



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:17 AM UTC

PDB ID : 2XIN / pdb_00002xin
Title : PROTEIN ENGINEERING OF XYLOSE (GLUCOSE) ISOMERASE FROM ACTINOPLANES MISSOURIENSIS. 1. CRYSTALLOGRAPHY AND SITE-DIRECTED MUTAGENESIS OF METAL BINDING SITES
Authors : Janin, J.
Deposited on : 1992-04-06
Resolution : 2.30 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
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

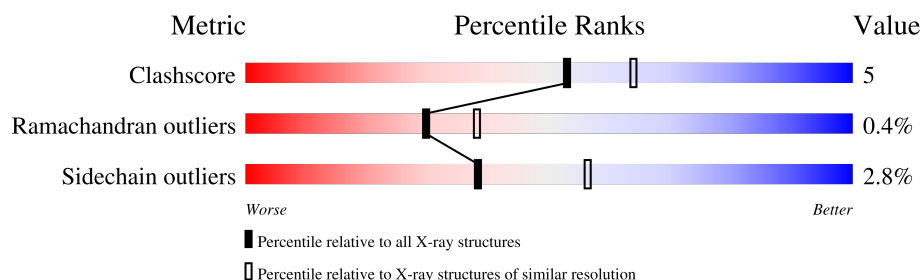
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	393	72% 23% 5%
1	B	393	74% 23% ..
1	C	393	74% 23% .
1	D	393	77% 20% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13160 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.

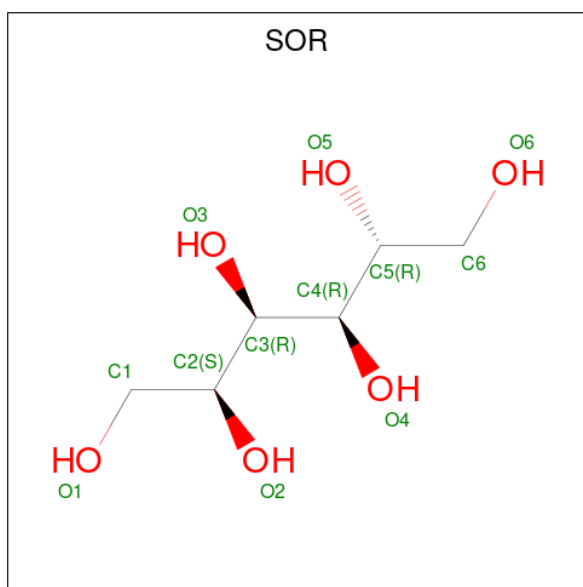
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3051	1937	531	579	4			
1	B	392	Total	C	N	O	S	0	0	0
			3051	1937	531	579	4			
1	C	392	Total	C	N	O	S	0	0	0
			3051	1937	531	579	4			
1	D	392	Total	C	N	O	S	0	0	0
			3051	1937	531	579	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	ASN	HIS	conflict	UNP P12851
B	290	ASN	HIS	conflict	UNP P12851
C	290	ASN	HIS	conflict	UNP P12851
D	290	ASN	HIS	conflict	UNP P12851

- Molecule 2 is sorbitol (CCD ID: SOR) (formula: C₆H₁₄O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Co	0	0
			2	2		
3	B	2	Total	Co	0	0
			2	2		
3	C	2	Total	Co	0	0
			2	2		
3	D	2	Total	Co	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	230	Total	O	0	0
			230	230		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	221	Total 221	O 221	0	0
4	C	231	Total 231	O 231	0	0
4	D	218	Total 218	O 218	0	0

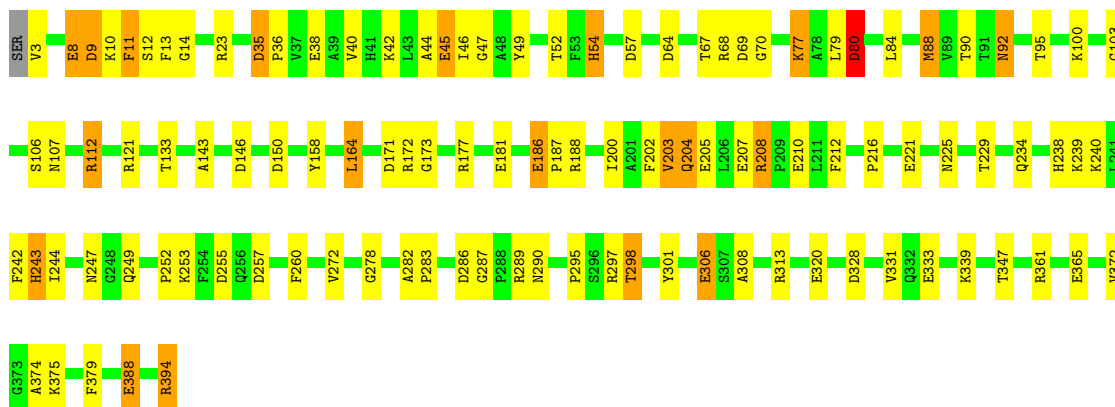
3 Residue-property plots

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.

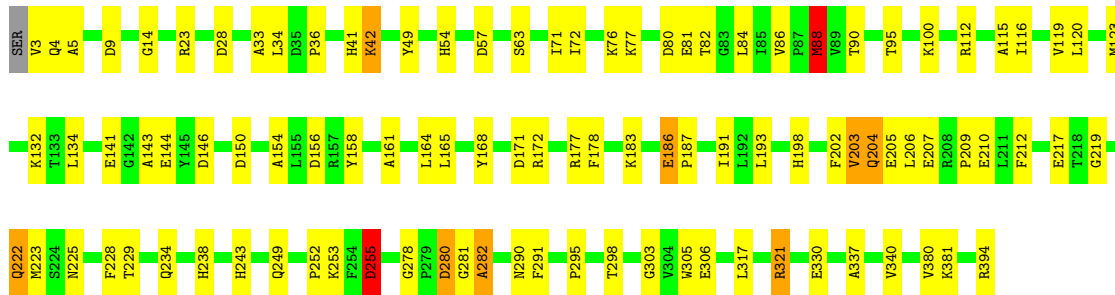
• Molecule 1: D-XYLOSE ISOMERASE

Chain A: 



