



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2EIB / pdb_00002eib
Title : Crystal Structure of Galactose Oxidase, W290H mutant
Authors : Phillips, S.E.; McPherson, M.J.; Knowles, P.F.; Wilmot, C.
Deposited on : 2007-03-12
Resolution : 2.10 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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

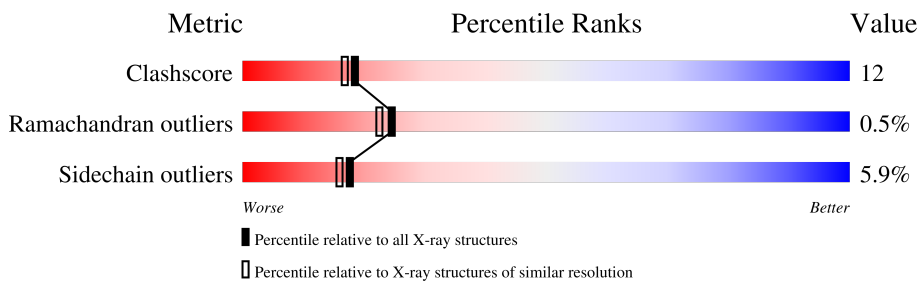
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	639	 41% 44% 14% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5171 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 Galactose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	639	4826	3012	841	954	19	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	HIS	TRP	engineered mutation	UNP Q01745

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	326	Total 326	O 326	0	0

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: Galactose oxidase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.00Å 89.40Å 86.70Å 90.00° 117.80° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.157 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5171	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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: ACT, NA, SO4, CU

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	1.36	17/4954 (0.3%)	2.68	437/6757 (6.5%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	590	ILE	N-CA	7.65	1.52	1.46
1	A	619	MET	N-CA	7.42	1.54	1.46
1	A	62	THR	CA-CB	6.46	1.61	1.53
1	A	440	THR	C-O	6.09	1.31	1.23
1	A	491	ILE	CA-C	-5.96	1.45	1.52
1	A	315	ALA	C-N	-5.81	1.25	1.33
1	A	391	ALA	N-CA	5.66	1.53	1.46
1	A	396	ILE	CA-CB	5.65	1.61	1.54
1	A	359	THR	CA-CB	5.45	1.61	1.53
1	A	250	THR	CA-CB	5.39	1.62	1.53
1	A	170	VAL	N-CA	5.33	1.50	1.46
1	A	403	PRO	CA-CB	-5.33	1.46	1.53
1	A	188	SER	N-CA	5.16	1.52	1.46
1	A	435	LEU	C-N	-5.06	1.27	1.33
1	A	356	TRP	NE1-CE2	-5.04	1.31	1.37
1	A	631	VAL	N-CA	5.03	1.52	1.46
1	A	497	SER	N-CA	5.02	1.51	1.45

All (437) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	ARG	CD-NE-CZ	30.97	167.76	124.40
1	A	406	GLN	CA-C-O	-13.62	106.62	121.33
1	A	406	GLN	O-C-N	12.72	137.75	123.25
1	A	84	ARG	CD-NE-CZ	12.32	141.65	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	559	ARG	CD-NE-CZ	12.15	141.41	124.40
1	A	333	ASN	CA-CB-CG	11.70	124.30	112.60
1	A	273	GLN	OE1-CD-NE2	-11.39	111.21	122.60
1	A	104	SER	O-C-N	11.27	136.97	123.33
1	A	466	ASP	CA-CB-CG	11.16	123.76	112.60
1	A	489	ASN	OD1-CG-ND2	11.06	133.66	122.60
1	A	506	ARG	CD-NE-CZ	10.99	139.79	124.40
1	A	609	ASP	CA-CB-CG	10.39	122.99	112.60
1	A	218	THR	O-C-N	10.21	134.86	123.22
1	A	224	HIS	CA-CB-CG	10.19	123.99	113.80
1	A	28	ASN	CA-CB-CG	10.10	122.70	112.60
1	A	265	ASP	CA-CB-CG	10.05	122.65	112.60
1	A	493	ARG	NE-CZ-NH2	-10.02	110.18	119.20
1	A	632	ALA	CA-C-O	-9.91	110.97	121.87
1	A	283	VAL	CA-C-O	9.84	130.72	120.39
1	A	369	GLY	CA-C-N	9.83	137.19	122.93
1	A	369	GLY	C-N-CA	9.83	137.19	122.93
1	A	286	ILE	O-C-N	9.74	133.44	122.82
1	A	330	ARG	NE-CZ-NH1	9.66	131.16	121.50
1	A	46	ASN	CA-CB-CG	9.48	122.08	112.60
1	A	69	SER	CB-CA-C	9.46	130.56	109.56
1	A	345	VAL	CA-C-O	9.46	129.61	120.25
1	A	587	GLN	OE1-CD-NE2	9.38	131.98	122.60
1	A	417	ILE	CA-C-O	-9.18	110.75	120.48
1	A	487	ASN	CA-CB-CG	-8.97	103.63	112.60
1	A	342	LYS	N-CA-CB	-8.94	98.52	111.84
1	A	286	ILE	CA-C-O	-8.89	112.56	121.45
