	1:A:613:TYR:CE1	2.52	0.43
1:B:66:ILE:O	1:B:66:ILE:CG1	2.61	0.43
1:B:404:GLU:HG3	1:B:433:ILE:CD1	2.48	0.43
1:A:57:VAL:CG2	1:A:86:TYR:CE2	3.02	0.43
1:A:82:TYR:HB3	1:A:85:VAL:CG1	2.49	0.43
1:A:160:ARG:CD	1:A:336:GLU:HG3	2.49	0.43
1:A:220:LYS:HE3	1:A:243:GLN:CD	2.44	0.43
1:B:160:ARG:HH22	3:B:702:2ED:H19B	1.84	0.43
1:B:349:ASN:CG	1:B:352:LEU:HB2	2.44	0.42
1:A:585:GLN:HB2	1:A:601:SER:OG	2.19	0.42
1:B:162:LEU:O	1:B:166:LEU:HG	2.19	0.42
1:B:578:THR:HG22	1:B:580:ASN:H	1.85	0.42
1:A:115:VAL:O	1:A:115:VAL:HG12	2.18	0.42
1:B:145:ARG:NE	7:B:1107:HOH:O	2.51	0.42
1:B:360:THR:OG1	1:B:361:GLY:N	2.52	0.42
1:A:202:PRO:O	1:A:203:VAL:HB	2.20	0.42
1:A:256:LYS:HD2	1:A:256:LYS:C	2.45	0.42
1:A:562:VAL:CG2	1:A:577:ALA:HB3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:VAL:O	1:B:115:VAL:HG12	2.19	0.42
1:A:6:ARG:HG2	1:A:6:ARG:NH1	2.34	0.42
1:A:164:SER:O	1:A:167:LYS:HB2	2.20	0.42
1:A:307:LEU:HA	1:A:308:PRO:HD3	1.91	0.42
1:A:408:ALA:HA	1:A:409:PRO:HD3	1.78	0.42
1:A:578:THR:CG2	7:A:674:HOH:O	2.64	0.42
1:B:262:PHE:HD1	1:B:267:ASP:CB	2.25	0.42
1:A:120:GLU:HG2	1:A:124:ASN:ND2	2.34	0.42
1:B:209:THR:HG21	1:B:257:PRO:HB2	2.02	0.42
1:B:588:TRP:NE1	1:B:596:SER:HB2	2.35	0.42
1:A:3:LEU:CD2	1:A:4:PRO:HD2	2.50	0.41
1:A:331:ALA:CB	1:A:334:SER:OG	2.68	0.41
1:A:345:GLU:C	1:A:347:GLY:N	2.78	0.41
1:A:540:VAL:O	1:A:601:SER:HA	2.20	0.41
3:A:701:2ED:H3	3:A:701:2ED:H	1.57	0.41
1:B:82:TYR:HB3	1:B:85:VAL:CG1	2.49	0.41
1:B:160:ARG:NH1	1:B:336:GLU:HG2	2.16	0.41
1:B:406:LEU:HD21	1:B:424:VAL:HG21	2.02	0.41
1:A:110:MET:CG	7:A:785:HOH:O	2.66	0.41
1:A:404:GLU:HG3	1:A:433:ILE:CD1	2.49	0.41
1:B:68:GLN:HG3	7:B:807:HOH:O	2.18	0.41
1:B:310:ARG:HG3	1:B:477:GLN:NE2	2.35	0.41
1:B:484:VAL:HG23	7:B:757:HOH:O	2.21	0.41
1:A:64:GLY:O	1:A:65:MET:HB3	2.20	0.41
1:B:162:LEU:HD23	1:B:162:LEU:HA	1.93	0.41
1:B:171:ILE:HG22	1:B:415:MET:SD	2.60	0.41
1:B:299:PHE:CD2	1:B:299:PHE:C	2.98	0.41
