



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:59 AM UTC

PDB ID : 8XIM / pdb_00008xim
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 : 1992-04-01
Resolution : 2.40 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

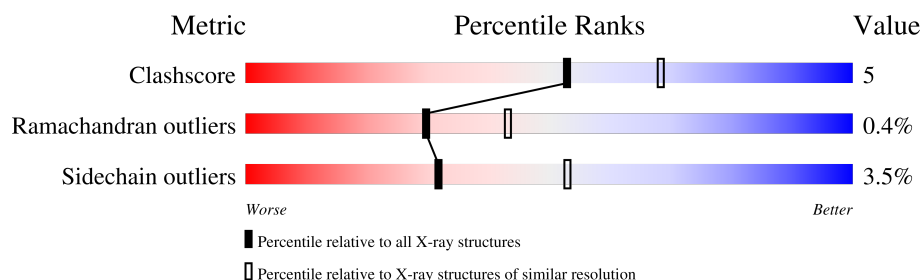
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	 78% 19% .
1	B	393	 76% 22% ..
1	C	393	 73% 22% . ..
1	D	393	 76% 20% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13203 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.

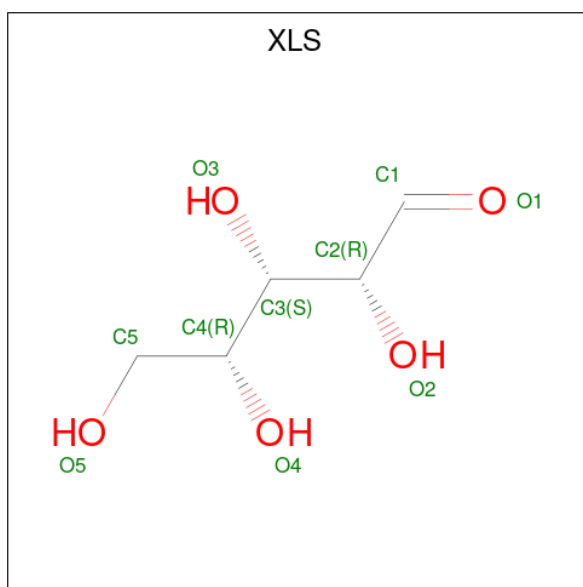
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3049	1937	533	575	4			
1	B	392	Total	C	N	O	S	0	0	0
			3049	1937	533	575	4			
1	C	391	Total	C	N	O	S	0	0	0
			3042	1932	532	574	4			
1	D	392	Total	C	N	O	S	0	0	0
			3048	1936	533	575	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	GLN	GLU	conflict	UNP P12851
B	186	GLN	GLU	conflict	UNP P12851
C	186	GLN	GLU	conflict	UNP P12851
D	186	GLN	GLU	conflict	UNP P12851

- Molecule 2 is D-xylose (CCD ID: XLS) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		
2	C	1	Total	C	O	0	0
			10	5	5		
2	D	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	240	Total	O	0	0
			240	240		

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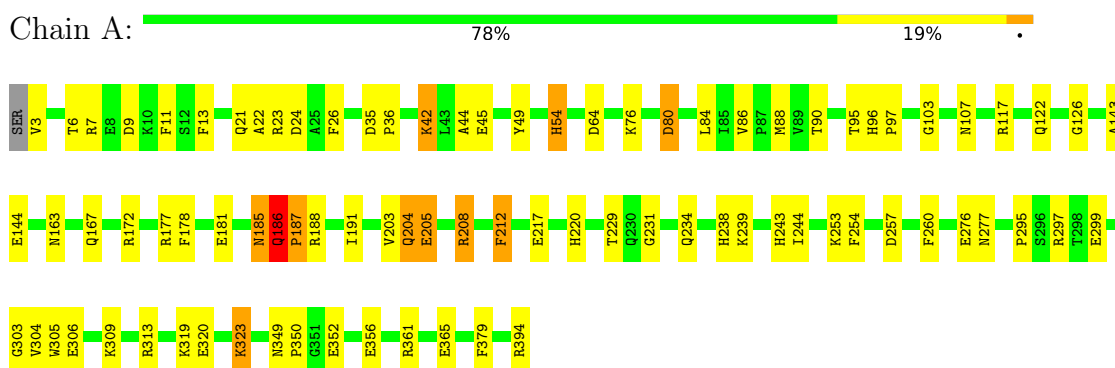
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	235	Total 235	O 235	0	0
4	C	254	Total 254	O 254	0	0
4	D	242	Total 242	O 242	0	0

3 Residue-property plots

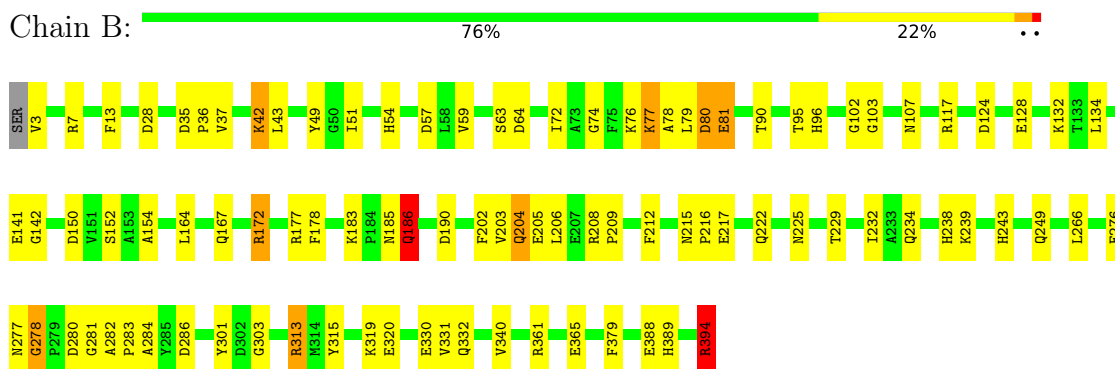
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