1	A	283	VAL	O-C-N	-8.87	113.68	123.26
1	A	401	GLY	CA-C-O	-8.83	113.46	122.56
1	A	589	ARG	CD-NE-CZ	-8.79	112.09	124.40
1	A	370	LYS	N-CA-C	8.76	123.69	109.59
1	A	208	ASP	CA-CB-CG	-8.69	103.91	112.60
1	A	30	ALA	CA-C-O	-8.69	108.69	119.38
1	A	71	LEU	N-CA-C	-8.57	97.19	109.62
1	A	200	GLY	N-CA-C	8.56	126.75	115.36
1	A	439	ARG	NE-CZ-NH2	8.52	126.87	119.20
1	A	578	THR	CA-CB-OG1	-8.52	96.83	109.60
1	A	131	GLU	N-CA-C	-8.49	96.82	110.32
1	A	200	GLY	CA-C-O	8.47	128.43	119.02
1	A	342	LYS	N-CA-C	8.42	122.99	111.54
1	A	416	ILE	N-CA-CB	8.42	122.58	111.64
1	A	589	ARG	CA-C-N	-8.38	111.47	123.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	589	ARG	C-N-CA	-8.38	111.47	123.28
1	A	333	ASN	O-C-N	8.25	132.19	122.94
1	A	425	SER	CB-CA-C	8.24	119.56	110.08
1	A	249	LYS	CA-C-N	8.17	134.48	122.39
1	A	249	LYS	C-N-CA	8.17	134.48	122.39
1	A	631	VAL	N-CA-C	-8.14	98.31	109.55
1	A	593	THR	CB-CA-C	8.10	123.74	110.78
1	A	440	THR	CA-CB-OG1	-8.02	97.57	109.60
1	A	506	ARG	NE-CZ-NH1	7.98	129.48	121.50
1	A	422	PRO	CB-CA-C	7.96	121.58	111.39
1	A	169	ILE	CA-C-O	-7.91	113.61	121.67
1	A	114	SER	N-CA-CB	7.89	123.70	110.69
1	A	184	LEU	CA-C-O	7.88	129.02	120.43
1	A	506	ARG	NH1-CZ-NH2	-7.87	109.07	119.30
1	A	170	VAL	N-CA-C	-7.86	99.83	107.76
1	A	53	HIS	N-CA-C	-7.82	97.21	109.72
1	A	595	THR	CA-CB-OG1	-7.79	97.91	109.60
1	A	495	TYR	CB-CA-C	7.76	121.48	109.84
1	A	578	THR	OG1-CB-CG2	7.75	124.79	109.30
1	A	169	ILE	O-C-N	7.74	131.51	123.00
1	A	282	ARG	CD-NE-CZ	7.74	135.23	124.40
1	A	92	ASP	CA-CB-CG	7.71	120.31	112.60
1	A	20	SER	N-CA-CB	7.71	125.87	111.53
1	A	439	ARG	CA-CB-CG	7.71	129.51	114.10
1	A	61	THR	CA-C-N	7.70	133.67	121.66
1	A	61	THR	C-N-CA	7.70	133.67	121.66
1	A	99	PRO	CA-C-O	-7.70	112.66	121.36
1	A	104	SER	CA-C-O	-7.65	111.42	120.60
1	A	493	ARG	NH1-CZ-NH2	7.62	129.20	119.30
1	A	586	ASP	CA-CB-CG	-7.62	104.98	112.60
1	A	130	THR	N-CA-C	7.55	120.93	109.23
1	A	330	ARG	NE-CZ-NH2	-7.53	112.42	119.20
1	A	485	LYS	CB-CG-CD	7.53	128.62	111.30
1	A	20	SER	O-C-N	7.52	132.00	123.27
1	A	364	ASP	CA-C-O	7.51	129.34	121.38
1	A	137	TRP	N-CA-C	7.50	121.61	110.52
1	A	255	SER	CA-C-O	7.45	128.45	120.55
1	A	50	LYS	O-C-N	7.44	129.87	121.53
1	A	299	GLY	CA-C-O	-7.44	112.57	122.24
1	A	238	GLN	OE1-CD-NE2	7.43	130.03	122.60
1	A	593	THR	CA-C-O	7.42	128.26	120.54
1	A	575	ARG	CA-C-N	7.42	131.28	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	ARG	C-N-CA	7.42	131.28	120.82
1	A	142	GLU	CA-C-N	7.38	133.99	122.70
1	A	142	GLU	C-N-CA	7.38	133.99	122.70
1	A	384	GLY	N-CA-C	-7.36	101.01	112.85
1	A	566	SER	O-C-N	7.31	131.58	123.25
1	A	20	SER	CA-CB-OG	7.29	125.67	111.10
1	A	167	LEU	N-CA-C	7.28	120.81	110.40
1	A	453	PHE	CA-C-N	7.25	132.75	123.10
1	A	453	PHE	C-N-CA	7.25	132.75	123.10
1	A	309	TRP	CA-C-O	-7.25	113.02	120.71
1	A	230	GLY	CA-C-O	-7.25	114.80	121.18
1	A	556	VAL	CA-C-O	-7.25	113.39	121.36
1	A	315	ALA	CA-C-N	7.24	131.08	120.95
1	A	315	ALA	C-N-CA	7.24	131.08	120.95
1	A	318	ASN	CB-CA-C	7.21	128.02	112.38
1	A	41	THR	CA-C-O	-7.19	113.67	121.94
1	A	182	ARG	CA-CB-CG	-7.17	99.75	114.10
1	A	77	ASN	CA-C-N	7.17	134.28	121.66
1	A	77	ASN	C-N-CA	7.17	134.28	121.66
1	A	253	TYR	O-C-N	7.17	131.73	123.27
1	A	362	SER	N-CA-C	-7.15	105.39	112.97
1	A	282	ARG	NE-CZ-NH1	7.15	128.65	121.50
1	A	128	ALA	CA-C-O	-7.14	112.94	120.58
1	A	587	GLN	CA-C-O	7.14	129.34	121.56
1	A	565	ASP	N-CA-C	-7.13	104.60	113.38