1:B:395:ILE:O	1:B:482:MET:HE1	2.21	0.41
1:A:258:GLY:CA	1:A:262:PHE:O	2.66	0.41
1:B:66:ILE:HD11	1:B:442:ALA:C	2.45	0.41
1:A:7:PHE:HA	1:A:46:VAL:O	2.20	0.41
1:A:346:GLU:CB	1:A:352:LEU:HD13	2.49	0.41
1:B:452:ARG:CD	1:B:469:PRO:HB2	2.50	0.41
1:A:171:ILE:HG22	1:A:415:MET:SD	2.60	0.41
1:B:510:THR:HG22	1:B:511:GLY:N	2.36	0.41
1:B:566:GLY:HA3	1:B:571:GLN:HG2	2.02	0.41
1:B:560:LEU:HG	1:B:600:ILE:HG23	2.02	0.41
1:A:58:TYR:OH	1:A:439:ASN:ND2	2.51	0.41
1:A:66:ILE:HD13	1:A:66:ILE:N	2.32	0.41
1:A:74:VAL:O	1:A:78:LEU:HG	2.21	0.41
1:A:168:ASN:HB2	1:A:171:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:SER:O	1:B:344:LEU:HD11	2.20	0.41
1:B:531:ARG:HB2	1:B:531:ARG:NH2	2.35	0.41
1:A:66:ILE:HD11	1:A:442:ALA:C	2.46	0.41
1:A:114:SER:HB3	1:A:344:LEU:HD21	2.03	0.41
1:A:209:THR:HA	1:A:337:ASP:OD2	2.21	0.41
1:A:427:ALA:O	1:A:487:ARG:HD3	2.21	0.41
1:A:560:LEU:C	1:A:560:LEU:CD2	2.94	0.41
1:A:588:TRP:NE1	1:A:596:SER:HB2	2.35	0.41
1:A:644:THR:O	1:A:644:THR:OG1	2.39	0.41
1:B:86:TYR:OH	1:B:138:GLN:NE2	2.54	0.41
1:B:560:LEU:O	1:B:560:LEU:HD22	2.21	0.41
1:B:585:GLN:HB2	1:B:601:SER:OG	2.20	0.41
1:A:331:ALA:HB1	1:A:334:SER:OG	2.21	0.41
1:B:256:LYS:HG3	1:B:337:ASP:CG	2.45	0.41
1:B:379:ASP:OD1	1:B:379:ASP:C	2.64	0.40
1:A:38:MET:HE2	1:A:582:TRP:HE3	1.85	0.40
1:A:549:PRO:HD3	1:A:588:TRP:CD1	2.56	0.40
1:B:82:TYR:O	1:B:85:VAL:HG13	2.21	0.40
1:B:331:ALA:CB	1:B:334:SER:HA	2.51	0.40
1:B:345:GLU:HG2	1:B:348:ASN:HD21	1.85	0.40
1:B:6:ARG:HA	1:B:142:GLN:O	2.21	0.40
1:B:140:ARG:HH11	1:B:140:ARG:HG3	1.87	0.40
1:B:555:THR:O	1:B:556:GLU:HB2	2.20	0.40
1:A:626:THR:O	1:A:627:GLN:HB2	2.21	0.40
1:B:127:VAL:CG2	1:B:128:ASP:N	2.85	0.40
1:A:99:HIS:NE2	3:A:701:2ED:H19A	2.36	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	A	641/646 (99%)	603 (94%)	26 (4%)	12 (2%)	6	4
1	B	641/646 (99%)	586 (91%)	43 (7%)	12 (2%)	6	4
All	All	1282/1292 (99%)	1189 (93%)	69 (5%)	24 (2%)	6	4

