



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:13 PM UTC

PDB ID : 1FBE / pdb_00001fbe
Title : CRYSTALLOGRAPHIC STUDIES OF THE CATALYTIC MECHANISM OF
THE NEUTRAL FORM OF FRUCTOSE-1,6-BISPHOSPHATASE
Authors : Zhang, Y.; Liang, J.-Y.; Huang, S.; Ke, H.; Lipscomb, W.N.
Deposited on : 1992-10-16
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 ⓘ 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

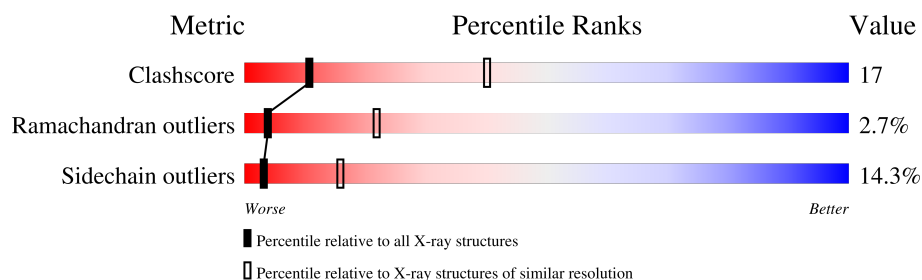
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	335	43% 37% 13% • 7%
1	B	335	38% 38% 16% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5909 atoms, of which 1069 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 FRUCTOSE 1,6-BISPHOSPHATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	313	Total	C	H	N	O	S	0	0	1
			2921	1520	530	403	453	15			
1	B	315	Total	C	H	N	O	S	0	0	1
			2938	1532	531	405	455	15			

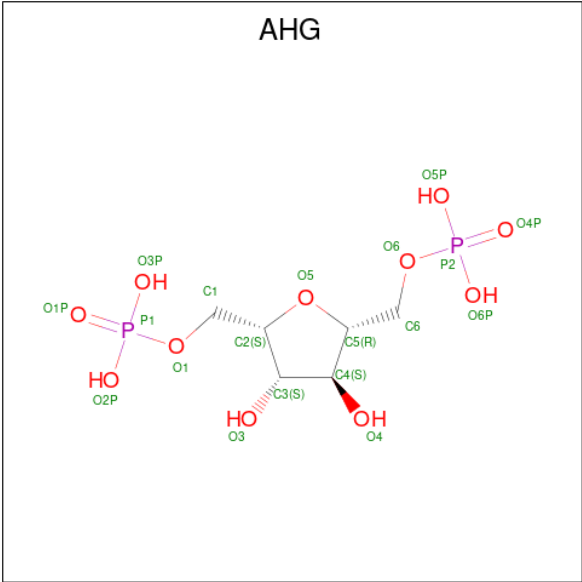
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLN	GLU	conflict	UNP P00636
A	96	THR	SER	conflict	UNP P00636
A	199	ASN	ASP	conflict	UNP P00636
B	20	GLN	GLU	conflict	UNP P00636
B	96	THR	SER	conflict	UNP P00636
B	199	ASN	ASP	conflict	UNP P00636

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

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

- Molecule 3 is 2,5-anhydro-1,6-di-O-phosphono-D-glucitol (CCD ID: AHG) (formula: C₆H₁₄O₁₁P₂).



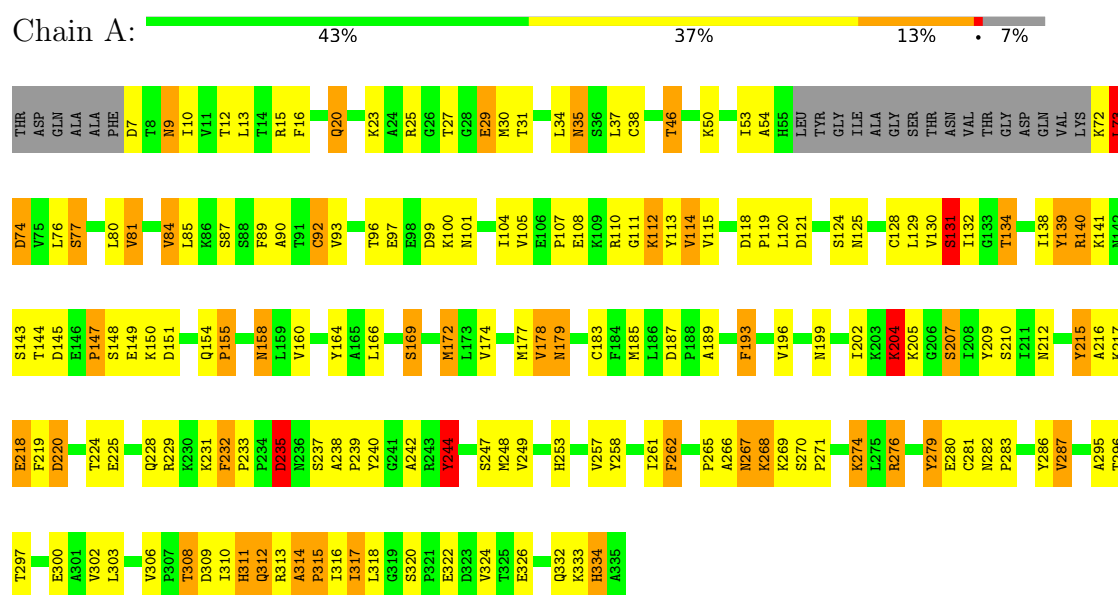
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	P	0	0
			23	6	4	11	2		
3	B	1	Total	C	H	O	P	0	0
			23	6	4	11	2		