1	A	68	LEU	CA-CB-CG	7.12	141.22	116.30
1	A	633	SER	N-CA-C	-7.11	97.81	109.40
1	A	530	PRO	CB-CA-C	7.11	120.26	110.95
1	A	102	SER	CA-C-O	-7.08	113.31	121.10
1	A	299	GLY	O-C-N	7.08	132.23	122.82
1	A	236	ASN	CA-CB-CG	7.07	119.67	112.60
1	A	266	MET	O-C-N	7.07	130.91	122.85
1	A	137	TRP	O-C-N	7.06	130.85	122.94
1	A	402	SER	O-C-N	7.06	126.23	121.71
1	A	233	MET	N-CA-C	-7.05	97.75	108.96
1	A	201	ILE	O-C-N	7.04	130.87	123.05
1	A	99	PRO	O-C-N	7.04	131.83	122.89
1	A	457	GLY	CA-C-N	7.02	133.59	122.21
1	A	457	GLY	C-N-CA	7.02	133.59	122.21
1	A	290	HIS	CA-C-O	7.02	128.04	119.97
1	A	635	ILE	CB-CG1-CD1	7.01	128.52	113.80
1	A	217	ARG	CB-CG-CD	7.00	127.41	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	GLY	O-C-N	6.99	129.54	122.90
1	A	446	VAL	O-C-N	-6.99	114.98	122.95
1	A	255	SER	N-CA-C	6.99	118.89	111.28
1	A	526	GLN	OE1-CD-NE2	6.96	129.56	122.60
1	A	465	GLU	CA-C-O	6.94	127.86	120.36
1	A	374	ASN	OD1-CG-ND2	-6.92	115.68	122.60
1	A	506	ARG	O-C-N	-6.91	115.20	122.94
1	A	575	ARG	N-CA-CB	-6.90	99.83	109.97
1	A	548	ARG	NE-CZ-NH1	6.88	128.38	121.50
1	A	603	SER	O-C-N	6.87	131.24	123.27
1	A	285	THR	CA-CB-OG1	-6.86	99.31	109.60
1	A	299	GLY	N-CA-C	6.86	119.88	112.33
1	A	514	LEU	CA-C-O	6.84	130.29	120.51
1	A	69	SER	O-C-N	-6.82	115.36	123.27
1	A	70	MET	O-C-N	6.81	131.99	123.14
1	A	217	ARG	CG-CD-NE	6.79	126.94	112.00
1	A	332	ASP	CA-CB-CG	6.78	119.38	112.60
1	A	192	ASP	N-CA-C	6.77	121.51	112.30
1	A	34	ASN	OD1-CG-ND2	6.76	129.36	122.60
1	A	318	ASN	O-C-N	-6.76	114.13	120.55
1	A	273	GLN	CG-CD-NE2	6.75	126.53	116.40
1	A	266	MET	N-CA-C	-6.74	101.45	110.55
1	A	140	ILE	CA-C-O	-6.72	113.59	120.25
1	A	339	GLY	N-CA-C	-6.72	102.40	111.54
1	A	478	PRO	CA-C-N	6.72	129.29	120.28
1	A	478	PRO	C-N-CA	6.72	129.29	120.28
1	A	41	THR	O-C-N	6.72	130.91	122.65
1	A	213	ILE	CB-CA-C	-6.71	102.43	111.15
1	A	247	ALA	CA-C-O	-6.69	111.71	119.61
1	A	511	GLY	O-C-N	6.68	129.54	122.86
1	A	58	ASP	N-CA-CB	6.66	121.18	110.65
1	A	185	MET	CG-SD-CE	6.65	115.53	100.90
1	A	298	ASN	N-CA-CB	6.64	119.55	110.38
1	A	220	THR	CA-C-N	6.63	129.88	120.53
1	A	220	THR	C-N-CA	6.63	129.88	120.53
1	A	141	ALA	CA-C-N	6.63	132.96	122.62
1	A	141	ALA	C-N-CA	6.63	132.96	122.62
1	A	48	ASP	O-C-N	6.62	127.45	121.42
1	A	138	THR	CA-CB-OG1	-6.62	99.67	109.60
1	A	216	ASP	CA-CB-CG	6.59	119.19	112.60
1	A	74	GLN	OE1-CD-NE2	6.57	129.17	122.60
1	A	274	SER	O-C-N	6.57	131.44	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	627	GLY	O-C-N	6.57	129.79	122.50
1	A	617	TYR	CA-C-O	-6.56	113.49	121.36
1	A	182	ARG	CD-NE-CZ	-6.55	115.22	124.40
1	A	546	ILE	N-CA-CB	6.52	119.42	111.60
1	A	168	PRO	CB-CA-C	-6.50	102.19	111.68
1	A	66	ASN	CA-CB-CG	6.48	119.08	112.60
1	A	399	PHE	N-CA-C	6.45	118.88	109.07
1	A	417	ILE	CA-C-N	-6.43	114.04	123.05
1	A	417	ILE	C-N-CA	-6.43	114.04	123.05
1	A	566	SER	CA-CB-OG	6.43	123.97	111.10
1	A	364	ASP	O-C-N	-6.38	116.56	123.26
1	A	434	GLY	CA-C-O	-6.37	116.00	122.56
1	A	482	THR	CA-CB-OG1	-6.37	100.04	109.60
1	A	170	VAL	CA-CB-CG1	6.36	121.22	110.40
1	A	257	SER	CA-CB-OG	6.36	123.81	111.10
1	A	632	ALA	O-C-N	6.35	130.18	122.75
1	A	411	THR	CA-C-O	6.33	129.15	121.68
1	A	352	THR	N-CA-C	-6.33	104.30	111.07
1	A	218	THR	CA-CB-OG1	-6.29	100.16	109.60
1	A	467	SER	CA-C-N	6.29	137.15	121.80
1	A	467	SER	C-N-CA	6.29	137.15	121.80
1	A	69	SER	N-CA-C	-6.27	99.52	109.23
1	A	278	MET	N-CA-CB	-6.25	100.77	110.46
1	A	395	LYS	O-C-N	6.25	130.32	123.13