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	LEU
1	A	256	LYS
1	A	257	PRO
1	A	332	ALA
1	A	336	GLU
1	A	337	ASP
1	A	346	GLU
1	B	255	LEU
1	B	257	PRO
1	B	261	PRO
1	B	262	PHE
1	B	569	GLY
1	A	50	ALA
1	A	203	VAL
1	A	341	PRO
1	A	259	SER
1	A	331	ALA
1	B	53	GLY
1	B	235	SER
1	B	259	SER
1	B	334	SER
1	B	256	LYS
1	B	203	VAL
1	B	339	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	516/520 (99%)	462 (90%)	54 (10%)	6	6
1	B	516/520 (99%)	464 (90%)	52 (10%)	7	7
All	All	1032/1040 (99%)	926 (90%)	106 (10%)	7	7

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	21	VAL
1	A	23	MET
1	A	29	LEU
1	A	52	SER
1	A	66	ILE
1	A	74	VAL
1	A	75	LEU
1	A	85	VAL
1	A	88	GLU
1	A	110	MET
1	A	153	LEU
1	A	155	ASN
1	A	162	LEU
1	A	167	LYS
1	A	194	LEU
1	A	210	ASN
1	A	233	ARG
1	A	245	ASN
1	A	253	LEU
1	A	256	LYS
1	A	274	LEU
1	A	279	LYS
1	A	295	LEU
1	A	300	ARG
1	A	321	LEU
1	A	334	SER
1	A	336	GLU
1	A	337	ASP
1	A	339	PRO
1	A	345	GLU
1	A	346	GLU
1	A	352	LEU
1	A	358	LEU
1	A	360	THR

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Mol	Chain	Res	Type
1	A	365	GLN
1	A	367	LEU
1	A	369	GLN
1	A	373	GLU
1	A	402	GLN
1	A	403	LEU
1	A	492	VAL
1	A	493	GLU
1	A	494	THR
1	A	531	ARG
1	A	535	ARG
1	A	553	LEU
1	A	560	LEU
1	A	570	LYS
1	A	575	THR
1	A	578	THR
1	A	591	VAL
1	A	628	LYS
1	A	644	THR
1	B	6	ARG
1	B	23	MET
1	B	29	LEU
1	B	30	GLU
1	B	66	ILE
1	B	75	LEU
1	B	85	VAL
1	B	88	GLU
1	B	110	MET
1	B	153	LEU
1	B	162	LEU
1	B	194	LEU
1	B	210	ASN
1	B	245	ASN
1	B	253	LEU
1	B	256	LYS
1	B	257	PRO
1	B	262	PHE
1	B	274	LEU
1	B	279	LYS
1	B	295	LEU
1	B	300	ARG
1	B	321	LEU

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Mol	Chain	Res	Type
1	B	335	THR
1	B	336	GLU
1	B	341	PRO
1	B	342	LEU
1	B	346	GLU
1	B	348	ASN
1	B	352	LEU
1	B	358	LEU
1	B	359	LEU
1	B	362	VAL
1	B	365	GLN
1	B	367	LEU
1	B	373	GLU
1	B	402	GLN
1	B	403	LEU
1	B	450	THR
1	B	492	VAL
1	B	493	GLU
1	B	494	THR
1	B	502	SER
1	B	531	ARG
1	B	535	ARG
1	B	560	LEU
1	B	567	LYS
1	B	570	LYS
1	B	578	THR
1	B	591	VAL
1	B	628	LYS
1	B	644	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	112	ASN
1	A	119	GLN
1	A	124	ASN
1	A	138	GLN
1	A	159	ASN
1	A	213	HIS
1	A	252	ASN
1	A	254	ASN

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Mol	Chain	Res	Type
1	A	268	ASN
1	A	288	GLN
1	A	317	GLN
1	A	320	GLN
1	A	348	ASN
1	A	369	GLN
1	A	382	ASN
1	A	402	GLN
1	A	439	ASN
1	A	443	ASN
1	A	477	GLN
1	A	585	GLN
1	A	612	HIS
1	B	40	GLN
1	B	112	ASN
1	B	119	GLN
1	B	124	ASN
1	B	138	GLN
1	B	210	ASN
1	B	213	HIS
1	B	254	ASN
1	B	264	ASN
1	B	288	GLN
1	B	317	GLN
1	B	320	GLN
1	B	348	ASN
1	B	382	ASN
1	B	402	GLN
1	B	425	GLN
1	B	439	ASN
1	B	443	ASN
1	B	477	GLN
1	B	571	GLN
1	B	585	GLN
1	B	612	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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$
3	2ED	B	702	-	11,12,23	0.37	0	11,14,25	1.47	3 (27%)
4	FMT	B	648	-	2,2,2	0.69	0	1,1,1	0.23	0
4	FMT	A	650	-	2,2,2	0.78	0	1,1,1	0.15	0
4	FMT	A	648	-	2,2,2	0.71	0	1,1,1	0.23	0
4	FMT	A	649	-	2,2,2	0.67	0	1,1,1	0.18	0
6	DMS	B	652	-	3,3,3	2.84	1 (33%)	3,3,3	0.87	0
3	2ED	A	701	-	11,12,23	0.37	0	11,14,25	1.48	3 (27%)
4	FMT	B	651	-	2,2,2	0.66	0	1,1,1	0.20	0
6	DMS	B	653	-	3,3,3	2.80	1 (33%)	3,3,3	1.10	0
4	FMT	A	651	-	2,2,2	0.67	0	1,1,1	0.17	0
4	FMT	B	650	-	2,2,2	0.66	0	1,1,1	0.22	0
4	FMT	B	649	-	2,2,2	0.71	0	1,1,1	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2ED	B	702	-	1/1/3/6	6/14/14/25	-
3	2ED	A	701	-	-	9/14/14/25	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	652	DMS	O-S	4.81	1.81	1.50
6	B	653	DMS	O-S	4.54	1.80	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	2ED	C2-C1-N	-2.77	104.97	109.66
3	A	701	2ED	C-C1-N	-2.74	104.96	109.28
3	B	702	2ED	C2-C1-N	-2.73	105.02	109.66
3	B	702	2ED	C-C1-N	-2.72	104.99	109.28
3	A	701	2ED	C2-C3-C4	-2.27	119.99	124.69
3	B	702	2ED	C2-C3-C4	-2.26	120.02	124.69