3 Residue-property plots

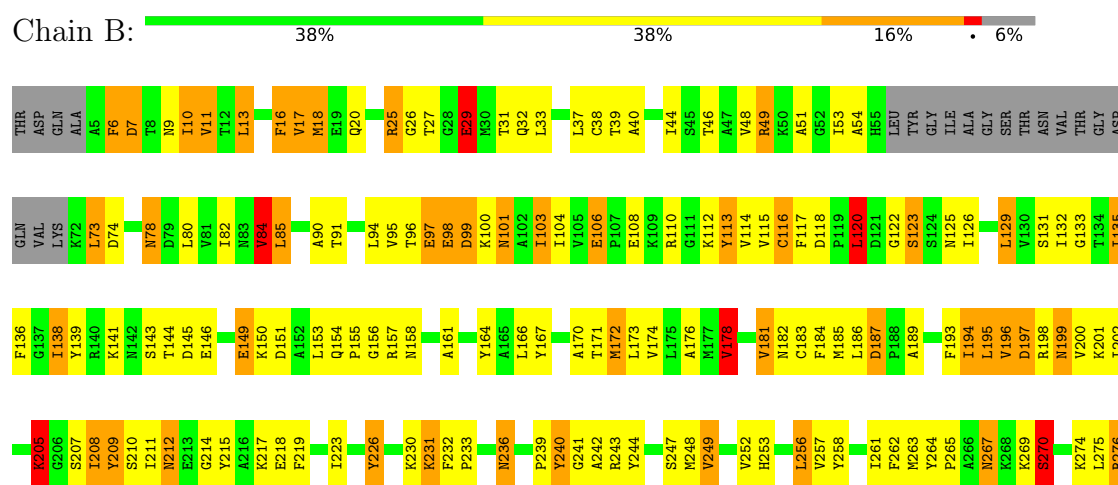
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

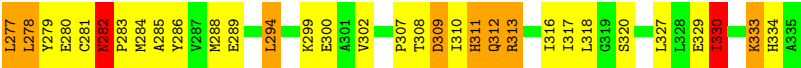
Note EDS was not executed.

• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE



• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.00Å 132.00Å 67.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5909	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.28	14/2430 (0.6%)	2.18	93/3286 (2.8%)
1	B	1.13	11/2447 (0.4%)	2.14	95/3309 (2.9%)
All	All	1.21	25/4877 (0.5%)	2.16	188/6595 (2.9%)

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	10
1	B	0	8
All	All	0	18

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	HIS	CD2-NE2	-7.96	1.29	1.37
1	A	178	VAL	CA-CB	7.93	1.64	1.54
1	A	35	ASN	CA-CB	-7.66	1.41	1.53
1	A	121	ASP	CA-CB	-7.45	1.43	1.53
1	B	178	VAL	CA-CB	6.76	1.63	1.54
1	B	311	HIS	CD2-NE2	-6.73	1.30	1.37
1	A	253	HIS	CD2-NE2	-6.69	1.30	1.37
1	A	253	HIS	CG-ND1	-6.44	1.31	1.38
1	B	193	PHE	CA-CB	-6.40	1.44	1.53
1	B	54	ALA	C-N	-6.38	1.24	1.33
1	A	54	ALA	C-N	-6.34	1.24	1.33
1	A	296	THR	CA-CB	6.32	1.63	1.53
1	B	174	VAL	CA-CB	-6.05	1.47	1.54
1	A	334	HIS	CD2-NE2	-5.95	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	LEU	CA-C	-5.92	1.46	1.52
1	B	253	HIS	CD2-NE2	-5.79	1.31	1.37
1	B	196	VAL	CA-CB	5.68	1.62	1.54
1	B	311	HIS	CG-ND1	-5.67	1.32	1.38
1	B	334	HIS	CD2-NE2	-5.52	1.31	1.37
1	A	37	LEU	CA-CB	-5.41	1.45	1.53
1	A	12	THR	CA-CB	5.39	1.61	1.53
1	A	147	PRO	CA-CB	-5.09	1.46	1.53
1	B	120	LEU	C-O	5.08	1.30	1.24
1	A	160	VAL	CA-CB	5.07	1.61	1.54
1	B	282	ASN	N-CA	-5.05	1.43	1.46