1	A	449	ASP	CA-C-O	-6.25	111.72	119.28
1	A	294	VAL	CA-C-O	-6.24	112.57	120.86
1	A	146	PHE	CA-CB-CG	-6.23	107.57	113.80
1	A	517	ASP	N-CA-C	6.23	118.87	111.71
1	A	519	THR	CA-CB-OG1	-6.21	100.28	109.60
1	A	270	ARG	N-CA-CB	-6.21	100.89	111.69
1	A	358	TYR	CA-C-O	-6.20	114.15	121.16
1	A	273	GLN	N-CA-C	-6.18	102.21	110.55
1	A	544	PRO	N-CA-C	-6.17	101.57	111.38
1	A	639	GLN	N-CA-CB	6.17	120.98	110.50
1	A	109	SER	O-C-N	6.15	129.82	122.26
1	A	170	VAL	N-CA-CB	6.14	118.82	111.08
1	A	91	SER	N-CA-C	-6.14	105.95	113.50
1	A	555	LYS	CA-C-O	-6.13	114.49	121.72
1	A	119	ARG	CD-NE-CZ	6.12	132.97	124.40
1	A	236	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	A	596	ASN	OD1-CG-ND2	6.10	128.70	122.60
1	A	38	PHE	CA-CB-CG	6.09	119.89	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	SER	N-CA-CB	6.09	122.02	111.13
1	A	596	ASN	CB-CG-ND2	-6.06	107.32	116.40
1	A	601	SER	O-C-N	6.05	130.39	123.31
1	A	230	GLY	N-CA-C	-6.05	100.91	111.62
1	A	582	THR	CA-C-N	6.04	130.26	121.80
1	A	582	THR	C-N-CA	6.04	130.26	121.80
1	A	625	SER	O-C-N	6.03	130.78	122.46
1	A	345	VAL	O-C-N	-6.01	116.84	123.03
1	A	50	LYS	CA-C-O	-6.00	114.16	120.88
1	A	94	THR	CA-C-O	5.98	126.76	119.64
1	A	108	ASP	CA-CB-CG	5.98	118.58	112.60
1	A	265	ASP	O-C-N	5.98	129.71	122.96
1	A	418	THR	CA-CB-OG1	-5.96	100.65	109.60
1	A	313	PRO	CA-C-O	-5.96	110.66	119.18
1	A	19	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	317	VAL	CA-C-O	5.94	126.89	120.47
1	A	526	GLN	CB-CG-CD	-5.93	102.52	112.60
1	A	439	ARG	NH1-CZ-NH2	-5.93	111.59	119.30
1	A	344	SER	O-C-N	5.92	129.59	122.85
1	A	442	HIS	CA-C-O	-5.91	115.14	121.94
1	A	267	GLN	O-C-N	5.91	128.89	122.15
1	A	429	VAL	CA-C-O	-5.91	115.78	121.63
1	A	54	THR	N-CA-CB	-5.90	100.31	111.00
1	A	352	THR	CA-CB-OG1	-5.90	100.74	109.60
1	A	418	THR	CA-C-O	-5.90	113.83	120.32
1	A	507	VAL	CA-CB-CG1	5.89	120.41	110.40
1	A	484	TYR	O-C-N	5.86	130.16	123.31
1	A	456	GLY	CA-C-O	-5.82	113.26	122.28
1	A	399	PHE	CA-CB-CG	5.81	119.61	113.80
1	A	370	LYS	CB-CA-C	-5.81	98.92	109.38
1	A	464	PHE	O-C-N	5.81	128.10	121.88
1	A	10	SER	N-CA-CB	5.79	118.58	109.83
1	A	318	ASN	N-CA-CB	-5.79	99.13	110.08
1	A	310	THR	N-CA-CB	5.79	121.47	111.00
1	A	437	PHE	N-CA-C	5.79	117.84	108.41
1	A	491	ILE	CA-C-O	-5.79	114.38	120.57
1	A	277	THR	CA-CB-OG1	-5.78	100.92	109.60
1	A	129	ILE	N-CA-C	-5.78	105.45	111.58
1	A	30	ALA	N-CA-C	-5.78	105.49	112.54
1	A	22	GLN	CA-CB-CG	-5.77	102.56	114.10
1	A	464	PHE	CA-C-N	-5.75	114.89	122.99
1	A	464	PHE	C-N-CA	-5.75	114.89	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	606	VAL	N-CA-C	-5.73	103.70	108.63
1	A	52	PRO	O-C-N	5.72	131.97	121.10
1	A	615	PRO	CB-CA-C	5.72	118.55	111.23
1	A	589	ARG	O-C-N	5.72	130.66	123.23
1	A	23	SER	CA-C-N	-5.71	116.64	123.44
1	A	23	SER	C-N-CA	-5.71	116.64	123.44
1	A	144	ASN	OD1-CG-ND2	5.71	128.31	122.60
1	A	318	ASN	OD1-CG-ND2	5.71	128.31	122.60
1	A	58	ASP	CB-CA-C	5.69	119.89	110.74
1	A	489	ASN	CA-CB-CG	-5.68	106.92	112.60
1	A	22	GLN	CB-CG-CD	5.68	122.26	112.60
1	A	402	SER	CA-C-O	-5.68	115.27	120.50
1	A	68	LEU	CB-CA-C	5.67	119.96	110.43
1	A	618	TRP	CA-C-N	-5.67	114.71	122.93
1	A	618	TRP	C-N-CA	-5.67	114.71	122.93
1	A	243	GLY	O-C-N	5.67	129.01	122.61
1	A	141	ALA	O-C-N	-5.65	115.93	122.03
1	A	439	ARG	CG-CD-NE	5.65	124.43	112.00
1	A	514	LEU	O-C-N	-5.65	115.07	122.59
1	A	151	TYR	N-CA-CB	5.62	119.42	110.65
1	A	128	ALA	N-CA-C	-5.62	99.36	108.41