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	702	2ED	C1

All (15) torsion outliers are listed below:

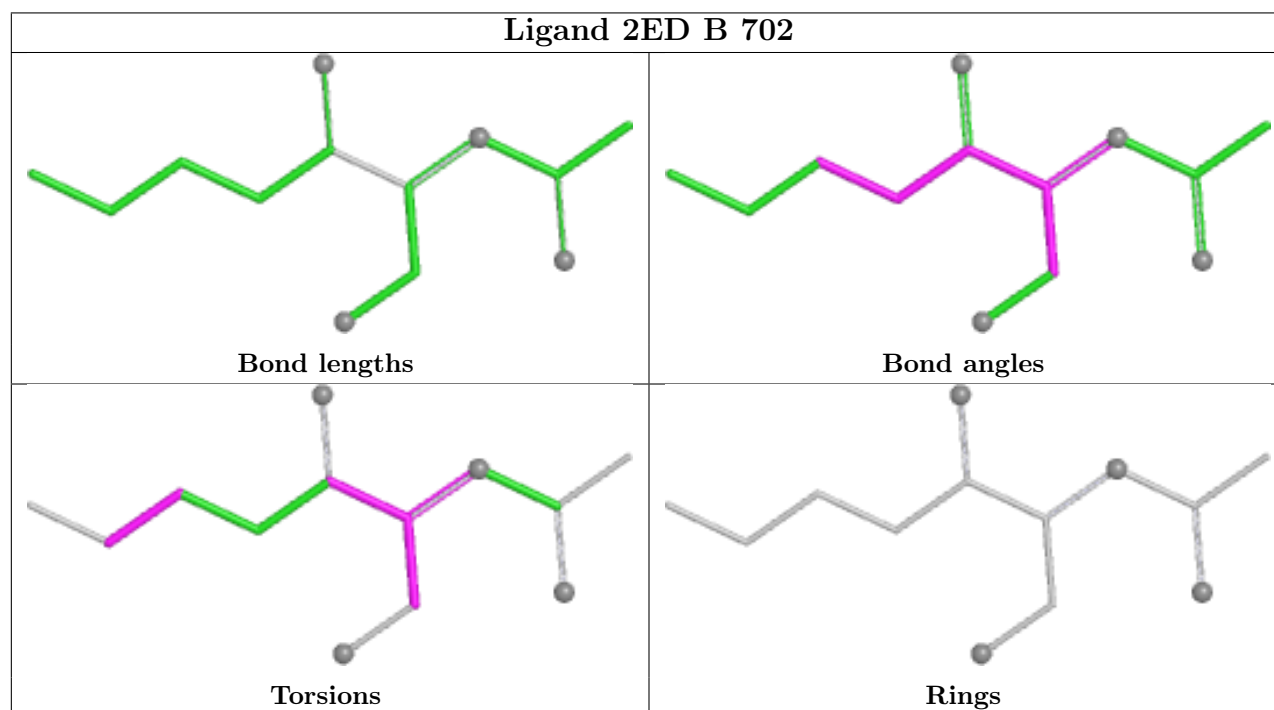
Mol	Chain	Res	Type	Atoms
3	A	701	2ED	N-C1-C2-C3
3	A	701	2ED	C-C1-C2-O1
3	A	701	2ED	C-C1-C2-C3
3	A	701	2ED	O3-C-C1-C2
3	B	702	2ED	C-C1-C2-O1
3	B	702	2ED	C-C1-N-C18
3	A	701	2ED	O3-C-C1-N
3	A	701	2ED	N-C1-C2-O1
3	B	702	2ED	O3-C-C1-C2
3	A	701	2ED	C3-C4-C5-C6
3	A	701	2ED	O1-C2-C3-C4
3	B	702	2ED	O3-C-C1-N
3	A	701	2ED	C1-C2-C3-C4
3	B	702	2ED	C-C1-C2-C3
3	B	702	2ED	C3-C4-C5-C6