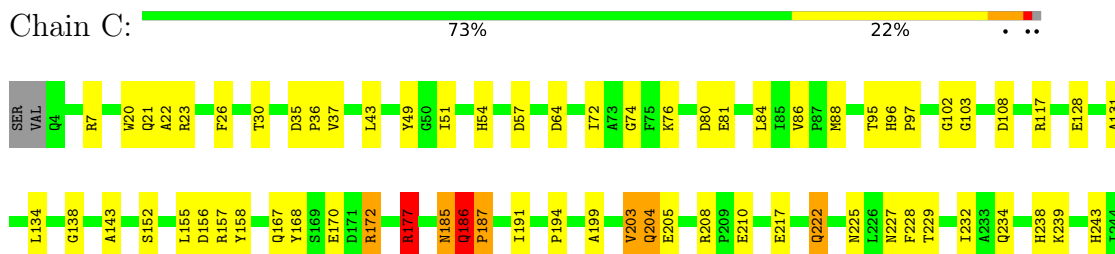
• Molecule 1: D-XYLOSE ISOMERASE

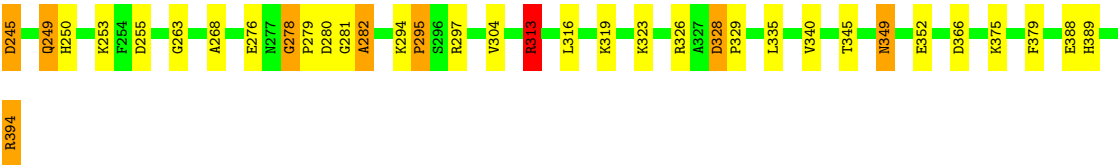


• Molecule 1: D-XYLOSE ISOMERASE

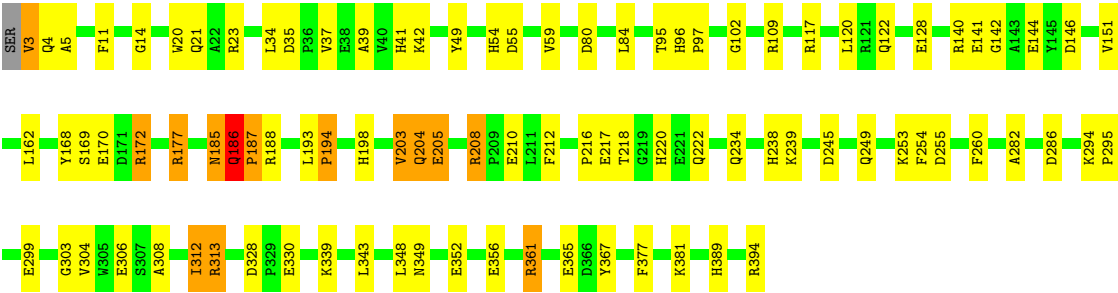
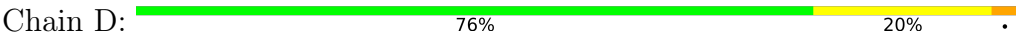


• Molecule 1: D-XYLOSE ISOMERASE





● 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) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.146 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13203	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: MG, XLS

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	0.94	1/3121 (0.0%)	1.87	61/4228 (1.4%)
1	B	0.93	2/3121 (0.1%)	1.87	68/4228 (1.6%)
1	C	0.93	0/3114	1.90	81/4218 (1.9%)
1	D	0.99	1/3119 (0.0%)	1.90	62/4224 (1.5%)
All	All	0.95	4/12475 (0.0%)	1.89	272/16898 (1.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	169	SER	C-N	-17.01	1.12	1.33
1	B	103	GLY	CA-C	6.49	1.55	1.51
1	A	103	GLY	CA-C	5.54	1.55	1.51
1	B	102	GLY	C-N	-5.13	1.29	1.33