1	A	479	GLU	CB-CG-CD	5.62	122.16	112.60
1	A	234	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	161	TRP	CB-CG-CD2	-5.61	118.94	126.80
1	A	572	SER	O-C-N	5.59	129.65	123.33
1	A	385	ASN	CB-CG-ND2	5.59	124.79	116.40
1	A	633	SER	N-CA-CB	5.59	120.56	110.83
1	A	184	LEU	O-C-N	-5.59	116.96	123.27
1	A	543	ARG	NH1-CZ-NH2	5.58	126.56	119.30
1	A	217	ARG	CD-NE-CZ	5.58	132.21	124.40
1	A	184	LEU	CB-CA-C	5.57	118.94	109.75
1	A	231	ILE	N-CA-CB	5.57	120.60	111.58
1	A	268	VAL	CA-CB-CG1	5.57	119.87	110.40
1	A	416	ILE	CA-C-N	-5.57	116.29	123.19
1	A	416	ILE	C-N-CA	-5.57	116.29	123.19
1	A	595	THR	CA-C-N	-5.57	114.79	122.30
1	A	595	THR	C-N-CA	-5.57	114.79	122.30
1	A	416	ILE	O-C-N	5.55	129.08	123.20
1	A	173	ALA	CA-C-O	5.55	127.26	120.60
1	A	25	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	A	221	VAL	CA-C-O	-5.54	115.29	121.05
1	A	192	ASP	CB-CG-OD2	5.54	131.13	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	SER	N-CA-C	-5.53	99.02	110.80
1	A	62	THR	CA-C-O	-5.53	114.04	120.62
1	A	252	LEU	O-C-N	5.53	129.88	123.30
1	A	48	ASP	N-CA-C	5.53	119.03	108.97
1	A	557	GLY	N-CA-C	-5.52	108.51	115.08
1	A	574	ILE	CB-CA-C	5.52	118.60	110.77
1	A	137	TRP	CB-CA-C	-5.51	100.19	109.83
1	A	522	HIS	O-C-N	5.51	131.36	122.99
1	A	554	VAL	N-CA-CB	-5.51	101.74	111.93
1	A	320	MET	CA-C-O	-5.50	112.91	119.35
1	A	638	THR	CB-CA-C	5.50	119.44	109.37
1	A	217	ARG	NE-CZ-NH1	5.49	126.99	121.50
1	A	51	PRO	CB-CA-C	5.49	117.61	110.92
1	A	144	ASN	CA-CB-CG	-5.49	107.11	112.60
1	A	218	THR	CA-C-O	-5.48	114.35	120.54
1	A	316	LYS	CB-CA-C	-5.48	101.12	109.89
1	A	298	ASN	O-C-N	5.48	129.52	122.23
1	A	472	THR	CA-C-O	5.48	122.85	119.29
1	A	166	ASP	O-C-N	5.47	129.44	123.04
1	A	551	THR	O-C-N	5.47	128.40	123.26
1	A	161	TRP	CB-CG-CD1	5.46	135.10	126.90
1	A	558	GLY	O-C-N	-5.46	115.55	122.82
1	A	395	LYS	CA-C-N	-5.45	116.00	123.14
1	A	395	LYS	C-N-CA	-5.45	116.00	123.14
1	A	104	SER	CA-CB-OG	-5.45	100.20	111.10
1	A	22	GLN	O-C-N	5.44	129.47	123.16
1	A	526	GLN	O-C-N	5.44	130.40	123.11
1	A	26	GLU	CG-CD-OE2	5.43	130.88	118.40
1	A	579	ALA	N-CA-C	5.42	117.64	109.23
1	A	344	SER	CA-C-N	5.42	130.99	122.70
1	A	344	SER	C-N-CA	5.42	130.99	122.70
1	A	70	MET	N-CA-C	-5.41	98.45	107.80
1	A	374	ASN	CA-CB-CG	5.41	118.00	112.60
1	A	532	TYR	CB-CA-C	5.40	122.04	110.21
1	A	495	TYR	CA-C-O	5.40	126.84	120.96
1	A	583	VAL	N-CA-C	5.39	116.52	108.54
1	A	118	THR	N-CA-CB	5.39	117.94	109.69
1	A	459	ARG	CB-CA-C	5.39	121.37	110.38
1	A	74	GLN	CG-CD-NE2	-5.38	108.32	116.40
1	A	128	ALA	O-C-N	5.38	129.39	122.93
1	A	252	LEU	CA-C-O	-5.38	114.55	120.36
1	A	247	ALA	N-CA-C	5.38	119.33	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	546	ILE	CB-CG1-CD1	5.37	125.08	113.80
1	A	318	ASN	CA-C-O	5.37	123.57	118.63
1	A	527	ILE	CA-CB-CG1	5.37	119.53	110.40
1	A	296	GLU	CA-CB-CG	5.37	124.83	114.10
1	A	334	HIS	N-CA-CB	-5.37	103.94	111.62
1	A	413	ASN	N-CA-CB	5.37	118.22	109.69
1	A	637	VAL	CA-CB-CG1	5.37	119.52	110.40
1	A	468	THR	CA-CB-CG2	5.36	119.61	110.50
1	A	545	LYS	CA-C-N	5.36	129.60	122.95
1	A	545	LYS	C-N-CA	5.36	129.60	122.95
1	A	274	SER	CA-C-O	-5.36	115.10	121.16
1	A	526	GLN	CA-C-N	-5.36	116.55	123.19
1	A	526	GLN	C-N-CA	-5.36	116.55	123.19
1	A	53	HIS	CA-CB-CG	-5.36	108.44	113.80
1	A	160	ARG	CB-CA-C	-5.36	98.51	109.38
1	A	243	GLY	CA-C-N	-5.35	110.93	121.41
1	A	243	GLY	C-N-CA	-5.35	110.93	121.41
1	A	373	SER	CA-C-N	5.35	128.44	120.31