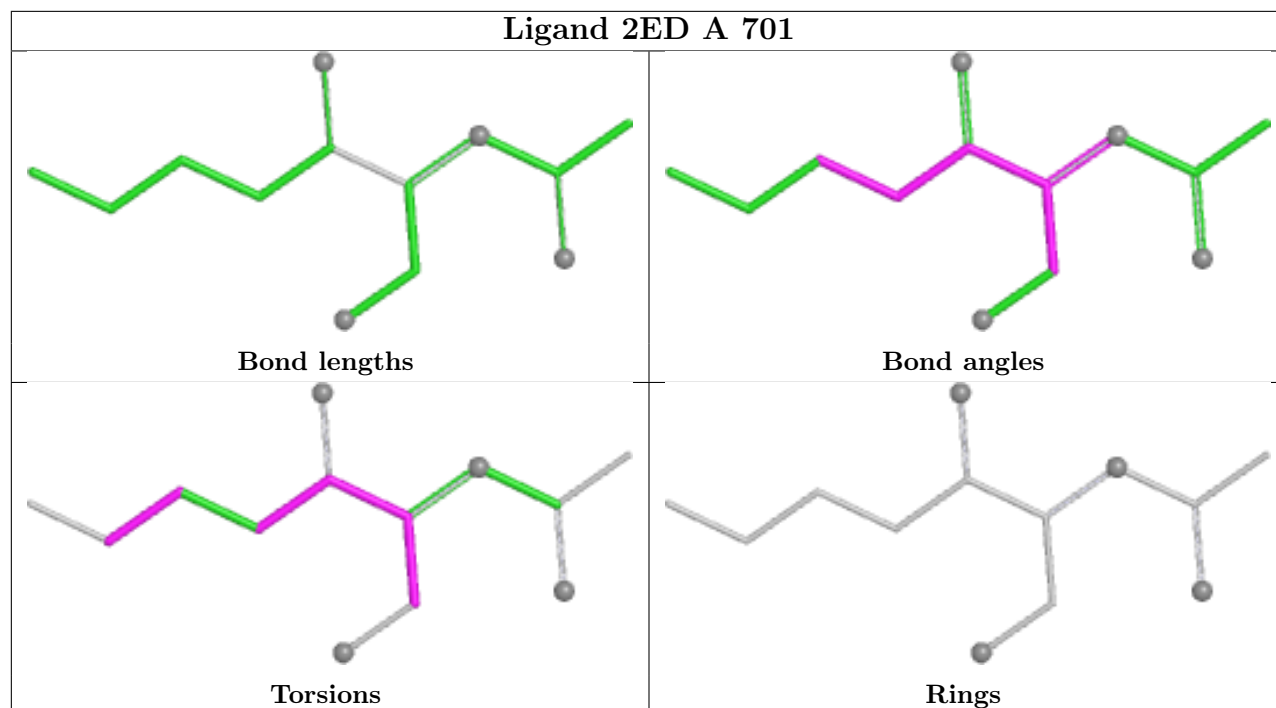
There are no ring outliers.