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	ARG	CD-NE-CZ	15.93	146.71	124.40
1	C	204	GLN	OE1-CD-NE2	-14.41	108.19	122.60
1	C	313	ARG	CD-NE-CZ	13.81	143.74	124.40
1	A	204	GLN	OE1-CD-NE2	-12.67	109.93	122.60
1	D	204	GLN	OE1-CD-NE2	-12.61	109.99	122.60
1	D	169	SER	CA-C-O	-11.21	109.05	120.82
1	A	80	ASP	CA-CB-CG	-11.21	101.39	112.60
1	B	204	GLN	OE1-CD-NE2	-9.91	112.69	122.60
1	D	170	GLU	N-CA-CB	8.84	123.11	109.94
1	B	394	ARG	N-CA-CB	8.83	125.51	110.50
1	C	328	ASP	CA-C-O	8.72	126.17	119.46
1	C	208	ARG	CD-NE-CZ	-8.66	112.28	124.40
1	A	394	ARG	NH1-CZ-NH2	8.42	130.25	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	389	HIS	CA-CB-CG	-8.41	105.39	113.80
1	B	394	ARG	CD-NE-CZ	-8.36	112.69	124.40
1	B	117	ARG	NE-CZ-NH1	8.27	129.77	121.50
1	C	253	LYS	CA-C-O	-8.09	112.44	121.25
1	D	95	THR	N-CA-C	8.07	119.86	111.14
1	D	328	ASP	CB-CA-C	8.06	119.03	109.85
1	A	107	ASN	CA-CB-CG	7.87	120.47	112.60
1	C	326	ARG	NE-CZ-NH2	7.76	126.19	119.20
1	D	188	ARG	NE-CZ-NH2	7.75	126.17	119.20
1	C	54	HIS	N-CA-C	-7.65	98.16	110.32
1	A	172	ARG	CD-NE-CZ	7.64	135.09	124.40
1	C	313	ARG	NH1-CZ-NH2	-7.37	109.72	119.30
1	A	319	LYS	CA-C-O	7.28	128.69	120.90
1	D	313	ARG	CA-CB-CG	7.24	128.58	114.10
1	A	126	GLY	CA-C-N	7.21	129.94	120.28
1	A	126	GLY	C-N-CA	7.21	129.94	120.28
1	A	23	ARG	CD-NE-CZ	7.18	134.46	124.40
1	B	59	VAL	O-C-N	7.17	127.52	120.92
1	D	349	ASN	CA-CB-CG	-7.15	105.45	112.60
1	D	312	ILE	O-C-N	7.13	129.17	121.83
1	A	320	GLU	CB-CG-CD	7.12	124.71	112.60
1	B	102	GLY	N-CA-C	-7.04	104.97	112.08
1	C	313	ARG	NE-CZ-NH1	7.04	128.53	121.50
1	D	54	HIS	N-CA-C	-7.03	98.85	110.17
1	C	281	GLY	N-CA-C	-7.03	96.52	113.18
1	A	379	PHE	CA-CB-CG	7.01	120.81	113.80
1	D	328	ASP	CA-CB-CG	6.99	119.59	112.60
1	D	349	ASN	OD1-CG-ND2	6.95	129.55	122.60
1	A	244	ILE	CA-C-O	-6.93	113.49	120.90
1	A	95	THR	N-CA-C	6.87	118.66	111.03
1	B	13	PHE	CA-CB-CG	6.86	120.66	113.80
1	C	340	VAL	CB-CA-C	6.84	120.63	111.88
1	B	286	ASP	CA-C-O	-6.81	111.44	119.48
1	C	117	ARG	NE-CZ-NH1	6.80	128.30	121.50
1	C	389	HIS	CA-CB-CG	-6.79	107.01	113.80
1	D	253	LYS	CA-C-O	-6.79	113.85	121.25
1	A	144	GLU	N-CA-C	-6.78	105.55	113.88
1	D	286	ASP	CA-C-O	-6.74	111.52	119.48
1	B	313	ARG	NE-CZ-NH1	6.73	128.23	121.50
1	B	286	ASP	CA-CB-CG	-6.72	105.88	112.60
1	D	389	HIS	CA-CB-CG	-6.71	107.09	113.80
1	C	225	ASN	OD1-CG-ND2	-6.70	115.91	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	GLU	CA-C-O	-6.67	113.48	120.55
1	A	257	ASP	CA-CB-CG	6.67	119.27	112.60
1	B	57	ASP	CA-CB-CG	6.66	119.25	112.60
1	D	144	GLU	N-CA-C	-6.66	105.45	113.97
1	C	64	ASP	CA-CB-CG	-6.65	105.95	112.60
1	D	59	VAL	O-C-N	6.65	127.04	120.92
1	B	79	LEU	CA-C-O	6.63	127.45	120.42
1	B	64	ASP	N-CA-C	-6.58	101.84	110.53
1	B	95	THR	N-CA-C	6.54	119.38	111.40
1	C	394	ARG	CD-NE-CZ	-6.54	115.25	124.40
1	D	210	GLU	CB-CG-CD	6.54	123.71	112.60
1	C	328	ASP	CA-CB-CG	6.53	119.12	112.60
1	D	122	GLN	OE1-CD-NE2	-6.47	116.13	122.60
1	B	394	ARG	NE-CZ-NH2	-6.44	113.40	119.20
1	C	204	GLN	CG-CD-NE2	6.44	126.06	116.40
1	B	202	PHE	CA-C-N	6.44	129.28	120.46
1	B	202	PHE	C-N-CA	6.44	129.28	120.46
1	C	394	ARG	NE-CZ-NH1	-6.40	115.10	121.50
1	B	134	LEU	CA-C-O	-6.38	113.30	120.32
1	C	229	THR	CA-CB-OG1	-6.37	100.05	109.60
1	D	55	ASP	O-C-N	6.34	128.69	122.09
1	A	103	GLY	N-CA-C	-6.33	104.45	110.21
1	D	208	ARG	CD-NE-CZ	-6.32	115.56	124.40
1	B	54	HIS	N-CA-C	-6.29	100.31	110.32
1	C	349	ASN	N-CA-C	-6.29	101.05	110.24
1	D	14	GLY	N-CA-C	-6.29	103.56	112.37
1	B	183	LYS	O-C-N	6.29	126.75	121.84
1	D	330	GLU	CG-CD-OE2	-6.29	103.94	118.40
1	B	215	ASN	CA-CB-CG	-6.26	106.34	112.60
1	A	204	GLN	CB-CG-CD	6.26	123.23	112.60
1	C	23	ARG	CA-C-O	-6.26	113.53	120.60
1	B	150	ASP	CA-CB-CG	-6.25	106.35	112.60
1	C	328	ASP	CB-CA-C	6.24	119.48	109.51
1	D	313	ARG	CD-NE-CZ	-6.22	115.69	124.40
1	D	349	ASN	O-C-N	6.22	128.49	121.53
1	C	23	ARG	N-CA-C	-6.20	99.06	108.67