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ASP	CA-CB-CG	24.96	137.56	112.60
1	A	20	GLN	OE1-CD-NE2	-12.16	110.44	122.60
1	B	120	LEU	O-C-N	11.92	138.45	122.59
1	B	118	ASP	CA-CB-CG	11.70	124.30	112.60
1	A	235	ASP	CA-CB-CG	10.93	123.53	112.60
1	A	35	ASN	CA-CB-CG	-10.90	101.70	112.60
1	B	49	ARG	N-CA-C	-10.69	99.16	111.03
1	B	78	ASN	OD1-CG-ND2	-10.61	111.99	122.60
1	A	232	PHE	CA-CB-CG	10.29	124.09	113.80
1	B	145	ASP	CA-CB-CG	10.03	122.62	112.60
1	A	7	ASP	CA-CB-CG	9.78	122.38	112.60
1	A	120	LEU	O-C-N	9.63	134.91	123.36
1	B	212	ASN	CA-CB-CG	9.18	121.78	112.60
1	A	311	HIS	CA-CB-CG	9.08	122.88	113.80
1	A	333	LYS	N-CA-C	-8.98	99.68	111.71
1	B	101	ASN	N-CA-C	-8.55	99.00	110.55
1	B	329	GLU	CA-CB-CG	8.50	131.10	114.10
1	B	282	ASN	CA-C-O	-8.47	111.34	119.13
1	A	120	LEU	CA-C-O	8.40	129.81	119.98
1	A	179	ASN	CA-CB-CG	-8.32	104.28	112.60
1	A	118	ASP	CB-CG-OD2	-8.26	99.41	118.40
1	B	112	LYS	N-CA-C	8.23	122.90	113.02
1	B	197	ASP	CA-CB-CG	8.23	120.83	112.60
1	B	247	SER	N-CA-C	-8.08	95.75	109.24
1	A	282	ASN	OD1-CG-ND2	-7.93	114.67	122.60
1	A	20	GLN	CB-CG-CD	7.91	126.05	112.60
1	A	308	THR	N-CA-C	-7.86	103.53	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	LYS	CA-CB-CG	7.77	129.63	114.10
1	B	334	HIS	CA-CB-CG	7.75	121.55	113.80
1	A	97	GLU	N-CA-C	-7.71	102.48	111.03
1	B	187	ASP	CA-CB-CG	7.67	120.27	112.60
1	B	126	ILE	CB-CA-C	-7.64	102.03	112.04
1	B	329	GLU	CB-CA-C	-7.57	98.99	110.88
1	A	257	VAL	N-CA-C	7.42	118.02	110.82
1	B	9	ASN	CA-CB-CG	7.41	120.01	112.60
1	B	199	ASN	OD1-CG-ND2	-7.40	115.20	122.60
1	B	214	GLY	N-CA-C	-7.36	103.96	112.50
1	B	51	ALA	N-CA-C	7.31	123.44	111.37
1	B	73	LEU	CA-C-O	-7.23	110.17	120.51
1	B	18	MET	CA-CB-CG	-7.20	99.69	114.10
1	B	39	THR	CA-CB-OG1	-7.12	98.91	109.60
1	A	118	ASP	N-CA-C	-6.93	97.57	109.15
1	B	16	PHE	CA-CB-CG	-6.90	106.90	113.80
1	A	112	LYS	N-CA-C	6.88	121.28	113.02
1	A	155	PRO	O-C-N	6.85	131.32	123.10
1	B	209	TYR	N-CA-C	-6.83	98.59	109.59
1	B	104	ILE	N-CA-C	-6.79	98.65	108.36
1	A	187	ASP	CA-C-N	6.78	127.36	120.04
1	A	187	ASP	C-N-CA	6.78	127.36	120.04
1	B	125	ASN	OD1-CG-ND2	-6.76	115.84	122.60
1	B	117	PHE	O-C-N	-6.75	115.93	123.48
1	B	267	ASN	CA-CB-CG	6.71	119.31	112.60
1	A	149	GLU	CA-CB-CG	6.70	127.50	114.10
1	A	228	GLN	OE1-CD-NE2	-6.64	115.96	122.60
1	A	89	PHE	CA-CB-CG	-6.63	107.17	113.80
1	B	187	ASP	CA-C-N	6.63	126.26	119.56
1	B	187	ASP	C-N-CA	6.63	126.26	119.56
1	B	138	ILE	CA-C-O	6.62	127.38	120.36
1	A	247	SER	N-CA-C	-6.60	97.30	108.26
1	B	193	PHE	N-CA-C	-6.58	96.95	108.20
1	B	151	ASP	CA-CB-CG	6.57	119.17	112.60
1	A	204	LYS	N-CA-C	6.57	118.13	110.97
1	A	113	TYR	N-CA-C	6.57	120.40	109.95
1	B	7	ASP	CA-CB-CG	6.55	119.15	112.60
1	B	232	PHE	N-CA-C	-6.54	96.60	109.10
1	A	196	VAL	CA-C-O	-6.51	112.65	120.78
1	B	110	ARG	N-CA-C	6.47	119.08	110.53
1	A	267	ASN	O-C-N	-6.47	115.72	122.84
1	A	312	GLN	OE1-CD-NE2	-6.46	116.14	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	ASN	OD1-CG-ND2	-6.45	116.15	122.60
1	B	223	ILE	N-CA-C	-6.40	104.51	110.53
1	A	202	ILE	N-CA-C	6.40	117.03	110.05
1	A	267	ASN	CA-CB-CG	6.38	118.98	112.60
1	B	117	PHE	N-CA-C	6.38	118.85	108.76
1	B	84	VAL	CB-CA-C	-6.36	103.45	112.22
1	A	187	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	205	LYS	N-CA-C	-6.28	99.92	109.85
1	A	274	LYS	CA-C-O	6.28	126.33	119.24
1	A	312	GLN	CG-CD-NE2	6.25	125.77	116.40
1	A	87	SER	CA-CB-OG	-6.21	98.69	111.10
1	B	10	ILE	N-CA-C	6.18	116.77	108.11
1	B	97	GLU	OE1-CD-OE2	6.12	137.60	122.90
1	B	46	THR	CA-CB-OG1	-6.12	100.42	109.60
1	A	112	LYS	CA-CB-CG	6.11	126.33	114.10
1	A	30	MET	CA-C-O	-6.11	114.36	120.90
1	B	236	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	A	50	LYS	N-CA-C	-6.05	104.01	113.02
1	B	199	ASN	CB-CG-ND2	6.05	125.47	116.40
1	B	78	ASN	CB-CG-ND2	6.04	125.45	116.40
1	B	85	LEU	O-C-N	6.03	128.28	122.07
1	A	73	LEU	N-CA-C	5.99	123.55	110.80
1	B	144	THR	N-CA-C	-5.98	105.81	112.57
1	A	145	ASP	N-CA-C	5.97	119.11	109.79