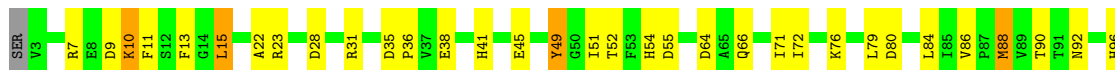
• Molecule 1: D-XYLOSE ISOMERASE

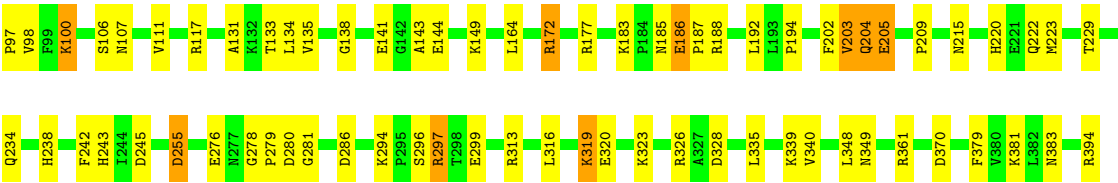
Chain B: 



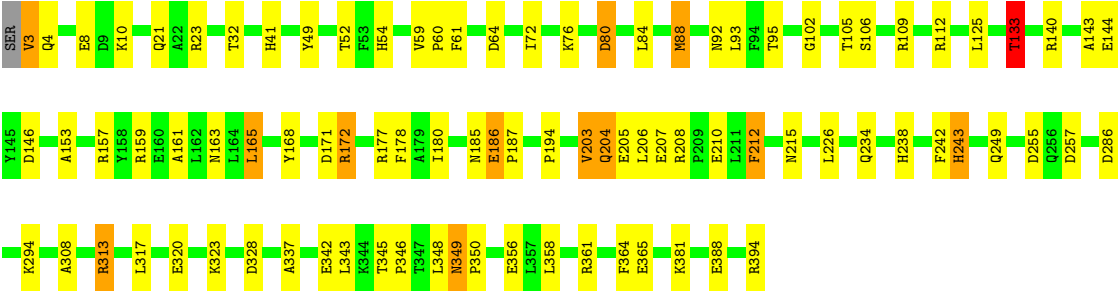
• Molecule 1: D-XYLOSE ISOMERASE

Chain C: 





● Molecule 1: D-XYLOSE ISOMERASE



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	143.45Å 143.45Å 231.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.154 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13160	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: CO, SOR

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	0.97	0/3122	2.08	106/4229 (2.5%)
1	B	0.95	1/3122 (0.0%)	1.97	83/4229 (2.0%)
1	C	0.95	0/3122	1.99	90/4229 (2.1%)
1	D	0.94	0/3122	1.94	69/4229 (1.6%)
All	All	0.95	1/12488 (0.0%)	1.99	348/16916 (2.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	LYS	C-O	5.20	1.29	1.24