1	A	13	PHE	CA-C-O	-6.19	113.88	121.06
1	A	394	ARG	NE-CZ-NH1	-6.18	115.32	121.50
1	B	320	GLU	CB-CG-CD	6.17	123.09	112.60
1	A	244	ILE	O-C-N	6.16	130.24	123.09
1	C	102	GLY	CA-C-O	-6.13	117.36	122.33
1	B	77	LYS	O-C-N	6.12	128.38	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	143	ALA	O-C-N	6.08	129.37	123.29
1	D	304	VAL	CA-C-O	-6.05	114.75	121.17
1	B	80	ASP	CA-CB-CG	-6.03	106.57	112.60
1	D	306	GLU	CB-CA-C	-6.02	101.43	110.88
1	C	95	THR	N-CA-C	5.97	117.59	111.14
1	B	177	ARG	CA-C-O	-5.97	114.42	121.16
1	C	194	PRO	N-CA-C	5.96	121.31	113.86
1	A	88	MET	CA-C-O	-5.96	114.90	121.33
1	D	212	PHE	N-CA-C	5.93	118.57	108.90
1	C	222	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	C	57	ASP	N-CA-CB	5.90	119.00	110.20
1	C	278	GLY	CA-C-N	5.90	127.21	119.84
1	C	278	GLY	C-N-CA	5.90	127.21	119.84
1	A	295	PRO	N-CA-C	-5.89	101.91	110.80
1	A	243	HIS	CA-CB-CG	5.88	119.68	113.80
1	A	177	ARG	CB-CA-C	5.88	120.59	109.37
1	D	367	TYR	O-C-N	5.86	129.90	123.04
1	A	319	LYS	CA-C-N	5.86	128.13	120.28
1	A	319	LYS	C-N-CA	5.86	128.13	120.28
1	B	63	SER	O-C-N	5.85	130.03	123.19
1	C	134	LEU	CA-C-O	-5.84	113.89	120.32
1	A	24	ASP	CA-CB-CG	5.83	118.43	112.60
1	D	203	VAL	CB-CA-C	5.82	119.67	112.04
1	C	227	ASN	OD1-CG-ND2	5.81	128.41	122.60
1	A	253	LYS	CA-C-O	-5.80	115.11	121.31
1	C	245	ASP	CA-C-O	-5.79	113.94	120.32
1	A	21	GLN	CB-CG-CD	-5.79	102.75	112.60
1	D	245	ASP	CA-CB-CG	5.78	118.38	112.60
1	C	138	GLY	CA-C-N	5.78	127.36	120.14
1	C	138	GLY	C-N-CA	5.78	127.36	120.14
1	C	108	ASP	CA-CB-CG	-5.77	106.83	112.60
1	D	216	PRO	CA-C-O	-5.77	114.63	121.67
1	A	208	ARG	CD-NE-CZ	-5.76	116.33	124.40
1	D	218	THR	CA-C-O	-5.75	114.75	121.07
1	B	394	ARG	NH1-CZ-NH2	5.73	126.75	119.30
1	C	81	GLU	CB-CG-CD	5.73	122.34	112.60
1	B	141	GLU	CB-CG-CD	5.72	122.32	112.60
1	B	225	ASN	CB-CG-ND2	5.72	124.98	116.40
1	A	304	VAL	CA-C-O	-5.71	115.18	121.29
1	C	57	ASP	CA-CB-CG	5.67	118.27	112.60
1	C	243	HIS	CA-CB-CG	5.67	119.47	113.80
1	C	128	GLU	CB-CG-CD	5.66	122.23	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	282	ALA	N-CA-C	5.64	118.33	110.20
1	B	117	ARG	NE-CZ-NH2	-5.64	114.13	119.20
1	A	13	PHE	O-C-N	5.62	129.79	123.27
1	A	276	GLU	N-CA-C	5.61	120.25	112.45
1	B	330	GLU	CG-CD-OE2	-5.60	105.52	118.40
1	B	96	HIS	CA-CB-CG	-5.60	108.20	113.80
1	C	335	LEU	O-C-N	5.60	128.05	122.12
1	C	185	ASN	O-C-N	5.59	128.88	123.29
1	B	243	HIS	CA-C-O	-5.56	115.49	121.38
1	A	143	ALA	N-CA-CB	-5.55	102.24	111.57
1	A	117	ARG	NE-CZ-NH1	5.55	127.05	121.50
1	C	316	LEU	CA-C-O	-5.54	114.55	120.42
1	D	198	HIS	CA-C-O	-5.53	114.69	120.55
1	A	229	THR	CA-CB-OG1	-5.52	101.32	109.60
1	D	23	ARG	CA-C-O	-5.52	114.67	120.58
1	B	276	GLU	N-CA-C	5.52	120.14	113.41
1	C	64	ASP	N-CA-C	-5.51	103.25	110.53
1	D	377	PHE	CA-C-O	-5.51	112.62	119.18
1	C	157	ARG	CD-NE-CZ	-5.50	116.70	124.40
1	A	191	ILE	CA-C-O	-5.50	114.50	121.48
1	A	181	GLU	O-C-N	5.48	127.37	121.12
1	A	54	HIS	N-CA-C	-5.47	101.62	110.32
1	B	243	HIS	CA-CB-CG	5.47	119.27	113.80
1	C	170	GLU	CA-C-O	-5.47	115.07	120.70
1	B	229	THR	CA-CB-OG1	-5.46	101.41	109.60
1	A	187	PRO	N-CA-C	5.46	126.30	112.10
1	A	26	PHE	CA-C-O	-5.46	113.04	119.48
1	B	183	LYS	CA-C-O	-5.46	113.67	119.13
1	C	268	ALA	N-CA-C	-5.46	105.41	111.36
1	C	282	ALA	N-CA-C	5.45	117.41	109.84
1	B	107	ASN	N-CA-C	-5.42	105.47	111.71
1	D	194	PRO	N-CA-C	5.42	120.68	113.57
1	D	204	GLN	CB-CG-CD	5.42	121.82	112.60
1	A	188	ARG	CD-NE-CZ	5.42	131.99	124.40
1	D	23	ARG	N-CA-C	-5.42	99.69	108.41
1	C	37	VAL	N-CA-C	-5.40	105.26	110.72
1	C	185	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	C	379	PHE	CA-CB-CG	5.39	119.19	113.80
1	C	103	GLY	N-CA-C	-5.39	100.40	113.18
1	A	394	ARG	N-CA-CB	5.39	119.66	110.50
1	B	340	VAL	CB-CA-C	5.39	118.78	111.88
1	C	366	ASP	CA-CB-CG	5.38	117.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	394	ARG	NH1-CZ-NH2	5.38	126.29	119.30