1	A	373	SER	C-N-CA	5.35	128.44	120.31
1	A	20	SER	CB-CA-C	-5.35	97.69	109.56
1	A	16	VAL	CA-C-N	5.34	130.97	122.74
1	A	16	VAL	C-N-CA	5.34	130.97	122.74
1	A	316	LYS	N-CA-C	5.34	117.97	109.96
1	A	571	ALA	CA-C-O	5.33	126.97	120.99
1	A	46	ASN	N-CA-C	-5.33	106.83	113.38
1	A	276	ALA	N-CA-C	5.32	117.06	108.34
1	A	300	GLU	CA-CB-CG	5.32	124.74	114.10
1	A	19	ASP	CA-C-N	5.32	131.06	122.29
1	A	19	ASP	C-N-CA	5.32	131.06	122.29
1	A	390	ASP	CA-C-N	-5.31	112.24	120.31
1	A	390	ASP	C-N-CA	-5.31	112.24	120.31
1	A	113	TYR	CA-C-N	5.31	131.15	123.13
1	A	113	TYR	C-N-CA	5.31	131.15	123.13
1	A	148	ALA	N-CA-C	-5.31	102.66	110.52
1	A	69	SER	CA-CB-OG	5.30	121.70	111.10
1	A	60	LYS	O-C-N	5.27	129.60	122.59
1	A	151	TYR	CB-CA-C	-5.26	101.42	110.16
1	A	471	PHE	O-C-N	5.26	129.31	122.42
1	A	282	ARG	NH1-CZ-NH2	-5.25	112.47	119.30
1	A	624	ASN	O-C-N	5.25	128.61	121.74
1	A	520	THR	O-C-N	5.25	128.96	122.19
1	A	303	SER	CB-CA-C	5.24	115.99	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	591	PRO	CB-CA-C	5.24	117.24	111.11
1	A	602	TYR	CB-CG-CD1	5.21	128.62	120.80
1	A	176	ILE	CA-C-O	-5.21	114.41	121.02
1	A	524	ASP	O-C-N	5.20	128.45	123.04
1	A	449	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	596	ASN	CB-CA-C	5.19	118.88	110.22
1	A	318	ASN	N-CA-C	5.18	119.99	113.25
1	A	460	ARG	NH1-CZ-NH2	5.17	126.02	119.30
1	A	155	GLN	N-CA-C	-5.16	103.56	110.07
1	A	118	THR	CB-CA-C	-5.16	101.85	109.90
1	A	496	HIS	CA-CB-CG	-5.16	108.64	113.80
1	A	621	PHE	CA-C-O	-5.15	115.29	121.11
1	A	569	SER	CA-C-O	-5.15	113.71	120.00
1	A	436	TYR	CA-C-N	5.15	130.26	123.00
1	A	436	TYR	C-N-CA	5.15	130.26	123.00
1	A	552	GLN	CB-CG-CD	5.15	121.35	112.60
1	A	445	VAL	O-C-N	5.14	128.87	123.00
1	A	563	SER	N-CA-C	-5.14	101.49	109.72
1	A	436	TYR	CB-CA-C	-5.14	102.11	110.85
1	A	295	PHE	CA-C-N	-5.14	114.34	121.99
1	A	295	PHE	C-N-CA	-5.14	114.34	121.99
1	A	365	VAL	N-CA-C	-5.13	100.49	108.81
1	A	366	LYS	N-CA-CB	-5.13	102.19	110.81
1	A	310	THR	N-CA-C	-5.13	100.68	109.24
1	A	296	GLU	CB-CA-C	5.12	119.33	110.77
1	A	34	ASN	N-CA-CB	-5.12	102.66	110.65
1	A	439	ARG	CA-C-N	5.12	130.74	122.29
1	A	439	ARG	C-N-CA	5.12	130.74	122.29
1	A	13	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	460	ARG	N-CA-C	-5.11	99.64	108.69
1	A	21	ALA	CA-C-O	5.11	126.38	120.14
1	A	504	ASP	CA-C-O	-5.11	113.38	119.35
1	A	439	ARG	N-CA-CB	-5.09	102.05	111.52
1	A	119	ARG	O-C-N	5.09	127.17	121.32
1	A	334	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	A	93	GLY	CA-C-O	-5.08	113.38	119.02
1	A	237	GLY	CA-C-O	5.07	124.89	119.06
1	A	396	ILE	N-CA-CB	-5.07	104.42	111.41
1	A	171	PRO	CA-C-O	-5.06	115.62	123.16
1	A	338	PHE	CE1-CZ-CE2	5.05	129.10	120.00
1	A	119	ARG	NE-CZ-NH2	-5.05	114.65	119.20
1	A	333	ASN	CB-CG-ND2	5.04	123.96	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	GLY	N-CA-C	-5.04	103.93	110.38
1	A	108	ASP	CB-CA-C	5.04	122.29	111.91
1	A	259	SER	CA-C-O	5.04	127.36	121.46
1	A	229	PRO	N-CA-CB	-5.03	97.96	103.25
1	A	8	ALA	O-C-N	5.03	129.06	122.87
1	A	588	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	A	385	ASN	CB-CG-OD1	-5.02	110.76	120.80
1	A	498	ILE	CA-CB-CG1	5.02	118.93	110.40
1	A	264	PRO	CA-C-O	5.01	128.50	122.08
1	A	211	THR	CB-CA-C	5.01	118.37	109.65
1	A	308	THR	CA-C-O	-5.01	115.58	121.44
1	A	604	PHE	CA-C-N	-5.00	115.68	122.93
1	A	604	PHE	C-N-CA	-5.00	115.68	122.93

There are no chirality outliers.