All (348) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	GLN	OE1-CD-NE2	-16.65	105.95	122.60
1	B	204	GLN	OE1-CD-NE2	-14.73	107.86	122.60
1	D	204	GLN	OE1-CD-NE2	-13.04	109.56	122.60
1	A	80	ASP	CA-CB-CG	-12.70	99.90	112.60
1	C	204	GLN	OE1-CD-NE2	-11.67	110.93	122.60
1	B	255	ASP	CA-CB-CG	11.07	123.67	112.60
1	A	172	ARG	CD-NE-CZ	10.12	138.56	124.40
1	A	379	PHE	CA-CB-CG	10.06	123.86	113.80
1	B	394	ARG	NE-CZ-NH2	-10.01	110.19	119.20
1	D	255	ASP	CA-CB-CG	9.95	122.55	112.60
1	A	333	GLU	CA-CB-CG	9.95	134.00	114.10
1	A	204	GLN	CB-CG-CD	9.06	128.00	112.60
1	D	286	ASP	CA-CB-CG	-9.02	103.58	112.60
1	A	69	ASP	CA-CB-CG	-8.89	103.71	112.60
1	A	80	ASP	O-C-N	8.81	131.20	122.03
1	C	134	LEU	CA-C-O	-8.74	110.71	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	255	ASP	N-CA-CB	-8.72	95.76	110.49
1	A	244	ILE	CA-C-O	-8.55	111.75	120.90
1	D	8	GLU	CB-CG-CD	8.50	127.06	112.60
1	C	54	HIS	N-CA-C	-8.41	98.08	110.52
1	C	222	GLN	OE1-CD-NE2	-8.28	114.32	122.60
1	C	23	ARG	CA-C-O	-8.19	111.82	120.58
1	A	247	ASN	OD1-CG-ND2	-8.13	114.47	122.60
1	A	52	THR	CA-CB-OG1	-8.09	97.46	109.60
1	B	177	ARG	CD-NE-CZ	-7.92	113.31	124.40
1	C	64	ASP	CA-CB-CG	-7.79	104.81	112.60
1	B	41	HIS	CA-CB-CG	-7.78	106.02	113.80
1	D	41	HIS	CA-CB-CG	-7.75	106.05	113.80
1	A	177	ARG	N-CA-C	-7.75	97.61	109.85
1	B	229	THR	CA-CB-OG1	-7.68	98.08	109.60
1	D	144	GLU	N-CA-C	-7.66	104.16	113.97
1	A	394	ARG	NH1-CZ-NH2	7.52	129.08	119.30
1	A	216	PRO	CA-C-O	-7.49	112.53	121.67
1	B	321	ARG	NE-CZ-NH2	-7.44	112.50	119.20
1	C	185	ASN	O-C-N	7.40	130.69	123.29
1	A	95	THR	N-CA-C	7.39	119.23	111.03
1	A	10	LYS	CB-CA-C	-7.37	100.75	112.09
1	B	150	ASP	CA-CB-CG	-7.32	105.28	112.60
1	A	188	ARG	CA-C-O	-7.31	113.19	121.81
1	C	379	PHE	CA-CB-CG	7.27	121.07	113.80
1	B	177	ARG	N-CA-C	-7.26	98.89	110.14
1	C	361	ARG	NE-CZ-NH2	7.26	125.73	119.20
1	D	54	HIS	N-CA-C	-7.24	98.52	110.17
1	B	95	THR	N-CA-C	7.18	120.15	111.40
1	B	207	GLU	CA-C-O	-7.17	112.82	120.42
1	C	23	ARG	CD-NE-CZ	7.16	134.43	124.40
1	A	313	ARG	NE-CZ-NH1	7.15	128.65	121.50
1	A	255	ASP	N-CA-CB	-7.12	97.92	109.60
1	A	306	GLU	CB-CA-C	-7.12	99.70	110.88
1	D	328	ASP	CA-CB-CG	7.12	119.72	112.60
1	A	207	GLU	CA-C-O	-7.07	112.40	120.24
1	B	255	ASP	N-CA-CB	-6.98	98.69	110.49
1	A	207	GLU	CA-CB-CG	6.97	128.03	114.10
1	B	134	LEU	CA-C-O	-6.93	113.05	120.46
1	C	66	GLN	N-CA-C	-6.92	103.66	111.07
1	A	44	ALA	N-CA-C	-6.92	103.74	111.28
1	A	9	ASP	N-CA-C	-6.92	104.65	113.23
1	A	92	ASN	OD1-CG-ND2	6.91	129.51	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	GLU	CB-CG-CD	6.89	124.31	112.60
1	D	313	ARG	N-CA-CB	6.88	119.99	110.01
1	C	13	PHE	CA-C-O	-6.87	113.09	121.06
1	A	68	ARG	CD-NE-CZ	6.86	134.01	124.40
1	A	212	PHE	N-CA-C	6.83	120.53	109.40
1	C	185	ASN	CA-C-O	-6.81	114.00	121.28
1	D	23	ARG	CA-C-O	-6.79	113.32	120.58
1	B	82	THR	N-CA-C	6.76	120.74	112.23
1	C	172	ARG	CD-NE-CZ	-6.70	115.02	124.40
1	A	8	GLU	CA-CB-CG	-6.70	100.71	114.10
1	D	95	THR	N-CA-C	6.66	119.52	111.40
1	B	177	ARG	N-CA-CB	6.63	121.06	110.85
1	C	340	VAL	CB-CA-C	6.63	120.36	111.88
1	B	228	PHE	CA-C-O	-6.58	114.09	121.00
1	C	229	THR	CA-CB-OG1	-6.58	99.73	109.60
1	D	10	LYS	CB-CA-C	-6.56	103.07	111.86
1	D	144	GLU	N-CA-CB	6.55	119.78	110.67
1	B	202	PHE	CA-C-N	6.54	129.42	120.46
1	B	202	PHE	C-N-CA	6.54	129.42	120.46
1	C	328	ASP	CA-C-N	6.52	126.45	119.28
1	C	328	ASP	C-N-CA	6.52	126.45	119.28
1	D	212	PHE	N-CA-C	6.51	120.00	109.40
1	B	54	HIS	N-CA-C	-6.50	99.70	110.17
1	B	146	ASP	CA-C-O	-6.49	113.67	120.55
1	A	278	GLY	N-CA-C	-6.48	104.39	112.23
1	C	64	ASP	N-CA-C	-6.46	102.46	110.41
1	A	14	GLY	N-CA-C	-6.42	101.04	112.54
1	C	143	ALA	N-CA-CB	-6.42	100.79	111.57