1	A	394	ARG	NE-CZ-NH2	-5.37	114.37	119.20
1	B	315	TYR	CA-C-O	-5.37	115.19	120.82
1	D	109	ARG	NE-CZ-NH2	-5.37	114.37	119.20
1	D	205	GLU	CG-CD-OE2	5.37	130.74	118.40
1	C	155	LEU	CB-CA-C	5.36	119.69	110.79
1	C	199	ALA	CA-C-O	-5.35	114.75	120.42
1	B	280	ASP	N-CA-C	-5.35	104.03	111.52
1	C	304	VAL	CA-C-O	-5.35	115.71	121.27
1	A	117	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	B	124	ASP	O-C-N	5.34	127.57	122.07
1	A	23	ARG	N-CA-C	-5.33	99.84	108.41
1	A	163	ASN	O-C-N	5.32	127.75	122.12
1	A	260	PHE	CA-CB-CG	-5.30	108.50	113.80
1	D	169	SER	N-CA-C	-5.30	105.40	111.07
1	D	239	LYS	O-C-N	5.30	129.51	122.41
1	B	277	ASN	N-CA-C	-5.29	102.25	109.71
1	D	151	VAL	N-CA-C	5.29	116.01	110.62
1	C	57	ASP	N-CA-C	-5.28	105.19	111.69
1	C	177	ARG	N-CA-C	-5.28	101.09	109.59
1	A	231	GLY	CA-C-N	5.28	127.69	120.46
1	A	231	GLY	C-N-CA	5.28	127.69	120.46
1	B	303	GLY	N-CA-C	-5.28	106.02	112.77
1	B	90	THR	CA-CB-OG1	-5.27	101.69	109.60
1	D	41	HIS	CA-CB-CG	-5.27	108.53	113.80
1	A	86	VAL	O-C-N	5.27	127.11	121.10
1	C	295	PRO	N-CA-C	-5.26	102.85	110.80
1	B	278	GLY	N-CA-C	-5.26	105.86	112.23
1	C	187	PRO	N-CA-C	5.25	125.75	112.10
1	D	239	LYS	CB-CA-C	-5.25	104.28	111.73
1	B	185	ASN	OD1-CG-ND2	-5.25	117.35	122.60
1	C	281	GLY	CA-C-N	5.24	128.62	120.60
1	C	281	GLY	C-N-CA	5.24	128.62	120.60
1	D	255	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	64	ASP	N-CA-C	-5.22	103.99	110.41
1	D	177	ARG	N-CA-C	-5.22	101.19	109.59
1	D	361	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	A	122	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	B	330	GLU	OE1-CD-OE2	5.21	135.39	122.90
1	C	156	ASP	O-C-N	5.19	127.42	122.07
1	D	308	ALA	N-CA-C	-5.19	105.53	111.14
1	B	81	GLU	CA-CB-CG	5.19	124.48	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	GLN	CB-CG-CD	-5.18	103.79	112.60
1	B	57	ASP	N-CA-C	-5.18	105.32	111.69
1	D	260	PHE	CA-C-O	-5.18	115.32	120.96
1	D	142	GLY	CA-C-O	-5.16	117.35	120.91
1	C	167	GLN	CA-C-O	5.16	126.23	120.82
1	C	276	GLU	CG-CD-OE2	5.16	130.26	118.40
1	D	128	GLU	CA-CB-CG	5.16	124.41	114.10
1	B	74	GLY	O-C-N	5.15	127.19	122.19
1	B	284	ALA	N-CA-C	-5.15	106.94	113.18
1	C	249	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	D	330	GLU	OE1-CD-OE2	5.15	135.25	122.90
1	C	74	GLY	CA-C-N	5.14	127.12	120.44
1	C	74	GLY	C-N-CA	5.14	127.12	120.44
1	C	394	ARG	N-CA-CB	5.14	119.23	110.50
1	D	21	GLN	OE1-CD-NE2	5.14	127.74	122.60
1	D	339	LYS	CB-CA-C	-5.13	104.44	111.73
1	B	102	GLY	CA-C-N	5.13	131.64	123.95
1	B	102	GLY	C-N-CA	5.13	131.64	123.95
1	C	158	TYR	CA-CB-CG	5.13	123.13	113.90
1	B	177	ARG	N-CA-C	-5.12	101.80	109.95
1	C	203	VAL	CB-CA-C	5.12	120.10	112.16
1	A	107	ASN	N-CA-C	-5.12	106.30	112.54
1	B	301	TYR	CA-CB-CG	-5.11	104.70	113.90
1	A	80	ASP	O-C-N	5.11	127.34	122.03
1	A	23	ARG	CA-C-O	-5.10	115.12	120.58
1	C	345	THR	O-C-N	5.09	126.82	121.42
1	D	117	ARG	NE-CZ-NH1	5.08	126.58	121.50
1	B	239	LYS	CB-CA-C	-5.08	104.72	111.63
1	B	217	GLU	CA-C-O	-5.07	115.22	120.70
1	B	332	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	A	205	GLU	CG-CD-OE2	5.07	130.06	118.40
1	B	103	GLY	N-CA-C	-5.07	105.60	110.21
1	B	28	ASP	O-C-N	5.06	128.62	122.85
1	C	185	ASN	CA-C-O	-5.05	115.87	121.28
1	A	212	PHE	N-CA-C	5.05	117.72	109.59
1	D	313	ARG	N-CA-C	-5.04	105.68	111.07
1	D	162	LEU	CA-C-O	-5.03	115.08	120.42
1	C	88	MET	CA-C-O	-5.03	115.90	121.33
1	A	177	ARG	N-CA-C	-5.03	101.20	109.40
1	B	379	PHE	CA-CB-CG	5.03	118.83	113.80
1	C	54	HIS	N-CA-CB	5.03	118.61	110.41
1	D	146	ASP	CA-C-O	-5.03	115.22	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	ILE	CA-CB-CG2	5.02	119.04	110.50
1	C	210	GLU	CB-CG-CD	5.02	121.14	112.60
1	A	44	ALA	N-CA-C	-5.01	105.82	111.28
1	D	203	VAL	N-CA-CB	-5.01	104.21	110.47
1	B	319	LYS	CA-C-N	5.00	126.99	120.28
1	B	319	LYS	C-N-CA	5.00	126.99	120.28
1	B	331	VAL	N-CA-C	-5.00	105.67	110.72