1	A	269	LYS	N-CA-C	-5.94	104.80	111.28
1	A	302	VAL	CB-CA-C	-5.94	104.12	112.14
1	A	332	GLN	OE1-CD-NE2	-5.93	116.67	122.60
1	B	233	PRO	CA-C-N	5.91	125.78	119.28
1	B	233	PRO	C-N-CA	5.91	125.78	119.28
1	B	311	HIS	N-CA-C	-5.89	103.44	111.56
1	B	26	GLY	CA-C-N	5.85	132.71	121.54
1	B	26	GLY	C-N-CA	5.85	132.71	121.54
1	B	270	SER	CA-C-N	5.84	125.55	119.82
1	B	270	SER	C-N-CA	5.84	125.55	119.82
1	A	154	GLN	CA-C-N	5.81	125.57	119.76
1	A	154	GLN	C-N-CA	5.81	125.57	119.76
1	B	329	GLU	N-CA-CB	5.75	118.34	110.01
1	A	104	ILE	CA-C-O	5.74	126.67	120.53
1	A	132	ILE	CB-CA-C	-5.74	101.51	110.52
1	A	154	GLN	OE1-CD-NE2	-5.73	116.87	122.60
1	A	276	ARG	CB-CG-CD	5.72	124.47	111.30
1	B	106	GLU	CA-C-O	5.72	125.15	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	GLN	CA-C-O	-5.71	115.25	121.87
1	A	267	ASN	OD1-CG-ND2	-5.70	116.90	122.60
1	B	233	PRO	CB-CA-C	5.68	117.85	110.92
1	A	148	SER	N-CA-C	5.68	117.70	109.07
1	A	322	GLU	CA-CB-CG	-5.67	102.75	114.10
1	B	219	PHE	N-CA-C	5.67	117.92	109.25
1	A	144	THR	N-CA-C	5.66	118.39	111.82
1	B	135	ILE	CB-CA-C	-5.63	103.30	112.03
1	B	84	VAL	N-CA-CB	5.58	118.95	110.58
1	B	231	LYS	CB-CA-C	-5.57	102.38	110.96
1	B	264	TYR	N-CA-C	-5.57	97.47	109.01
1	B	38	CYS	CA-C-O	-5.57	115.16	121.00
1	B	167	TYR	N-CA-CB	-5.54	103.77	110.53
1	B	49	ARG	CA-C-O	-5.52	115.21	120.90
1	B	267	ASN	O-C-N	-5.50	118.46	123.41
1	A	118	ASP	N-CA-CB	5.50	119.89	110.05
1	B	282	ASN	CA-C-N	5.50	125.59	119.32
1	B	282	ASN	C-N-CA	5.50	125.59	119.32
1	B	39	THR	CA-CB-CG2	5.47	119.81	110.50
1	B	309	ASP	CA-CB-CG	5.47	118.08	112.60
1	B	97	GLU	CG-CD-OE2	-5.46	105.84	118.40
1	A	96	THR	CA-CB-OG1	-5.44	101.44	109.60
1	A	104	ILE	O-C-N	5.43	129.46	123.10
1	B	29	GLU	N-CA-C	-5.40	105.40	111.28
1	B	123	SER	CA-CB-OG	5.40	121.89	111.10
1	B	333	LYS	CA-CB-CG	5.39	124.88	114.10
1	B	313	ARG	NE-CZ-NH1	5.38	126.89	121.50
1	B	113	TYR	N-CA-C	5.37	118.32	109.72
1	A	81	VAL	CA-C-O	-5.36	114.68	120.47
1	A	202	ILE	O-C-N	-5.36	115.83	122.52
1	B	116	CYS	O-C-N	-5.35	116.93	123.30
1	A	189	ALA	N-CA-C	-5.33	105.38	111.14
1	A	193	PHE	CA-CB-CG	-5.33	108.47	113.80
1	A	118	ASP	OD1-CG-OD2	5.33	135.69	122.90
1	A	314	ALA	CA-C-O	5.32	125.14	119.50
1	B	129	LEU	CA-C-O	5.31	127.60	121.28
1	B	13	LEU	CA-C-O	-5.30	114.90	120.63
1	A	158	ASN	N-CA-C	5.29	119.45	112.89
1	A	154	GLN	CA-CB-CG	5.29	124.67	114.10
1	A	262	PHE	N-CA-C	-5.28	101.28	109.72
1	B	25	ARG	CA-CB-CG	5.26	124.61	114.10
1	B	257	VAL	N-CA-C	5.24	118.40	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	LYS	N-CA-C	5.24	116.79	108.67
1	B	285	ALA	N-CA-C	5.23	117.66	111.33
1	B	187	ASP	N-CA-C	-5.23	99.11	108.47
1	B	149	GLU	CA-C-O	5.22	126.05	120.20
1	B	172	MET	O-C-N	-5.22	116.84	123.05
1	A	314	ALA	CB-CA-C	-5.21	101.89	109.45
1	A	207	SER	N-CA-C	5.21	119.13	112.26
1	B	82	ILE	CB-CA-C	-5.20	102.76	111.29
1	A	134	THR	O-C-N	-5.19	117.13	123.10
1	A	9	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	A	114	VAL	CA-C-N	-5.18	116.21	123.10
1	A	114	VAL	C-N-CA	-5.18	116.21	123.10
1	B	11	VAL	O-C-N	5.17	128.09	122.36
1	A	29	GLU	CA-C-O	-5.17	115.37	120.90
1	A	315	PRO	N-CA-C	-5.16	102.50	111.32
1	A	84	VAL	N-CA-C	-5.15	105.36	110.62
1	B	205	LYS	CA-C-O	-5.15	115.09	121.06
1	A	326	GLU	CA-CB-CG	-5.14	103.82	114.10
1	A	287	VAL	CA-CB-CG1	-5.12	101.69	110.40
1	A	131	SER	CA-C-N	5.12	129.99	123.03
1	A	131	SER	C-N-CA	5.12	129.99	123.03
1	B	219	PHE	CA-C-O	5.12	126.43	120.49
1	B	330	ILE	CB-CA-C	-5.11	105.24	112.14
1	A	160	VAL	CG1-CB-CG2	-5.11	99.56	110.80
1	A	244	TYR	N-CA-C	-5.11	98.60	107.49
1	B	195	LEU	N-CA-CB	-5.09	102.12	110.52
1	A	46	THR	N-CA-C	-5.06	105.66	111.07
1	A	154	GLN	N-CA-C	-5.05	102.38	110.10
1	A	87	SER	N-CA-C	5.02	118.90	112.87
1	A	220	ASP	CA-C-N	5.02	124.74	119.82
1	A	220	ASP	C-N-CA	5.02	124.74	119.82
1	A	53	ILE	CA-C-N	5.02	130.73	121.70
1	A	53	ILE	C-N-CA	5.02	130.73	121.70
1	A	25	ARG	O-C-N	5.01	129.02	122.86
1	B	330	ILE	N-CA-C	-5.00	105.52	110.62