1	A	243	HIS	CA-C-O	-6.41	114.58	121.38
1	A	13	PHE	CA-C-O	-6.40	113.63	121.06
1	C	141	GLU	CB-CG-CD	6.40	123.47	112.60
1	D	172	ARG	CD-NE-CZ	6.39	133.35	124.40
1	C	223	MET	N-CA-C	-6.36	104.62	112.38
1	B	394	ARG	N-CA-CB	6.36	121.31	110.50
1	D	194	PRO	N-CA-C	6.35	121.80	113.86
1	B	290	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	A	173	GLY	CA-C-O	-6.30	112.64	119.82
1	A	54	HIS	N-CA-C	-6.30	100.03	110.17
1	A	287	GLY	O-C-N	6.28	128.05	121.77
1	C	194	PRO	N-CA-C	6.28	121.79	113.57
1	A	146	ASP	CA-C-O	-6.28	113.90	120.55
1	B	63	SER	N-CA-C	-6.27	99.47	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ASN	CA-CB-CG	6.24	118.84	112.60
1	C	31	ARG	NE-CZ-NH1	6.23	127.73	121.50
1	A	67	THR	CA-CB-OG1	-6.17	100.34	109.60
1	A	240	LYS	O-C-N	6.17	129.65	122.19
1	B	23	ARG	NE-CZ-NH1	6.16	127.66	121.50
1	B	80	ASP	O-C-N	6.15	128.66	122.08
1	A	394	ARG	NE-CZ-NH1	-6.15	115.35	121.50
1	B	57	ASP	N-CA-C	-6.15	104.13	111.69
1	C	45	GLU	CA-CB-CG	6.12	126.34	114.10
1	C	394	ARG	NE-CZ-NH1	-6.10	115.40	121.50
1	C	328	ASP	CB-CA-C	6.09	119.26	109.51
1	D	109	ARG	CD-NE-CZ	6.09	132.93	124.40
1	C	316	LEU	CA-C-O	-6.08	114.10	120.55
1	C	370	ASP	O-C-N	6.08	128.56	122.12
1	A	229	THR	CA-CB-OG1	-6.07	100.49	109.60
1	C	135	VAL	O-C-N	6.06	129.35	122.93
1	B	161	ALA	CA-C-O	-6.04	114.01	120.42
1	C	117	ARG	NE-CZ-NH1	6.04	127.54	121.50
1	A	95	THR	CA-CB-OG1	-6.04	100.55	109.60
1	A	158	TYR	CA-C-O	6.03	126.81	120.42
1	D	207	GLU	CA-CB-CG	6.03	126.16	114.10
1	B	225	ASN	OD1-CG-ND2	-6.02	116.58	122.60
1	B	340	VAL	CB-CA-C	6.01	119.66	111.97
1	C	52	THR	CA-CB-OG1	-6.01	100.59	109.60
1	D	204	GLN	CB-CG-CD	5.99	122.79	112.60
1	A	388	GLU	CA-CB-CG	-5.99	102.12	114.10
1	C	55	ASP	CA-CB-CG	5.99	118.59	112.60
1	C	188	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	A	77	LYS	O-C-N	5.99	128.23	122.07
1	A	45	GLU	CA-C-O	-5.98	114.54	120.82
1	A	240	LYS	CA-C-O	-5.98	112.42	119.48
1	A	286	ASP	CA-CB-CG	-5.97	106.62	112.60
1	C	15	LEU	N-CA-CB	-5.97	101.03	110.22
1	B	144	GLU	N-CA-C	-5.97	106.33	113.97
1	D	349	ASN	OD1-CG-ND2	5.95	128.55	122.60
1	D	356	GLU	CB-CG-CD	5.94	122.70	112.60
1	D	133	THR	CB-CA-C	5.93	121.78	109.38
1	C	202	PHE	CA-C-O	5.92	127.04	120.82
1	B	337	ALA	O-C-N	5.92	129.15	122.22
1	B	217	GLU	CA-C-O	-5.91	113.97	120.36
1	A	103	GLY	CA-C-N	5.91	128.78	120.28
1	A	103	GLY	C-N-CA	5.91	128.78	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	32	THR	CA-CB-OG1	-5.90	100.75	109.60
1	B	158	TYR	N-CA-C	-5.89	104.77	111.14
1	C	177	ARG	N-CA-C	-5.88	100.31	109.72
1	A	177	ARG	CD-NE-CZ	-5.87	116.18	124.40
1	D	342	GLU	CG-CD-OE2	5.87	131.91	118.40
1	D	177	ARG	N-CA-C	-5.87	100.58	109.85
1	D	243	HIS	CA-CB-CG	-5.86	107.94	113.80
1	C	215	ASN	O-C-N	5.85	126.64	121.37
1	C	297	ARG	NE-CZ-NH2	5.85	124.46	119.20
1	A	112	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	B	172	ARG	NE-CZ-NH1	5.80	127.30	121.50
1	A	171	ASP	CA-C-O	-5.78	114.30	120.42
1	C	286	ASP	CA-CB-CG	-5.77	106.83	112.60
1	D	112	ARG	CD-NE-CZ	5.76	132.47	124.40
1	C	71	ILE	O-C-N	5.73	127.42	121.87
1	D	112	ARG	NE-CZ-NH1	5.73	127.23	121.50
1	B	330	GLU	OE1-CD-OE2	5.72	136.64	122.90
1	C	144	GLU	N-CA-C	-5.72	106.85	113.88
1	C	394	ARG	CD-NE-CZ	-5.68	116.45	124.40
1	D	112	ARG	NH1-CZ-NH2	-5.67	111.94	119.30
1	D	358	LEU	CA-C-O	5.66	126.50	120.10
1	A	298	THR	CA-CB-OG1	-5.65	101.12	109.60
1	A	257	ASP	CA-CB-CG	5.65	118.25	112.60
1	B	291	PHE	CA-CB-CG	-5.64	108.16	113.80
1	A	331	VAL	N-CA-C	-5.64	105.03	110.72
1	C	281	GLY	N-CA-C	-5.64	99.82	113.18
1	A	143	ALA	N-CA-CB	-5.62	102.13	111.57
1	B	210	GLU	CB-CG-CD	5.62	122.15	112.60
1	C	349	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	A	244	ILE	O-C-N	5.62	129.60	123.09