4 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	2ED	13	0
6	B	652	DMS	5	0
3	A	701	2ED	24	0
6	B	653	DMS	1	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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	643/646 (99%)	0.14	44 (6%)	23 20	14, 24, 58, 98	0
1	B	643/646 (99%)	0.16	44 (6%)	23 20	14, 25, 59, 96	0
All	All	1286/1292 (99%)	0.15	88 (6%)	23 20	14, 25, 59, 98	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	GLY	8.7
1	B	337	ASP	7.8
1	A	337	ASP	7.7
1	B	259	SER	7.4
1	B	258	GLY	7.3
1	B	332	ALA	6.8
1	A	261	PRO	6.7
1	B	338	GLY	6.4
1	B	260	GLY	6.1
1	A	336	GLU	6.0
1	B	257	PRO	6.0
1	A	338	GLY	5.5
1	B	341	PRO	5.3
1	A	333	GLY	5.3
1	B	261	PRO	5.3
1	B	331	ALA	5.2
1	B	342	LEU	5.2
1	A	257	PRO	4.9
1	A	259	SER	4.9
1	B	263	ASP	4.7
1	A	344	LEU	4.6
1	A	342	LEU	4.5
1	B	336	GLU	4.5
1	B	262	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	255	LEU	4.1
1	A	262	PHE	4.0
1	A	332	ALA	4.0
1	A	258	GLY	3.9
1	B	255	LEU	3.9
1	B	335	THR	3.9
1	A	346	GLU	3.9
1	B	344	LEU	3.8
1	A	52	SER	3.7
1	A	339	PRO	3.6
1	A	347	GLY	3.6
1	A	345	GLU	3.6
1	A	341	PRO	3.6
1	B	358	LEU	3.5
1	A	644	THR	3.5
1	B	359	LEU	3.5
1	A	51	ALA	3.5
1	A	343	GLY	3.4
1	B	340	GLY	3.4
1	A	335	THR	3.4
1	B	339	PRO	3.4
1	A	256	LYS	3.4
1	A	340	GLY	3.3
1	A	331	ALA	3.3
1	B	346	GLU	3.2
1	B	644	THR	3.2
1	A	358	LEU	3.1
1	A	334	SER	3.0
1	B	334	SER	2.9
1	B	333	GLY	2.8
1	B	155	ASN	2.8
1	B	253	LEU	2.7
1	A	50	ALA	2.7
1	B	254	ASN	2.7
1	B	347	GLY	2.7
1	B	360	THR	2.7
1	B	569	GLY	2.6
1	A	348	ASN	2.6
1	A	235	SER	2.6
1	A	359	LEU	2.5
1	A	360	THR	2.5
1	B	51	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	361	GLY	2.5
1	A	569	GLY	2.5
1	B	52	SER	2.4
1	B	53	GLY	2.4
1	B	343	GLY	2.4
1	A	330	LEU	2.4
1	B	361	GLY	2.4
1	A	504	CYS	2.4
1	B	256	LYS	2.3
1	B	504	CYS	2.2
1	B	625	TRP	2.2
1	B	568	ASP	2.2
1	A	643	GLY	2.2
1	A	450	THR	2.2
1	B	494	THR	2.2
1	A	49	GLU	2.1
1	A	53	GLY	2.1
1	A	171	ILE	2.1
1	B	270	ARG	2.1
1	B	345	GLU	2.1
1	B	357	GLY	2.1
1	A	2	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	2ED	B	702	13/24	0.54	0.28	56,61,66,66	0