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Sidechain
1	A	16	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	A	164	TYR	Sidechain
1	A	193	PHE	Sidechain
1	A	215	TYR	Sidechain
1	A	220	ASP	Peptide
1	A	240	TYR	Sidechain
1	A	244	TYR	Sidechain
1	A	258	TYR	Sidechain
1	A	279	TYR	Sidechain
1	B	106	GLU	Peptide
1	B	120	LEU	Mainchain
1	B	164	TYR	Sidechain
1	B	215	TYR	Sidechain
1	B	226	TYR	Sidechain
1	B	240	TYR	Sidechain
1	B	258	TYR	Sidechain
1	B	279	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2391	530	2448	70	0
1	B	2407	531	2462	96	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	19	4	10	1	0
3	B	19	4	10	5	0
All	All	4840	1069	4930	163	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 17.

All (163) 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:248:MET:HE1	1:A:280:GLU:HB3	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:VAL:HG11	1:B:284:MET:SD	2.21	0.80
1:B:211:ILE:HD12	1:B:263:MET:HB2	1.66	0.78
1:B:327:LEU:HD12	1:B:330:ILE:HD12	1.66	0.76
1:B:281:CYS:HB3	1:B:316:ILE:HD12	1.68	0.75
1:B:226:TYR:HE2	1:B:261:ILE:HG21	1.51	0.75
1:B:218:GLU:HB3	1:B:267:ASN:HB2	1.71	0.73
1:B:114:VAL:HB	1:B:139:TYR:HB2	1.71	0.71
1:A:185:MET:SD	1:B:53:ILE:HG13	2.32	0.69
1:A:155:PRO:HD2	1:A:158:ASN:ND2	2.07	0.69
1:B:209:TYR:HA	1:B:261:ILE:HG22	1.73	0.69
1:B:96:THR:HB	1:B:99:ASP:HB2	1.75	0.67
1:A:174:VAL:HG22	1:A:183:CYS:SG	2.35	0.67
1:A:155:PRO:HD2	1:A:158:ASN:HD22	1.59	0.66
1:A:107:PRO:HA	1:A:110:ARG:HG3	1.79	0.64
1:B:29:GLU:HA	1:B:32:GLN:OE1	1.99	0.62
1:B:44:ILE:O	1:B:48:VAL:HG23	2.01	0.60
1:A:125:ASN:HB3	1:A:130:VAL:HB	1.83	0.60
3:A:336:AHG:H2	3:A:336:AHG:O3P	1.99	0.60
1:B:96:THR:HG22	1:B:97:GLU:N	2.18	0.59
1:B:226:TYR:CE2	1:B:261:ILE:HG21	2.36	0.59
1:B:261:ILE:HG23	1:B:263:MET:HE2	1.84	0.59
1:B:150:LYS:HA	1:B:153:LEU:HD12	1.83	0.59
1:B:274:LYS:HZ3	3:B:336:AHG:H61	1.68	0.58
1:B:95:VAL:HB	1:B:116:CYS:HB2	1.84	0.58
1:A:112:LYS:HD2	1:A:140:ARG:NH2	2.19	0.58
1:B:288:MET:HG3	1:B:318:LEU:HD22	1.86	0.57
1:A:90:ALA:HA	1:A:111:GLY:HA3	1.86	0.57
1:B:187:ASP:HB2	1:B:194:ILE:HD11	1.86	0.57
1:A:172:MET:SD	1:A:183:CYS:HB3	2.46	0.56
1:B:274:LYS:NZ	3:B:336:AHG:H61	2.21	0.56
1:A:209:TYR:CZ	1:A:242:ALA:HB2	2.40	0.56
1:B:310:ILE:HG13	1:B:311:HIS:CD2	2.41	0.56
1:A:281:CYS:SG	1:A:314:ALA:HB3	2.46	0.55
1:B:96:THR:HG22	1:B:98:GLU:H	1.70	0.55
1:B:330:ILE:HG23	1:B:333:LYS:HZ2	1.71	0.55
1:A:15:ARG:HH11	1:A:15:ARG:HG2	1.71	0.55
1:B:182:ASN:ND2	1:B:198:ARG:HA	2.21	0.55
1:B:40:ALA:HB2	1:B:84:VAL:HG21	1.89	0.55
1:A:9:ASN:HD21	1:A:15:ARG:HH21	1.54	0.54
1:B:133:GLY:HA3	1:B:249:VAL:HG21	1.88	0.54
1:B:176:ALA:HB2	1:B:181:VAL:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:VAL:HG21	1:B:284:MET:CG	2.38	0.54
1:A:92:CYS:HA	1:A:105:VAL:HB	1.89	0.54
1:A:114:VAL:O	1:A:138:ILE:HA	2.07	0.54
1:B:330:ILE:HG23	1:B:333:LYS:NZ	2.22	0.54
1:B:11:VAL:HG12	1:B:16:PHE:HB2	1.90	0.54
1:A:283:PRO:O	1:A:287:VAL:HG23	2.08	0.53
1:B:210:SER:HB3	1:B:262:PHE:HA	1.90	0.53
1:A:81:VAL:HA	1:A:84:VAL:HG22	1.91	0.53
1:A:81:VAL:O	1:A:85:LEU:HG	2.08	0.53
1:B:136:PHE:O	1:B:283:PRO:HB3	2.09	0.53
1:B:120:LEU:HG	1:B:132:ILE:HD12	1.90	0.53
1:A:31:THR:O	1:A:35:ASN:HB2	2.10	0.52
1:B:277:LEU:HB3	1:B:312:GLN:O	2.11	0.51
1:A:209:TYR:CE1	1:A:242:ALA:HB2	2.45	0.51
1:A:212:ASN:HB2	1:A:244:TYR:CE2	2.45	0.51
1:B:263:MET:HG2	1:B:317:ILE:HG23	1.93	0.51
1:B:94:LEU:HB2	1:B:103:ILE:HD13	1.92	0.51
1:B:166:LEU:O	1:B:171:THR:HA	2.11	0.51
1:B:171:THR:HB	1:B:186:LEU:HD23	1.93	0.50
1:B:248:MET:N	3:B:336:AHG:O3	2.44	0.50
1:B:205:LYS:NZ	1:B:205:LYS:HB2	2.27	0.50
1:B:289:GLU:HG2	1:B:294:LEU:HA	1.94	0.50
1:A:235:ASP:HB2	1:A:237:SER:OG	2.12	0.49
1:B:330:ILE:HA	1:B:333:LYS:HG2	1.93	0.49
1:A:93:VAL:HB	1:A:114:VAL:HG13	1.94	0.49
1:B:212:ASN:HB2	1:B:244:TYR:CE2	2.47	0.49
1:B:103:ILE:H	1:B:103:ILE:HD12	1.77	0.49
1:B:116:CYS:SG	1:B:278:LEU:HD13	2.52	0.49
1:B:288:MET:HG3	1:B:318:LEU:HD13	1.94	0.49
1:B:280:GLU:O	1:B:283:PRO:HD2	2.13	0.49
1:A:179:ASN:H	1:A:179:ASN:ND2	2.11	0.48
1:B:154:GLN:O	1:B:307:PRO:HG3	2.14	0.48
1:B:210:SER:N	1:B:261:ILE:O	2.47	0.48