1	C	319	LYS	CA-C-N	5.62	127.80	120.28
1	C	319	LYS	C-N-CA	5.62	127.80	120.28
1	C	339	LYS	CB-CA-C	-5.62	102.64	111.51
1	B	303	GLY	N-CA-C	-5.61	105.85	113.37
1	B	305	TRP	CA-CB-CG	-5.61	102.95	113.60
1	C	278	GLY	CA-C-N	5.60	126.84	119.84
1	C	278	GLY	C-N-CA	5.60	126.84	119.84
1	D	203	VAL	CB-CA-C	5.59	120.22	112.05
1	C	90	THR	CA-C-N	5.58	131.76	122.73
1	C	90	THR	C-N-CA	5.58	131.76	122.73
1	D	106	SER	CA-C-O	-5.57	115.65	121.55
1	A	203	VAL	CA-C-N	5.57	129.51	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	VAL	C-N-CA	5.57	129.51	120.60
1	A	272	VAL	O-C-N	5.57	127.27	121.87
1	D	215	ASN	CB-CG-ND2	5.55	124.73	116.40
1	D	125	LEU	CA-C-O	-5.54	114.67	120.55
1	A	204	GLN	CG-CD-NE2	5.54	124.71	116.40
1	D	337	ALA	CA-C-O	-5.54	114.68	120.55
1	C	296	SER	CA-C-N	5.54	128.25	120.28
1	C	296	SER	C-N-CA	5.54	128.25	120.28
1	D	157	ARG	NE-CZ-NH2	5.53	124.17	119.20
1	D	286	ASP	CA-C-O	-5.52	112.96	119.48
1	B	281	GLY	CA-C-N	5.52	129.86	121.03
1	B	281	GLY	C-N-CA	5.52	129.86	121.03
1	A	295	PRO	N-CA-C	-5.51	102.47	110.80
1	D	294	LYS	CB-CA-C	-5.51	102.83	110.16
1	D	226	LEU	O-C-N	5.50	129.10	122.94
1	D	93	LEU	CA-C-O	-5.49	114.86	121.34
1	A	394	ARG	CD-NE-CZ	-5.49	116.72	124.40
1	C	313	ARG	CD-NE-CZ	5.49	132.08	124.40
1	B	71	ILE	O-C-N	5.48	127.28	121.91
1	A	249	GLN	CA-C-O	-5.47	115.42	121.33
1	C	10	LYS	CB-CA-C	-5.46	104.54	111.86
1	C	294	LYS	O-C-N	5.46	128.23	121.79
1	B	172	ARG	CD-NE-CZ	5.46	132.04	124.40
1	A	188	ARG	CD-NE-CZ	5.45	132.03	124.40
1	B	77	LYS	O-C-N	5.45	127.68	122.07
1	A	88	MET	CB-CG-SD	5.44	129.03	112.70
1	B	143	ALA	N-CA-CB	-5.44	102.43	111.57
1	B	156	ASP	O-C-N	5.43	127.88	122.12
1	B	54	HIS	CB-CA-C	-5.42	100.33	109.50
1	C	188	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	B	54	HIS	N-CA-CB	5.42	119.46	110.63
1	A	243	HIS	CA-CB-CG	-5.42	108.38	113.80
1	B	36	PRO	O-C-N	5.41	128.72	122.23
1	D	143	ALA	N-CA-CB	-5.41	103.34	111.56
1	A	11	PHE	CA-C-O	-5.41	114.43	120.54
1	B	207	GLU	CG-CD-OE2	-5.40	105.98	118.40
1	D	54	HIS	N-CA-CB	5.40	119.43	110.63
1	D	80	ASP	O-C-N	5.40	127.63	122.07
1	A	253	LYS	N-CA-C	-5.39	101.12	108.24
1	A	47	GLY	N-CA-C	5.39	122.76	115.00
1	B	330	GLU	CG-CD-OE2	-5.38	106.02	118.40
1	A	297	ARG	NE-CZ-NH2	5.37	124.04	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	282	ALA	N-CA-C	5.37	117.94	110.20
1	A	225	ASN	CA-CB-CG	-5.37	107.23	112.60
1	C	299	GLU	N-CA-C	5.37	118.82	110.17
1	C	177	ARG	CA-CB-CG	5.37	124.84	114.10
1	B	33	ALA	CA-C-O	-5.36	115.29	121.19
1	D	23	ARG	CD-NE-CZ	5.36	131.91	124.40
1	A	221	GLU	CA-C-O	-5.36	113.81	119.97
1	B	168	TYR	O-C-N	5.36	127.59	122.07
1	A	79	LEU	CA-C-O	5.35	126.15	120.10
1	C	320	GLU	CA-C-N	5.35	128.45	120.31
1	C	320	GLU	C-N-CA	5.35	128.45	120.31
1	A	328	ASP	CA-CB-CG	5.35	117.95	112.60
1	C	92	ASN	CA-CB-CG	-5.35	107.25	112.60
1	A	308	ALA	N-CA-C	-5.34	105.54	111.36
1	B	253	LYS	N-CA-CB	5.34	119.31	110.97
1	A	216	PRO	O-C-N	5.34	129.63	123.06
1	A	289	ARG	N-CA-C	-5.34	96.62	107.41
1	B	14	GLY	N-CA-C	-5.34	102.99	112.54
1	A	35	ASP	CB-CA-C	5.32	118.45	109.67
1	B	380	VAL	CA-C-O	-5.32	115.42	120.95
1	A	121	ARG	NE-CZ-NH2	-5.32	114.41	119.20
1	A	374	ALA	CA-C-O	-5.32	112.85	119.18
1	C	13	PHE	O-C-N	5.32	129.44	123.27
1	C	66	GLN	O-C-N	5.32	127.55	122.07
1	B	191	ILE	CA-C-O	-5.31	114.74	121.48
1	A	202	PHE	CA-C-N	5.30	129.32	120.62
1	A	202	PHE	C-N-CA	5.30	129.32	120.62
1	A	200	ILE	N-CA-CB	5.30	116.75	110.55
1	D	163	ASN	O-C-N	5.30	127.74	122.12
1	D	52	THR	CA-C-O	-5.29	115.25	121.44
1	D	255	ASP	CA-C-O	-5.28	112.95	120.51
1	B	28	ASP	O-C-N	5.28	129.14	122.65
1	B	225	ASN	CB-CG-ND2	5.28	124.32	116.40
1	A	290	ASN	CB-CG-ND2	5.27	124.30	116.40
1	D	249	GLN	OE1-CD-NE2	5.27	127.87	122.60