There are no planarity outliers.

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	4826	0	4599	113	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
5	A	12	0	9	0	0
6	A	326	0	0	11	0
All	All	5171	0	4608	113	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 12.

All (113) 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:22:GLN:NE2	1:A:46:ASN:HB2	1.81	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ARG:HD3	6:A:819:HOH:O	1.68	0.92
1:A:22:GLN:HE21	1:A:46:ASN:HB2	1.33	0.91
1:A:22:GLN:NE2	1:A:43:TYR:H	1.70	0.90
1:A:13:ASN:HB2	6:A:931:HOH:O	1.87	0.72
1:A:35:LYS:HE2	1:A:71:LEU:HD21	1.73	0.70
1:A:298:ASN:HD22	1:A:317:VAL:H	1.39	0.69
1:A:529:THR:HG23	1:A:533:LEU:HD12	1.73	0.69
1:A:326:GLN:HB3	6:A:840:HOH:O	1.93	0.67
1:A:21:ALA:HA	1:A:40:HIS:O	1.95	0.67
1:A:171:PRO:HD2	1:A:511:GLY:HA2	1.78	0.66
1:A:29:LYS:HD2	1:A:37:THR:HB	1.78	0.65
1:A:290:HIS:HD2	6:A:741:HOH:O	1.79	0.65
1:A:300:GLU:HG3	1:A:309:TRP:CE3	2.31	0.65
1:A:340:TRP:CG	1:A:341:LYS:H	2.15	0.64
1:A:174:ALA:HB3	1:A:498:ILE:HD13	1.80	0.62
1:A:9:ILE:HD12	1:A:145:VAL:HG12	1.83	0.61
1:A:84:ARG:NH1	6:A:978:HOH:O	2.34	0.61
1:A:504:ASP:OD1	1:A:506:ARG:HB2	2.01	0.60
1:A:103:GLY:HA3	1:A:166:ASP:O	2.02	0.59
1:A:469:PRO:HB3	1:A:492:VAL:HG13	1.84	0.59
1:A:51:PRO:HD3	1:A:136:PRO:HA	1.86	0.58
1:A:90:SER:HB2	1:A:96:TRP:CE3	2.40	0.57
1:A:298:ASN:ND2	1:A:317:VAL:H	2.01	0.57
1:A:72:PRO:HG2	1:A:109:SER:HA	1.88	0.56
1:A:17:THR:HG22	6:A:944:HOH:O	2.05	0.56
1:A:260:TRP:C	1:A:261:ILE:HG13	2.31	0.56
1:A:22:GLN:NE2	1:A:43:TYR:O	2.36	0.55
1:A:290:HIS:CD2	6:A:741:HOH:O	2.56	0.55
1:A:35:LYS:HE2	1:A:71:LEU:CD2	2.36	0.55
1:A:167:LEU:CD1	1:A:171:PRO:HG3	2.37	0.54
1:A:356:TRP:O	1:A:365:VAL:HA	2.06	0.54
1:A:459:ARG:HB2	6:A:849:HOH:O	2.06	0.54
1:A:63:GLN:O	1:A:120:PRO:HA	2.08	0.53
1:A:174:ALA:CB	1:A:498:ILE:HD13	2.38	0.53
1:A:334:HIS:CE1	1:A:581:HIS:HB3	2.42	0.53
1:A:22:GLN:HG3	1:A:42:PHE:HA	1.91	0.52
1:A:402:SER:HB2	1:A:408:SER:HB3	1.91	0.52
1:A:398:THR:O	1:A:414:ALA:HA	2.09	0.52
1:A:174:ALA:HA	1:A:184:LEU:O	2.09	0.52
1:A:227:PHE:O	1:A:244:GLY:HA3	2.10	0.51
1:A:576:TYR:HE2	1:A:634:THR:HG23	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:MET:HE2	1:A:124:VAL:HG23	1.92	0.51
1:A:169:ILE:HG22	1:A:191:ASN:HB2	1.93	0.50
1:A:20:SER:O	1:A:39:TRP:NE1	2.43	0.50
1:A:52:PRO:HA	1:A:128:ALA:O	2.11	0.49
1:A:39:TRP:O	1:A:139:SER:HA	2.13	0.49
1:A:458:GLN:HA	1:A:468:THR:O	2.13	0.49
1:A:282:ARG:HG2	1:A:303:SER:HA	1.95	0.49
1:A:261:ILE:HA	1:A:262:PRO:HD3	1.70	0.48
1:A:58:ASP:OD1	1:A:60:LYS:N	2.39	0.48
1:A:208:ASP:OD1	1:A:208:ASP:C	2.56	0.48
1:A:575:ARG:HD2	1:A:618:TRP:CZ2	2.49	0.48
1:A:448:PRO:HA	1:A:574:ILE:CD1	2.44	0.48
1:A:11:ARG:O	1:A:12:ASN:C	2.57	0.47
1:A:88:TYR:CE2	1:A:99:PRO:HD3	2.49	0.47
1:A:14:TRP:CD1	1:A:59:MET:HA	2.50	0.47
1:A:402:SER:HB2	1:A:403:PRO:HD2	1.96	0.47
1:A:317:VAL:O	1:A:320:MET:HG2	2.15	0.47
1:A:564:THR:HG21	1:A:568:ILE:HD13	1.97	0.46
1:A:35:LYS:O	6:A:926:HOH:O	2.21	0.46
1:A:59:MET:HB2	1:A:122:ARG:O	2.16	0.46
1:A:20:SER:HB2	1:A:41:THR:HA	1.98	0.46
1:A:89:LEU:CD2	1:A:124:VAL:HG22	2.45	0.46
1:A:448:PRO:HA	1:A:574:ILE:HD11	1.97	0.45
1:A:225:ASP:N	1:A:246:ASP:OD2	2.41	0.45
1:A:68:LEU:HA	1:A:144:ASN:O	2.16	0.45
1:A:5:ILE:HD12	1:A:490:SER:HB3	1.99	0.45