1:A:114:VAL:HB	1:A:139:TYR:HB2	1.96	0.48
1:B:276:ARG:NH1	1:B:313:ARG:HD3	2.29	0.48
1:B:252:VAL:HG21	1:B:284:MET:HG2	1.95	0.48
1:A:74:ASP:HA	1:A:77:SER:OG	2.13	0.48
1:A:128:CYS:O	1:A:129:LEU:HB2	2.14	0.47
1:A:20:GLN:O	1:A:23:LYS:HB2	2.14	0.47
1:A:141:LYS:HG3	1:A:151:ASP:OD1	2.14	0.47
1:A:286:TYR:HA	1:A:303:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:THR:HG22	1:A:315:PRO:O	2.14	0.47
1:B:122:GLY:H	3:B:336:AHG:P1	2.37	0.47
1:A:210:SER:HB3	1:A:262:PHE:HA	1.97	0.47
1:A:215:TYR:HB2	1:A:219:PHE:CE1	2.50	0.47
1:A:309:ASP:HB3	1:A:312:GLN:HB3	1.96	0.47
1:B:202:ILE:HG12	1:B:320:SER:OG	2.14	0.47
1:B:252:VAL:HG21	1:B:284:MET:SD	2.55	0.47
1:B:242:ALA:O	1:B:243:ARG:HG2	2.15	0.47
1:A:232:PHE:CD2	1:B:217:LYS:HG2	2.50	0.46
1:A:274:LYS:O	1:A:313:ARG:HD3	2.14	0.46
1:A:317:ILE:HG22	1:A:324:VAL:HG13	1.98	0.46
1:B:95:VAL:HG11	1:B:278:LEU:HD12	1.97	0.46
1:B:181:VAL:O	1:B:200:VAL:HG23	2.16	0.46
1:B:155:PRO:HB3	1:B:307:PRO:HD3	1.97	0.46
1:B:299:LYS:HG3	1:B:300:GLU:H	1.80	0.45
1:B:183:CYS:HB2	1:B:197:ASP:HB2	1.98	0.45
1:A:204:LYS:O	1:A:320:SER:HB3	2.16	0.45
1:A:231:LYS:O	1:A:239:PRO:HB3	2.16	0.45
1:B:275:LEU:O	1:B:281:CYS:SG	2.75	0.45
1:B:80:LEU:O	1:B:84:VAL:HG22	2.16	0.45
1:B:170:ALA:CB	1:B:185:MET:HE2	2.46	0.45
1:A:115:VAL:HG22	1:A:138:ILE:HG12	1.99	0.45
1:B:29:GLU:HB3	1:B:113:TYR:HE2	1.82	0.45
1:A:13:LEU:HD13	1:A:38:CYS:SG	2.56	0.44
1:A:72:LYS:HG2	1:A:73:LEU:H	1.81	0.44
1:B:90:ALA:O	1:B:113:TYR:HB2	2.16	0.44
1:A:80:LEU:O	1:A:84:VAL:HG13	2.17	0.44
1:B:37:LEU:HD21	1:B:136:PHE:CE2	2.53	0.44
1:B:161:ALA:HA	1:B:286:TYR:HE2	1.83	0.44
1:B:187:ASP:CB	1:B:194:ILE:HD11	2.48	0.44
1:B:226:TYR:HB2	1:B:327:LEU:HD13	1.99	0.44
1:B:231:LYS:O	1:B:239:PRO:HB3	2.18	0.44
1:B:282:ASN:HD22	1:B:302:VAL:HG12	1.82	0.44
1:A:267:ASN:O	1:A:271:PRO:HA	2.18	0.43
1:A:216:ALA:HA	1:A:219:PHE:CD2	2.52	0.43
1:A:218:GLU:HB3	1:A:268:LYS:HD2	1.99	0.43
1:B:197:ASP:HB3	1:B:200:VAL:HG22	2.00	0.43
1:A:119:PRO:HA	1:A:134:THR:HG23	2.00	0.43
1:B:230:LYS:HB3	1:B:240:TYR:HB2	2.01	0.43
1:A:177:MET:HB2	1:A:177:MET:HE3	1.83	0.43
1:B:308:THR:HB	1:B:312:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LYS:HG3	1:A:101:ASN:H	1.84	0.43
1:B:269:LYS:O	1:B:270:SER:HB2	2.17	0.43
1:A:232:PHE:CZ	1:B:217:LYS:HA	2.54	0.43
1:B:282:ASN:HD22	1:B:282:ASN:HA	1.72	0.43
1:B:17:VAL:O	1:B:20:GLN:HB2	2.19	0.43
1:B:122:GLY:N	3:B:336:AHG:O2P	2.51	0.42
1:B:288:MET:SD	1:B:318:LEU:HD13	2.59	0.42
1:A:295:ALA:CB	1:A:318:LEU:HB3	2.49	0.42
1:A:169:SER:O	1:B:49:ARG:HA	2.20	0.42
1:B:208:ILE:HA	1:B:241:GLY:O	2.19	0.42
1:A:310:ILE:HG13	1:A:311:HIS:N	2.34	0.42
1:B:115:VAL:HG13	1:B:138:ILE:HG12	2.01	0.42
1:B:226:TYR:HB2	1:B:327:LEU:CD1	2.50	0.42
1:A:233:PRO:HD3	1:A:239:PRO:HG3	2.01	0.42
1:B:244:TYR:HE1	1:B:262:PHE:HE1	1.68	0.42
1:A:13:LEU:C	1:A:13:LEU:HD23	2.45	0.42
1:A:29:GLU:HB3	1:A:90:ALA:HB1	2.02	0.42
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.81	0.42
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.70	0.42
1:A:212:ASN:O	1:A:219:PHE:HZ	2.02	0.42
1:A:281:CYS:SG	1:A:316:ILE:HD12	2.59	0.42
1:A:140:ARG:HD3	1:A:140:ARG:C	2.45	0.41
1:B:243:ARG:HG2	1:B:243:ARG:NH1	2.35	0.41
1:B:256:LEU:HD13	1:B:288:MET:HE1	2.03	0.41
1:B:261:ILE:HD12	1:B:261:ILE:HA	1.93	0.41
1:A:266:ALA:HB1	1:A:271:PRO:O	2.20	0.41
1:A:204:LYS:HZ2	1:A:204:LYS:HA	1.85	0.41
1:A:166:LEU:HD13	1:A:249:VAL:HG12	2.02	0.41
1:A:238:ALA:HA	1:A:239:PRO:HD3	1.93	0.41
1:B:187:ASP:OD1	1:B:189:ALA:HB3	2.20	0.41
1:B:78:ASN:CG	1:B:96:THR:HG21	2.46	0.41
1:B:172:MET:HA	1:B:184:PHE:O	2.21	0.41
1:A:141:LYS:HE3	1:A:143:SER:O	2.20	0.41
1:A:266:ALA:H	1:A:315:PRO:HB3	1.86	0.41
1:B:309:ASP:O	1:B:312:GLN:HB2	2.21	0.41
1:A:209:TYR:HA	1:A:261:ILE:HG23	2.03	0.40
1:A:130:VAL:HG12	1:A:131:SER:O	2.21	0.40
1:A:112:LYS:HD2	1:A:140:ARG:HH21	1.87	0.40
1:B:6:PHE:HD1	1:B:6:PHE:HA	1.66	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	309/335 (92%)	276 (89%)	31 (10%)	2 (1%)	21	56
1	B	311/335 (93%)	257 (83%)	39 (12%)	15 (5%)	2	11
All	All	620/670 (92%)	533 (86%)	70 (11%)	17 (3%)	4	22