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	3049	0	2952	28	0
1	B	3049	0	2952	35	0
1	C	3042	0	2943	38	0
1	D	3048	0	2946	37	0
2	A	10	0	8	0	0
2	B	10	0	8	0	0
2	C	10	0	8	1	0
2	D	10	0	9	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	240	0	0	3	0
4	B	235	0	0	1	0
4	C	254	0	0	3	0
4	D	242	0	0	8	0
All	All	13203	0	11826	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:A:204:GLN:OE1	1:C:204:GLN:OE1	1.54	1.26
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.66	1.13
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.19	0.90
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.18	0.89
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.21	0.88
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.29	0.79
1:B:388:GLU:CD	1:C:313:ARG:HH11	1.98	0.71
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.71	0.71
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.74	0.70
1:C:26:PHE:HE2	1:D:186:GLN:NE2	1.90	0.69
1:A:277:ASN:OD1	1:A:323:LYS:HE3	1.93	0.69
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.77	0.68
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.80	0.65
1:D:217:GLU:OE2	4:D:429:HOH:O	2.14	0.64
1:A:313:ARG:HG3	4:A:637:HOH:O	2.00	0.62
1:B:77:LYS:O	1:B:80:ASP:HB2	2.01	0.61
1:D:185:ASN:HD22	1:D:186:GLN:HB2	1.65	0.61
1:D:3:VAL:HG12	1:D:4:GLN:H	1.65	0.61
1:B:76:LYS:NZ	1:B:128:GLU:OE2	2.35	0.60
1:B:388:GLU:OE2	1:C:313:ARG:HD3	2.03	0.59
1:D:141:GLU:OE2	4:D:595:HOH:O	2.17	0.59
1:A:167:GLN:OE1	1:A:208:ARG:NH2	2.36	0.58
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.86	0.58
1:C:26:PHE:CE2	1:D:186:GLN:NE2	2.67	0.58
1:D:394:ARG:NH1	4:D:614:HOH:O	2.14	0.56
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.89	0.55
1:C:177:ARG:HD3	4:C:613:HOH:O	2.06	0.54
1:D:220:HIS:NE2	4:D:429:HOH:O	2.33	0.53
2:C:397:XLS:H1	4:C:581:HOH:O	2.08	0.53
1:D:168:TYR:CE1	1:D:172:ARG:HD3	2.44	0.53
1:B:72:ILE:O	1:B:76:LYS:HG3	2.09	0.53
1:D:5:ALA:HB2	1:D:312:ILE:HG21	1.91	0.52
1:D:35:ASP:OD1	1:D:37:VAL:HB	2.10	0.52
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.14	0.51
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.45	0.51
1:C:168:TYR:O	1:C:172:ARG:HG2	2.10	0.51
1:B:152:SER:HB2	4:D:413:HOH:O	2.10	0.51
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.10	0.51
1:B:43:LEU:HD12	1:B:51:ILE:HD12	1.93	0.51
1:A:6:THR:O	1:A:9:ASP:HB2	2.11	0.51
1:C:72:ILE:O	1:C:76:LYS:HG3	2.11	0.50
1:A:299:GLU:HB3	1:A:303:GLY:HA3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:PHE:CZ	1:C:232:ILE:HD11	2.47	0.49
1:A:254:PHE:CD1	1:B:186:GLN:HG2	2.48	0.49
1:A:217:GLU:OE2	4:A:398:HOH:O	2.20	0.48
1:C:349:ASN:O	1:C:352:GLU:HB2	2.14	0.48
1:D:3:VAL:HG23	4:D:582:HOH:O	2.12	0.48
1:B:172:ARG:HE	1:B:172:ARG:HB3	1.27	0.48
1:D:3:VAL:N	4:D:582:HOH:O	2.46	0.48
1:C:186:GLN:HG2	1:D:254:PHE:CD1	2.49	0.47
1:B:167:GLN:OE1	1:B:208:ARG:NH2	2.48	0.46
1:C:222:GLN:HE21	1:C:249:GLN:HB3	1.79	0.46
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.97	0.46
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.12	0.46
1:A:352:GLU:HG3	1:A:356:GLU:HB2	1.96	0.46
1:B:206:LEU:O	1:B:209:PRO:HD3	2.16	0.46
1:B:278:GLY:CA	1:B:282:ALA:O	2.64	0.45
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.52	0.45
1:B:37:VAL:HG13	1:B:78:ALA:HB2	1.99	0.44