1	A	23	ARG	CD-NE-CZ	5.27	131.77	124.40
1	C	177	ARG	NE-CZ-NH2	-5.25	114.48	119.20
1	D	349	ASN	CA-CB-CG	-5.25	107.35	112.60
1	B	57	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	90	THR	CA-CB-OG1	-5.24	101.74	109.60
1	C	188	ARG	CD-NE-CZ	5.24	131.74	124.40
1	B	207	GLU	CG-CD-OE1	5.24	130.45	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	349	ASN	O-C-N	5.24	127.15	121.60
1	A	64	ASP	N-CA-C	-5.23	103.98	110.41
1	C	106	SER	CA-C-O	-5.23	116.01	121.55
1	A	260	PHE	CA-CB-CG	-5.22	108.58	113.80
1	C	149	LYS	N-CA-C	5.22	116.91	108.34
1	A	150	ASP	CB-CG-OD1	5.22	130.41	118.40
1	C	203	VAL	N-CA-CB	-5.22	103.94	110.47
1	C	276	GLU	CG-CD-OE2	5.22	130.41	118.40
1	A	301	TYR	CB-CA-C	5.21	120.28	110.63
1	B	80	ASP	CA-CB-CG	-5.21	107.39	112.60
1	B	193	LEU	O-C-N	5.21	127.31	121.32
1	D	105	THR	CA-C-O	-5.20	113.66	119.95
1	D	146	ASP	CA-C-O	-5.20	115.04	120.55
1	D	346	PRO	CA-C-O	-5.20	115.61	121.43
1	D	313	ARG	CA-CB-CG	5.19	124.48	114.10
1	B	165	LEU	CA-C-O	-5.18	115.05	120.55
1	C	205	GLU	CG-CD-OE2	5.18	130.32	118.40
1	D	328	ASP	CB-CA-C	5.18	116.84	109.38
1	B	198	HIS	N-CA-CB	5.18	117.73	110.12
1	D	320	GLU	CA-CB-CG	5.18	124.45	114.10
1	C	107	ASN	N-CA-CB	5.17	118.18	110.22
1	D	165	LEU	CA-C-O	-5.17	115.39	120.82
1	A	112	ARG	CA-C-O	-5.16	115.08	120.55
1	D	92	ASN	OD1-CG-ND2	5.16	127.76	122.60
1	B	5	ALA	CA-C-O	-5.16	115.17	121.05
1	B	88	MET	CB-CA-C	-5.16	98.72	110.07
1	B	253	LYS	N-CA-C	-5.16	101.43	108.24
1	A	290	ASN	CA-C-O	-5.16	114.99	120.92
1	A	172	ARG	N-CA-C	-5.14	106.98	113.20
1	D	257	ASP	CA-C-O	-5.14	115.63	121.65
1	D	59	VAL	O-C-N	5.14	125.65	120.92
1	B	34	LEU	CA-C-O	-5.13	114.74	120.54
1	B	280	ASP	N-CA-C	-5.13	105.04	111.92
1	C	79	LEU	CA-C-O	5.13	126.20	120.82
1	B	141	GLU	CB-CG-CD	5.12	121.31	112.60
1	C	383	ASN	OD1-CG-ND2	5.12	127.72	122.60
1	A	57	ASP	N-CA-C	-5.11	105.40	111.69
1	C	209	PRO	O-C-N	5.11	128.81	122.22
1	C	335	LEU	O-C-N	5.11	127.54	122.12
1	D	21	GLN	CB-CG-CD	-5.11	103.92	112.60
1	D	171	ASP	CA-C-O	-5.11	115.14	120.55
1	A	88	MET	CA-C-O	-5.11	115.82	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	28	ASP	CA-CB-CG	5.10	117.70	112.60
1	C	138	GLY	CA-C-N	5.09	126.51	120.14
1	C	138	GLY	C-N-CA	5.09	126.51	120.14
1	D	308	ALA	N-CA-C	-5.09	105.64	111.14
1	C	134	LEU	O-C-N	5.08	129.27	123.27
1	C	177	ARG	N-CA-CB	5.08	119.77	111.08
1	A	181	GLU	O-C-N	5.08	126.91	121.12
1	C	100	LYS	CA-C-O	-5.08	114.36	120.10
1	D	345	THR	CA-C-O	-5.08	115.49	119.66
1	D	210	GLU	CB-CG-CD	5.07	121.22	112.60
1	A	328	ASP	CA-C-O	5.07	124.50	119.49
1	A	339	LYS	CB-CA-C	-5.06	103.51	111.51
1	A	188	ARG	NH1-CZ-NH2	-5.06	112.72	119.30
1	C	23	ARG	N-CA-C	-5.06	100.26	108.41
1	A	347	THR	CA-C-O	5.05	125.77	120.42
1	B	171	ASP	CA-C-O	-5.05	115.07	120.42
1	B	158	TYR	CB-CA-C	5.04	118.87	110.90
1	D	64	ASP	N-CA-C	-5.04	104.21	110.41
1	D	313	ARG	N-CA-C	-5.04	105.67	111.07
1	A	70	GLY	O-C-N	5.04	127.02	122.18
1	B	77	LYS	CB-CA-C	-5.04	102.97	110.88
1	B	255	ASP	CA-C-O	-5.04	113.31	120.51
1	B	203	VAL	N-CA-CB	-5.03	103.69	110.54
1	D	364	PHE	CA-CB-CG	-5.03	108.77	113.80
1	A	394	ARG	CA-CB-CG	5.02	124.14	114.10
1	A	12	SER	CA-C-O	-5.02	115.57	121.44
1	A	164	LEU	CA-C-O	-5.02	115.10	120.42
1	C	326	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	C	15	LEU	CA-C-O	5.01	125.77	120.10
1	C	281	GLY	CA-C-O	5.01	129.29	120.57
1	C	245	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	222	GLN	CB-CG-CD	5.01	121.12	112.60
1	B	380	VAL	O-C-N	5.00	126.72	121.87
1	B	9	ASP	CA-C-O	5.00	125.69	119.79
1	B	295	PRO	N-CA-C	-5.00	103.24	110.80
1	B	42	LYS	CG-CD-CE	5.00	122.81	111.30
1	C	7	ARG	N-CA-C	-5.00	106.44	112.54
1	D	153	ALA	N-CA-C	-5.00	105.83	111.28