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	B	27	THR
1	B	73	LEU
1	B	100	LYS
1	B	276	ARG
1	A	92	CYS
1	B	156	GLY
1	B	157	ARG
1	B	199	ASN
1	B	270	SER
1	B	277	LEU
1	B	178	VAL
1	B	236	ASN
1	B	6	PHE
1	B	74	ASP
1	B	256	LEU
1	B	31	THR

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	261/278 (94%)	226 (87%)	35 (13%)	4	18
1	B	262/278 (94%)	222 (85%)	40 (15%)	3	14
All	All	523/556 (94%)	448 (86%)	75 (14%)	3	16

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	27	THR
1	A	46	THR
1	A	73	LEU
1	A	74	ASP
1	A	76	LEU
1	A	77	SER
1	A	99	ASP
1	A	108	GLU
1	A	124	SER
1	A	131	SER
1	A	140	ARG
1	A	147	PRO
1	A	150	LYS
1	A	169	SER
1	A	172	MET
1	A	178	VAL
1	A	199	ASN
1	A	204	LYS
1	A	207	SER
1	A	218	GLU
1	A	224	THR
1	A	225	GLU
1	A	229	ARG
1	A	235	ASP
1	A	265	PRO
1	A	268	LYS
1	A	270	SER
1	A	276	ARG
1	A	279	TYR
1	A	300	GLU
1	A	306	VAL
1	A	308	THR
1	A	317	ILE

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Mol	Chain	Res	Type
1	A	334	HIS
1	B	7	ASP
1	B	10	ILE
1	B	13	LEU
1	B	17	VAL
1	B	18	MET
1	B	25	ARG
1	B	29	GLU
1	B	33	LEU
1	B	84	VAL
1	B	91	THR
1	B	98	GLU
1	B	99	ASP
1	B	101	ASN
1	B	103	ILE
1	B	108	GLU
1	B	120	LEU
1	B	123	SER
1	B	129	LEU
1	B	131	SER
1	B	135	ILE
1	B	143	SER
1	B	146	GLU
1	B	149	GLU
1	B	173	LEU
1	B	178	VAL
1	B	181	VAL
1	B	194	ILE
1	B	195	LEU
1	B	196	VAL
1	B	201	LYS
1	B	205	LYS
1	B	207	SER
1	B	208	ILE
1	B	249	VAL
1	B	265	PRO
1	B	278	LEU
1	B	282	ASN
1	B	294	LEU
1	B	312	GLN
1	B	330	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	32	GLN
1	A	142	ASN
1	A	179	ASN
1	A	199	ASN
1	A	332	GLN
1	B	182	ASN
1	B	199	ASN
1	B	282	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	AHG	B	336	2	19,19,19	0.67	0	27,29,29	0.89	1 (3%)
3	AHG	A	336	2	19,19,19	0.69	0	27,29,29	0.84	1 (3%)

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	AHG	B	336	2	-	11/12/28/28	0/1/1/1
3	AHG	A	336	2	-	11/12/28/28	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	336	AHG	O2P-P1-O1P	2.21	119.43	110.83
3	A	336	AHG	O2P-P1-O1P	2.10	119.01	110.83

There are no chirality outliers.

All (22) torsion outliers are listed below:

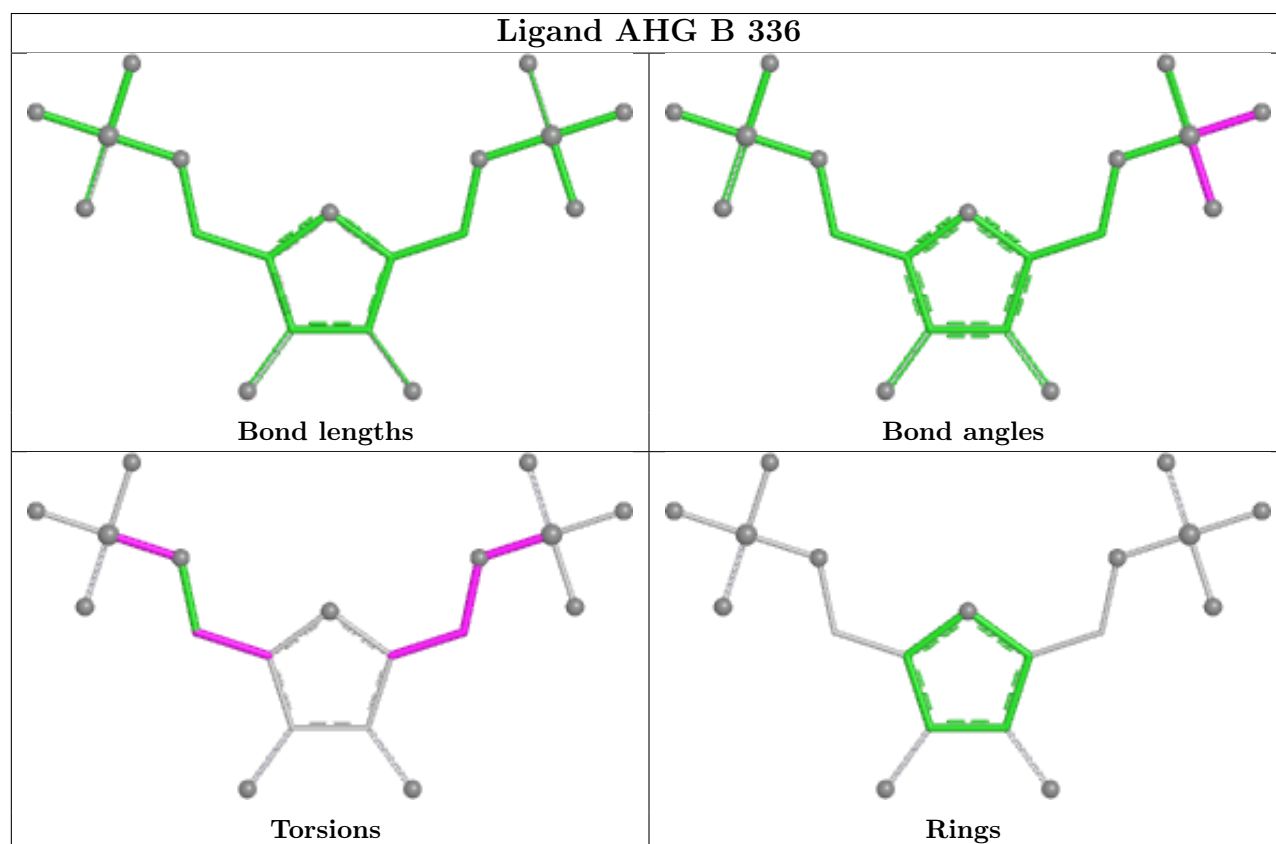
Mol	Chain	Res	Type	Atoms
3	A	336	AHG	C1-O1-P1-O1P
3	A	336	AHG	C1-O1-P1-O2P
3	A	336	AHG	C1-O1-P1-O3P
3	A	336	AHG	C2-C1-O1-P1
3	A	336	AHG	C6-O6-P2-O5P
3	A	336	AHG	C6-O6-P2-O6P
3	B	336	AHG	C1-O1-P1-O1P
3	B	336	AHG	C1-O1-P1-O2P
3	B	336	AHG	C1-O1-P1-O3P
3	B	336	AHG	C6-O6-P2-O4P
3	B	336	AHG	C6-O6-P2-O5P
3	B	336	AHG	C6-O6-P2-O6P
3	A	336	AHG	C4-C5-C6-O6
3	B	336	AHG	O1-C1-C2-C3
3	B	336	AHG	O1-C1-C2-O5
3	B	336	AHG	C4-C5-C6-O6
3	B	336	AHG	O5-C5-C6-O6
3	A	336	AHG	O5-C5-C6-O6
3	A	336	AHG	O1-C1-C2-O5
3	A	336	AHG	O1-C1-C2-C3
3	B	336	AHG	C2-C1-O1-P1
3	A	336	AHG	C6-O6-P2-O4P

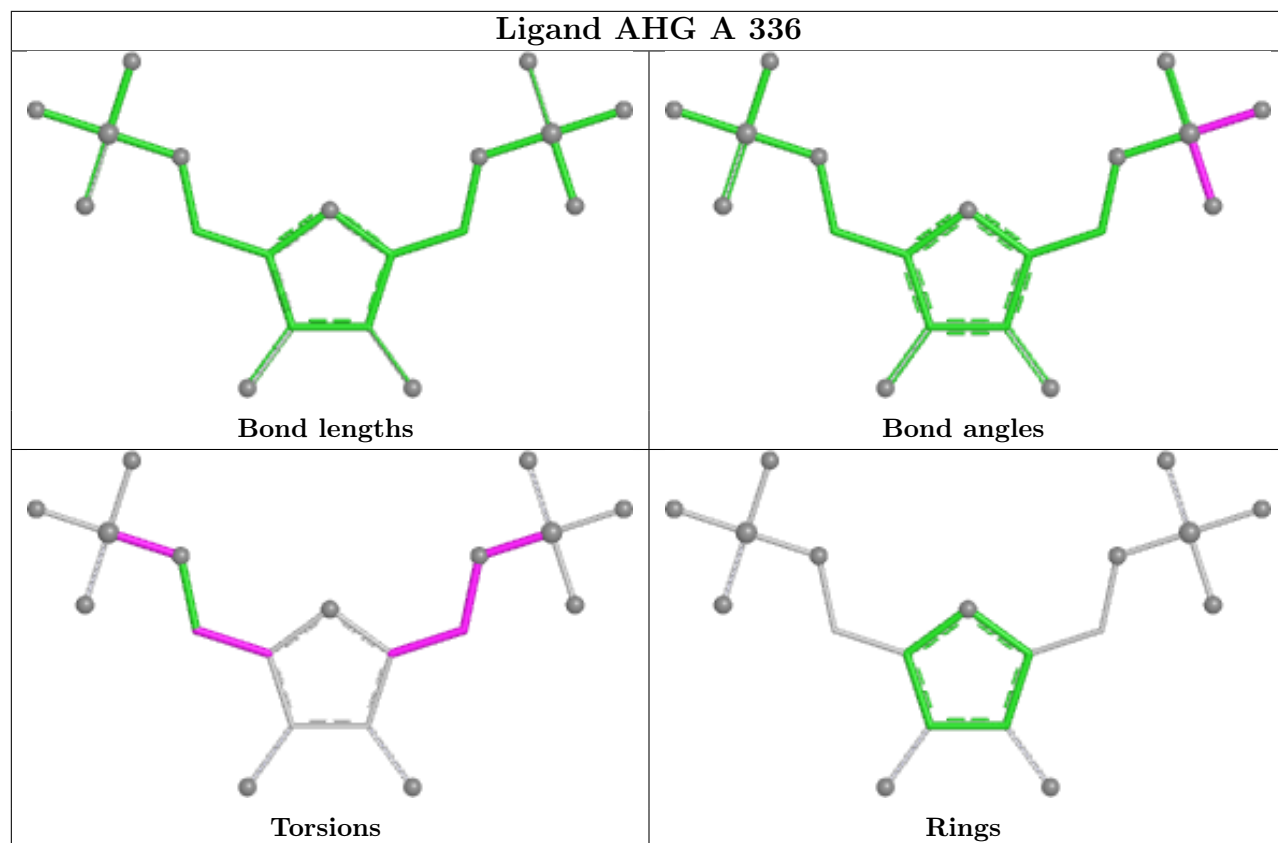
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	336	AHG	5	0
3	A	336	AHG	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.