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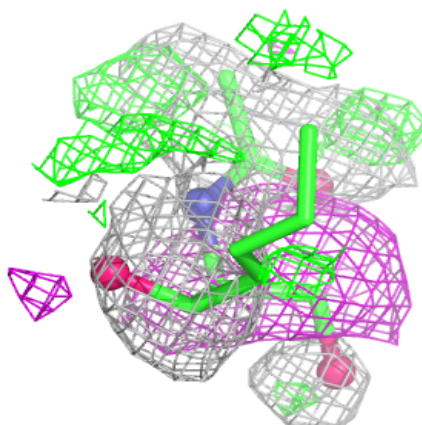
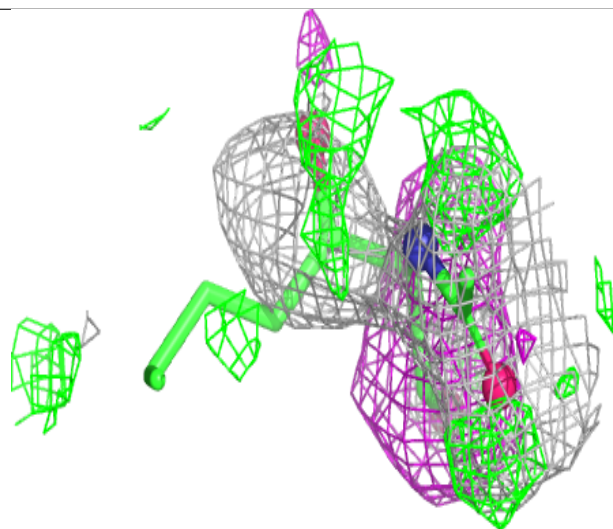
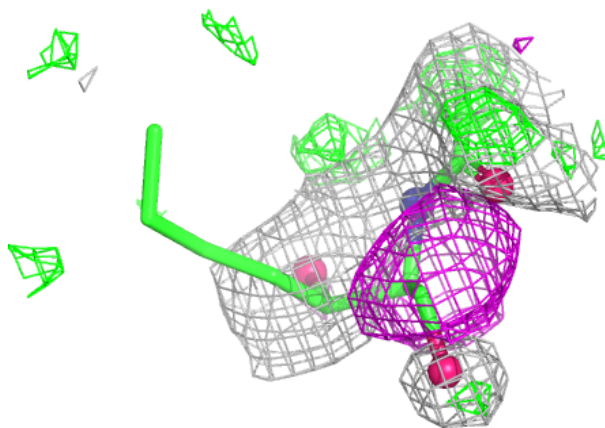
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	2ED	A	701	13/24	0.55	0.27	56,59,62,63	0
4	FMT	B	650	3/3	0.57	0.31	56,56,56,56	0
6	DMS	B	653	4/4	0.68	0.32	76,76,76,77	0
4	FMT	A	651	3/3	0.72	0.20	70,70,70,71	0
4	FMT	B	651	3/3	0.77	0.17	61,61,62,62	0
4	FMT	B	649	3/3	0.78	0.18	63,63,64,64	0
4	FMT	A	649	3/3	0.83	0.16	66,66,66,67	0
4	FMT	A	650	3/3	0.84	0.17	61,61,61,61	0
6	DMS	B	652	4/4	0.89	0.15	60,61,62,62	0
5	MG	B	654	1/1	0.90	0.08	29,29,29,29	0
5	MG	A	652	1/1	0.93	0.07	28,28,28,28	0
4	FMT	A	648	3/3	0.96	0.06	23,23,23,24	0
4	FMT	B	648	3/3	0.97	0.05	22,22,23,24	0
2	ZN	A	647	1/1	0.99	0.02	25,25,25,25	0
2	ZN	B	647	1/1	0.99	0.03	26,26,26,26	0

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.

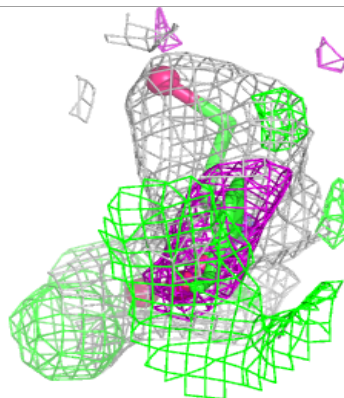
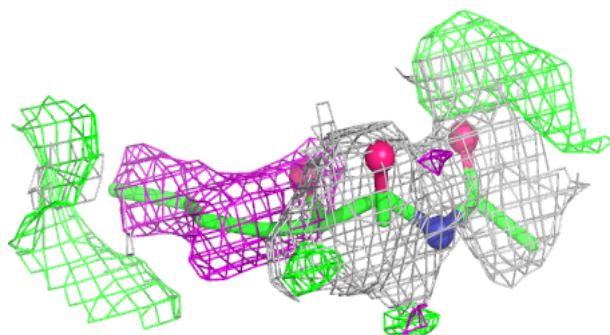
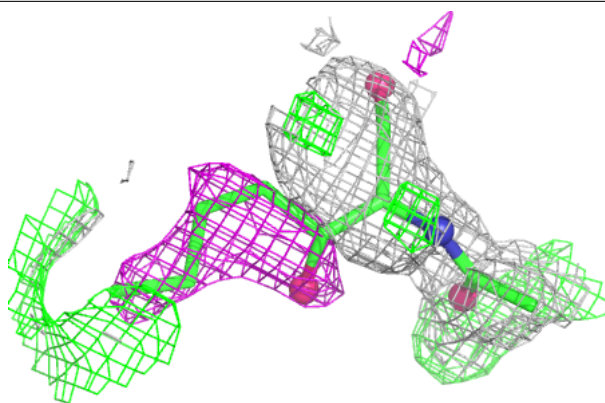
Electron density around 2ED B 702:

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



Electron density around 2ED A 701:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.