There are no chirality outliers.

There are no planarity outliers.

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	3051	0	2953	36	0
1	B	3051	0	2953	35	0
1	C	3051	0	2953	33	0
1	D	3051	0	2953	33	0
2	A	12	0	11	0	0
2	B	12	0	11	0	0
2	C	12	0	12	1	0
2	D	12	0	11	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	230	0	0	3	0
4	B	221	0	0	2	0
4	C	231	0	0	5	0
4	D	218	0	0	4	0
All	All	13160	0	11857	120	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 5.

All (120) 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:B:204:GLN:OE1	1:D:204:GLN:OE1	1.60	1.15
1:D:133:THR:HG21	1:D:243:HIS:NE2	1.69	1.07
1:A:204:GLN:OE1	1:C:204:GLN:OE1	1.75	1.02
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.13	0.95
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.49	0.94
1:D:133:THR:CG2	1:D:243:HIS:NE2	2.32	0.93
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.16	0.90
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.21	0.83
1:A:204:GLN:HG2	4:A:549:HOH:O	1.82	0.80
1:A:208:ARG:NH1	1:A:210:GLU:OE2	2.15	0.79
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LEU:CD1	1:D:348:LEU:HD11	2.19	0.71
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.04	0.70
1:C:183:LYS:NZ	1:C:255:ASP:OD2	2.21	0.70
1:C:133:THR:HG21	1:C:243:HIS:CD2	2.27	0.69
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.76	0.69
1:B:183:LYS:NZ	1:B:255:ASP:OD2	2.26	0.68
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.75	0.67
1:D:72:ILE:O	1:D:76:LYS:HG3	1.95	0.66
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.77	0.66
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.80	0.64
1:A:133:THR:OG1	1:A:243:HIS:HE1	1.81	0.63
1:D:88:MET:HE3	1:D:243:HIS:HD1	1.64	0.61
1:A:133:THR:OG1	1:A:243:HIS:CE1	2.55	0.60
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.36	0.60
1:A:164:LEU:C	1:A:164:LEU:HD23	2.26	0.60
1:A:242:PHE:O	1:A:243:HIS:ND1	2.34	0.59
1:D:394:ARG:HD2	4:D:608:HOH:O	2.02	0.58
1:B:183:LYS:CE	1:B:255:ASP:OD2	2.52	0.58
1:C:183:LYS:HG3	1:C:220:HIS:CG	2.40	0.56
1:C:242:PHE:O	1:C:243:HIS:CD2	2.59	0.56
1:B:219:GLY:O	1:B:223:MET:HG3	2.06	0.56
1:D:133:THR:HG23	1:D:243:HIS:NE2	2.20	0.56
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.89	0.55
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.90	0.55
1:C:234:GLN:HE21	1:C:238:HIS:CE1	2.09	0.55
1:B:164:LEU:HD12	1:D:348:LEU:CD1	2.28	0.55
1:C:15:LEU:HD13	1:C:51:ILE:HD11	1.89	0.55
1:C:243:HIS:HB3	4:C:620:HOH:O	2.08	0.54
1:A:306:GLU:HG2	1:D:381:LYS:HB2	1.90	0.53
1:B:243:HIS:HB3	4:B:608:HOH:O	2.08	0.53
1:C:88:MET:HG3	1:C:243:HIS:CE1	2.44	0.53
1:C:133:THR:CB	1:C:243:HIS:HE2	2.22	0.53
1:A:36:PRO:O	1:A:40:VAL:HG23	2.09	0.52
1:A:42:LYS:O	1:A:45:GLU:HB3	2.10	0.52
1:A:133:THR:CB	1:A:243:HIS:CE1	2.93	0.51
1:A:164:LEU:HD12	1:C:348:LEU:HD11	1.93	0.51
1:B:3:VAL:HG12	1:B:4:GLN:H	1.75	0.51
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.44	0.51
1:D:242:PHE:O	1:D:243:HIS:CD2	2.64	0.51
1:A:298:THR:HA	1:B:100:LYS:HD2	1.92	0.50
1:C:133:THR:CB	1:C:243:HIS:NE2	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:HIS:O	1:A:239:LYS:HB2	2.11	0.49
1:A:243:HIS:HB3	4:A:585:HOH:O	2.11	0.49
1:C:164:LEU:C	1:C:164:LEU:HD23	2.37	0.49
1:B:72:ILE:O	1:B:76:LYS:HG3	2.12	0.49
1:C:255:ASP:OD1	4:C:616:HOH:O	2.20	0.49
1:C:319:LYS:O	1:C:323:LYS:HG2	2.12	0.49
1:A:77:LYS:O	1:A:80:ASP:CB	2.61	0.48
1:A:234:GLN:HE21	1:A:238:HIS:CE1	2.14	0.48
1:B:381:LYS:NZ	4:B:550:HOH:O	2.39	0.47
1:C:72:ILE:O	1:C:76:LYS:HG3	2.14	0.47
1:C:86:VAL:O	1:C:131:ALA:HA	2.14	0.47
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.14	0.47
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.81	0.47
1:B:88:MET:HG3	1:B:243:HIS:CE1	2.50	0.47
1:D:102:GLY:HA2	1:D:140:ARG:HB2	1.97	0.47
1:B:115:ALA:O	1:B:119:VAL:HG23	2.15	0.46
1:C:100:LYS:NZ	4:C:626:HOH:O	2.48	0.46
1:D:60:PRO:O	1:D:61:PHE:C	2.58	0.46
1:A:35:ASP:HA	1:A:36:PRO:HD3	1.77	0.46
1:A:204:GLN:CD	1:C:204:GLN:OE1	2.53	0.46
1:A:372:VAL:HA	1:A:375:LYS:HD2	1.98	0.46
1:B:178:PHE:HB2	1:B:212:PHE:CD2	2.51	0.46
1:C:98:VAL:HG22	1:C:111:VAL:HG22	1.97	0.46
1:B:278:GLY:CA	1:B:282:ALA:O	2.64	0.45
1:A:243:HIS:HB3	4:A:521:HOH:O	2.16	0.45
1:D:388:GLU:HB3	1:D:394:ARG:HG3	1.99	0.45
1:A:8:GLU:H	1:A:8:GLU:HG3	1.53	0.44
1:B:317:LEU:O	1:B:321:ARG:HD2	2.17	0.44
1:C:172:ARG:HH11	1:C:172:ARG:HD2	1.67	0.44
1:A:252:PRO:HB2	1:B:252:PRO:HB2	1.98	0.44
1:B:86:VAL:HG12	1:B:86:VAL:O	2.17	0.44
1:A:92:ASN:OD1	1:A:92:ASN:C	2.61	0.44
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.81	0.44
1:D:317:LEU:HD23	1:D:317:LEU:HA	1.83	0.44
1:C:41:HIS:HE1	4:C:514:HOH:O	2.00	0.44
1:A:186:GLU:HA	1:A:187:PRO:HA	1.75	0.43
1:A:388:GLU:OE2	1:D:313:ARG:HD3	2.18	0.43
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.88	0.43
1:B:112:ARG:O	1:B:116:ILE:HG13	2.19	0.43
1:A:42:LYS:HD3	1:A:42:LYS:HA	1.57	0.43
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ASP:HB3	1:C:11:PHE:CE2	2.54	0.43
1:A:100:LYS:HD2	1:B:298:THR:HA	2.00	0.43
2:C:397:SOR:H12	4:C:544:HOH:O	2.18	0.43
1:A:106:SER:O	1:A:112:ARG:HD3	2.18	0.43
1:B:278:GLY:HA3	1:B:282:ALA:O	2.18	0.43
1:B:164:LEU:C	1:B:164:LEU:HD23	2.44	0.43
1:D:3:VAL:HG12	1:D:4:GLN:H	1.84	0.43
1:B:206:LEU:O	1:B:209:PRO:HD3	2.18	0.42
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.84	0.42
1:D:88:MET:HE2	4:D:474:HOH:O	2.20	0.42
1:B:42:LYS:HD3	1:B:42:LYS:HA	1.93	0.42
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.19	0.42
1:D:168:TYR:O	1:D:172:ARG:HG2	2.19	0.42
1:D:349:ASN:HB3	1:D:350:PRO:CD	2.48	0.42
1:D:178:PHE:HB2	1:D:212:PHE:CD2	2.55	0.42
1:D:159:ARG:HG3	1:D:206:LEU:HD23	2.01	0.42
1:B:154:ALA:HB2	1:D:343:LEU:HD21	2.02	0.42
1:D:161:ALA:O	1:D:165:LEU:HG	2.20	0.42
1:D:186:GLU:HA	1:D:187:PRO:HA	1.81	0.42
1:B:186:GLU:HA	1:B:187:PRO:HA	1.88	0.41
1:C:192:LEU:HA	1:C:192:LEU:HD23	1.87	0.41
1:D:243:HIS:HB3	4:D:474:HOH:O	2.20	0.41
1:C:10:LYS:HA	1:C:49:TYR:CD1	2.56	0.40
1:B:120:LEU:O	1:B:123:MET:HB2	2.22	0.40
1:D:3:VAL:HG23	4:D:597:HOH:O	2.21	0.40
1:B:280:ASP:C	1:B:282:ALA:H	2.28	0.40
1:C:186:GLU:HA	1:C:187:PRO:HA	1.91	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	390/393 (99%)	374 (96%)	15 (4%)	1 (0%)	36	46
1	B	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	36	46
1	C	390/393 (99%)	375 (96%)	12 (3%)	3 (1%)	16	20
1	D	390/393 (99%)	372 (95%)	17 (4%)	1 (0%)	36	46
All	All	1560/1572 (99%)	1497 (96%)	57 (4%)	6 (0%)	30	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	280	ASP
1	A	186	GLU
1	B	186	GLU
1	C	186	GLU
1	C	279	PRO
1	D	186	GLU