1:A:78:GLN:HG2	1:A:81:TRP:CH2	2.51	0.45
1:A:340:TRP:CG	1:A:341:LYS:N	2.85	0.45
1:A:495:TYR:O	1:A:496:HIS:HB2	2.17	0.45
1:A:56:THR:HG21	1:A:125:ARG:HH21	1.82	0.45
1:A:182:ARG:HH11	1:A:182:ARG:HD3	1.54	0.45
1:A:32:ASP:OD2	1:A:37:THR:OG1	2.35	0.44
1:A:228:CYS:N	1:A:229:PRO:HD3	2.32	0.44
1:A:192:ASP:HA	1:A:514:LEU:HD12	2.00	0.44
1:A:161:TRP:CE2	1:A:489:ASN:HB3	2.53	0.44
1:A:469:PRO:HB3	1:A:492:VAL:CG1	2.47	0.44
1:A:351:SER:O	1:A:371:ARG:NH1	2.45	0.44
1:A:576:TYR:CZ	1:A:619:MET:HG3	2.53	0.44
1:A:253:TYR:CE2	1:A:255:SER:HA	2.53	0.44
1:A:16:VAL:HG12	1:A:57:ILE:HG12	2.00	0.43
1:A:135:GLN:HB3	1:A:136:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLU:HG3	1:A:309:TRP:CZ3	2.54	0.43
1:A:29:LYS:HB3	1:A:37:THR:HB	2.01	0.43
1:A:290:HIS:HE1	6:A:1031:HOH:O	2.02	0.43
1:A:479:GLU:H	1:A:479:GLU:CD	2.27	0.43
1:A:529:THR:HA	1:A:530:PRO:HD3	1.81	0.43
1:A:67:GLY:HA2	1:A:114:SER:O	2.19	0.43
1:A:271:GLY:O	1:A:272:TYR:HB2	2.19	0.43
1:A:554:VAL:HG11	1:A:606:VAL:HG21	2.01	0.42
1:A:560:ILE:HG21	1:A:560:ILE:HD13	1.79	0.42
1:A:95:ASN:ND2	1:A:95:ASN:N	2.67	0.42
1:A:382:MET:HE2	1:A:382:MET:HB2	1.86	0.42
1:A:49:PRO:HB2	6:A:1022:HOH:O	2.18	0.42
1:A:72:PRO:HG2	1:A:109:SER:CA	2.50	0.42
1:A:233:MET:HE1	1:A:576:TYR:HB2	2.01	0.42
1:A:296:GLU:OE2	1:A:318:ASN:HB2	2.20	0.42
1:A:595:THR:O	1:A:602:TYR:HA	2.20	0.42
1:A:95:ASN:N	1:A:95:ASN:HD22	2.17	0.42
1:A:146:PHE:CD1	1:A:146:PHE:N	2.87	0.41
1:A:269:ALA:O	1:A:297:LYS:NZ	2.38	0.41
1:A:464:PHE:CD1	1:A:515:CYS:HB3	2.55	0.41
1:A:402:SER:HB2	1:A:403:PRO:CD	2.50	0.41
1:A:59:MET:C	1:A:61:THR:H	2.29	0.41
1:A:69:SER:HB3	1:A:146:PHE:CE1	2.56	0.41
1:A:35:LYS:HG3	1:A:74:GLN:HG3	2.04	0.40
1:A:412:THR:O	1:A:413:ASN:C	2.62	0.40
1:A:477:VAL:HA	1:A:478:PRO:HD2	1.98	0.40
1:A:283:VAL:O	1:A:301:VAL:HA	2.22	0.40
1:A:541:ALA:HB1	1:A:628:VAL:HG21	2.04	0.40
1:A:183:VAL:O	1:A:206:SER:HA	2.22	0.40
1:A:298:ASN:ND2	1:A:316:LYS:HA	2.37	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	637/639 (100%)	603 (95%)	31 (5%)	3 (0%)	24 22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	494	VAL
1	A	229	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	A	526/526 (100%)	495 (94%)	31 (6%)	18 16

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	17	THR
1	A	20	SER
1	A	61	THR
1	A	62	THR
1	A	68	LEU
1	A	84	ARG
1	A	94	THR
1	A	95	ASN
1	A	98	SER
1	A	108	ASP
1	A	152	THR
1	A	165	ILE
1	A	203	LEU
1	A	218	THR
1	A	229	PRO

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Mol	Chain	Res	Type
1	A	248	LYS
1	A	256	SER
1	A	305	SER
1	A	408	SER
1	A	445	VAL
1	A	498	ILE
1	A	532	TYR
1	A	536	SER
1	A	545	LYS
1	A	556	VAL
1	A	563	SER
1	A	570	LYS
1	A	593	THR
1	A	594	LEU
1	A	639	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	22	GLN
1	A	28	ASN
1	A	46	ASN
1	A	78	GLN
1	A	95	ASN
1	A	133	ASN
1	A	135	GLN
1	A	290	HIS
1	A	298	ASN
1	A	372	GLN
1	A	509	ASN
1	A	552	GLN
1	A	597	ASN
1	A	600	ASN

5.3.3 RNA

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, 2 are monoatomic - leaving 4 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	$\# Z > 2$
5	ACT	A	705	-	3,3,3	0.95	0	3,3,3	0.89	0
5	ACT	A	703	2	3,3,3	0.99	0	3,3,3	0.43	0
5	ACT	A	701	-	3,3,3	1.07	0	3,3,3	1.23	0
4	SO4	A	704	-	4,4,4	0.74	0	6,6,6	0.77	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.