1:D:102:GLY:HA2	1:D:140:ARG:HB2	1.98	0.44
4:A:542:HOH:O	1:C:152:SER:HB2	2.17	0.44
1:D:11:PHE:CE2	1:D:312:ILE:HG23	2.52	0.44
1:C:185:ASN:HD22	1:C:186:GLN:HB2	1.81	0.44
1:B:278:GLY:HA3	1:B:282:ALA:O	2.17	0.44
1:C:278:GLY:HA3	1:C:282:ALA:O	2.18	0.44
1:B:394:ARG:HH11	1:B:394:ARG:HD3	1.55	0.44
1:C:186:GLN:HA	1:C:187:PRO:HA	1.86	0.44
1:B:142:GLY:HA3	1:B:190:ASP:O	2.18	0.44
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.17	0.44
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.99	0.44
1:C:30:THR:HG22	1:D:97:PRO:HB3	2.00	0.44
1:D:42:LYS:HD2	4:D:581:HOH:O	2.18	0.43
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.99	0.43
1:C:328:ASP:HA	1:C:329:PRO:HD3	1.79	0.43
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.53	0.43
1:B:178:PHE:HB2	1:B:212:PHE:CD2	2.53	0.43
1:C:394:ARG:HH11	1:C:394:ARG:HD3	1.45	0.43
1:C:319:LYS:O	1:C:323:LYS:HG2	2.19	0.43
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.83	0.43
1:C:43:LEU:HD12	1:C:51:ILE:HD12	2.01	0.43
1:A:42:LYS:HB3	1:A:42:LYS:HE2	1.65	0.43
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.80	0.43
1:C:86:VAL:O	1:C:131:ALA:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:LYS:HA	1:C:295:PRO:HD3	1.89	0.43
1:D:186:GLN:HA	1:D:187:PRO:HA	1.80	0.43
1:B:42:LYS:HE2	1:B:42:LYS:HB3	1.64	0.43
1:C:217:GLU:HA	1:C:245:ASP:O	2.19	0.43
1:D:299:GLU:HB3	1:D:303:GLY:HA3	2.01	0.43
1:B:164:LEU:C	1:B:164:LEU:HD23	2.44	0.42
1:B:216:PRO:HG2	1:B:232:ILE:HD11	2.01	0.42
1:C:238:HIS:O	1:C:239:LYS:HB2	2.18	0.42
1:D:120:LEU:HD22	1:D:168:TYR:CD2	2.54	0.42
1:D:34:LEU:HD21	1:D:39:ALA:HB2	2.02	0.42
1:A:305:TRP:O	1:A:309:LYS:HG3	2.20	0.42
1:A:186:GLN:HA	1:A:187:PRO:HA	1.77	0.42
1:B:313:ARG:HH11	1:C:388:GLU:CD	2.27	0.42
1:D:222:GLN:HE21	1:D:249:GLN:HB3	1.83	0.42
1:B:361:ARG:HA	1:B:365:GLU:OE1	2.19	0.42
1:A:217:GLU:HB3	1:A:220:HIS:CG	2.54	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.91	0.41
1:B:7:ARG:HD3	4:B:497:HOH:O	2.21	0.41
1:D:20:TRP:CE3	1:D:294:LYS:HB3	2.55	0.41
1:A:306:GLU:HG2	1:D:381:LYS:HB2	2.03	0.41
1:A:238:HIS:O	1:A:239:LYS:HB2	2.20	0.41
1:B:388:GLU:OE1	1:C:313:ARG:NH1	2.52	0.41
1:D:294:LYS:HA	1:D:295:PRO:HD3	1.91	0.41
1:A:185:ASN:ND2	1:A:185:ASN:C	2.78	0.41
1:A:35:ASP:HA	1:A:36:PRO:HD3	1.90	0.41
1:A:178:PHE:HB2	1:A:212:PHE:CD2	2.55	0.41
1:B:35:ASP:HA	1:B:36:PRO:HD3	1.91	0.41
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.90	0.41
1:D:193:LEU:N	1:D:194:PRO:CD	2.84	0.41
1:B:266:LEU:HD23	1:B:266:LEU:HA	1.80	0.41
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.97	0.41
1:C:250:HIS:CE1	1:C:263:GLY:HA2	2.56	0.41
1:A:349:ASN:HB3	1:A:350:PRO:CD	2.51	0.40
1:C:177:ARG:NH2	4:C:590:HOH:O	2.40	0.40
1:A:204:GLN:CD	1:C:204:GLN:OE1	2.51	0.40
1:B:282:ALA:HB1	1:B:283:PRO:HD2	2.03	0.40
1:C:278:GLY:CA	1:C:282:ALA:O	2.70	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	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	36	50
1	B	390/393 (99%)	378 (97%)	10 (3%)	2 (0%)	24	37
1	C	389/393 (99%)	374 (96%)	12 (3%)	3 (1%)	16	25
1	D	390/393 (99%)	377 (97%)	12 (3%)	1 (0%)	36	50
All	All	1559/1572 (99%)	1505 (96%)	47 (3%)	7 (0%)	30	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	280	ASP
1	C	186	GLN
1	D	186	GLN
1	A	186	GLN
1	B	186	GLN
1	C	279	PRO
1	B	281	GLY