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	306/310 (99%)	296 (97%)	10 (3%)	33	50
1	B	306/310 (99%)	299 (98%)	7 (2%)	44	63
1	C	306/310 (99%)	300 (98%)	6 (2%)	48	67
1	D	306/310 (99%)	295 (96%)	11 (4%)	31	47
All	All	1224/1240 (99%)	1190 (97%)	34 (3%)	38	56

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	38	GLU
1	A	46	ILE
1	A	49	TYR
1	A	80	ASP

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Mol	Chain	Res	Type
1	A	84	LEU
1	A	88	MET
1	A	203	VAL
1	A	208	ARG
1	A	394	ARG
1	B	49	TYR
1	B	81	GLU
1	B	84	LEU
1	B	88	MET
1	B	132	LYS
1	B	203	VAL
1	B	255	ASP
1	C	38	GLU
1	C	49	TYR
1	C	80	ASP
1	C	84	LEU
1	C	88	MET
1	C	203	VAL
1	D	3	VAL
1	D	49	TYR
1	D	80	ASP
1	D	84	LEU
1	D	88	MET
1	D	133	THR
1	D	180	ILE
1	D	185	ASN
1	D	203	VAL
1	D	208	ARG
1	D	323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	238	HIS
1	A	243	HIS
1	B	204	GLN
1	B	222	GLN
1	B	230	GLN
1	B	238	HIS
1	B	290	ASN
1	C	222	GLN

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Mol	Chain	Res	Type
1	C	238	HIS
1	C	290	ASN
1	D	222	GLN
1	D	238	HIS

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 12 ligands modelled in this entry, 8 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	$\# Z > 2$
2	SOR	A	397	3	11,11,11	0.84	0	14,14,14	1.72	4 (28%)
2	SOR	C	397	3	11,11,11	1.11	1 (9%)	14,14,14	2.30	6 (42%)
2	SOR	B	397	3	11,11,11	0.99	1 (9%)	14,14,14	2.08	5 (35%)
2	SOR	D	397	3	11,11,11	1.27	1 (9%)	14,14,14	2.41	7 (50%)

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
2	SOR	A	397	3	-	2/16/16/16	-
2	SOR	C	397	3	-	2/16/16/16	-
2	SOR	B	397	3	-	3/16/16/16	-
2	SOR	D	397	3	-	7/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	397	SOR	C1-C2	2.95	1.59	1.52
2	C	397	SOR	C1-C2	2.40	1.58	1.52
2	B	397	SOR	C6-C5	2.26	1.57	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	397	SOR	O1-C1-C2	-5.02	100.61	111.16
2	D	397	SOR	O2-C2-C3	4.52	119.83	109.25
2	B	397	SOR	O6-C6-C5	-4.21	102.30	111.16
2	D	397	SOR	O6-C6-C5	-3.97	102.82	111.16
2	A	397	SOR	O6-C6-C5	-3.43	103.95	111.16
2	D	397	SOR	C1-C2-C3	-3.38	105.28	112.17
2	C	397	SOR	C2-C3-C4	3.00	117.08	112.48
2	D	397	SOR	O1-C1-C2	-2.90	105.07	111.16
2	B	397	SOR	O1-C1-C2	-2.89	105.08	111.16
2	B	397	SOR	O4-C4-C3	2.86	116.15	109.46
2	C	397	SOR	O3-C3-C4	2.69	115.74	109.46
2	C	397	SOR	O2-C2-C3	2.65	115.44	109.25
2	C	397	SOR	C6-C5-C4	-2.61	106.85	112.17
2	D	397	SOR	O2-C2-C1	-2.51	103.33	109.03
2	D	397	SOR	C5-C4-C3	2.50	116.32	112.48
2	A	397	SOR	O5-C5-C4	2.45	114.99	109.25
2	C	397	SOR	O6-C6-C5	-2.42	106.07	111.16
2	B	397	SOR	C5-C4-C3	2.40	116.16	112.48
2	A	397	SOR	O4-C4-C3	2.38	115.02	109.46
2	A	397	SOR	C5-C4-C3	2.32	116.05	112.48
2	B	397	SOR	O3-C3-C4	2.27	114.77	109.46
2	D	397	SOR	O5-C5-C4	2.23	114.47	109.25

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	397	SOR	C4-C5-C6-O6
2	A	397	SOR	O5-C5-C6-O6
2	D	397	SOR	O1-C1-C2-O2
2	D	397	SOR	O5-C5-C6-O6
2	A	397	SOR	C4-C5-C6-O6
2	B	397	SOR	C4-C5-C6-O6
2	C	397	SOR	C4-C5-C6-O6
2	B	397	SOR	O5-C5-C6-O6
2	C	397	SOR	O5-C5-C6-O6
2	B	397	SOR	O1-C1-C2-O2
2	D	397	SOR	O2-C2-C3-C4
2	D	397	SOR	O2-C2-C3-O3
2	D	397	SOR	C1-C2-C3-C4
2	D	397	SOR	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	397	SOR	1	0

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.