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	305/310 (98%)	294 (96%)	11 (4%)	31	52
1	B	305/310 (98%)	296 (97%)	9 (3%)	36	58
1	C	304/310 (98%)	293 (96%)	11 (4%)	31	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	304/310 (98%)	292 (96%)	12 (4%)	28	48
All	All	1218/1240 (98%)	1175 (96%)	43 (4%)	32	53

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	7	ARG
1	A	42	LYS
1	A	49	TYR
1	A	76	LYS
1	A	80	ASP
1	A	84	LEU
1	A	185	ASN
1	A	186	GLN
1	A	203	VAL
1	A	323	LYS
1	B	3	VAL
1	B	42	LYS
1	B	49	TYR
1	B	81	GLU
1	B	132	LYS
1	B	172	ARG
1	B	186	GLN
1	B	203	VAL
1	B	394	ARG
1	C	7	ARG
1	C	49	TYR
1	C	80	ASP
1	C	84	LEU
1	C	172	ARG
1	C	177	ARG
1	C	186	GLN
1	C	203	VAL
1	C	255	ASP
1	C	313	ARG
1	C	375	LYS
1	D	3	VAL
1	D	49	TYR
1	D	80	ASP
1	D	84	LEU
1	D	172	ARG

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Mol	Chain	Res	Type
1	D	177	ARG
1	D	185	ASN
1	D	186	GLN
1	D	187	PRO
1	D	203	VAL
1	D	208	ARG
1	D	313	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	238	HIS
1	B	222	GLN
1	B	230	GLN
1	B	238	HIS
1	C	222	GLN
1	C	238	HIS
1	D	41	HIS
1	D	185	ASN
1	D	204	GLN
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 8 ligands modelled in this entry, 4 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	XLS	B	397	3	8,9,9	2.22	1 (12%)	10,11,11	1.27	1 (10%)
2	XLS	C	397	3	8,9,9	2.06	1 (12%)	10,11,11	1.40	1 (10%)
2	XLS	D	397	3	8,9,9	2.07	1 (12%)	10,11,11	1.02	1 (10%)
2	XLS	A	397	3	8,9,9	2.16	1 (12%)	10,11,11	0.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XLS	B	397	3	-	3/11/12/12	-
2	XLS	C	397	3	-	1/11/12/12	-
2	XLS	D	397	3	-	2/11/12/12	-
2	XLS	A	397	3	-	3/11/12/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	397	XLS	O1-C1	6.18	1.43	1.20
2	A	397	XLS	O1-C1	6.05	1.43	1.20
2	C	397	XLS	O1-C1	5.76	1.41	1.20
2	D	397	XLS	O1-C1	5.74	1.41	1.20

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	XLS	O4-C4-C3	2.63	115.40	109.25
2	D	397	XLS	O2-C2-C1	-2.19	105.50	110.48
2	C	397	XLS	O3-C3-C2	2.08	112.99	109.13

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	397	XLS	O1-C1-C2-C3
2	B	397	XLS	O1-C1-C2-C3
2	C	397	XLS	O1-C1-C2-C3
2	D	397	XLS	O1-C1-C2-C3
2	B	397	XLS	O4-C4-C5-O5
2	A	397	XLS	O4-C4-C5-O5
2	A	397	XLS	C1-C2-C3-O3
2	B	397	XLS	C3-C4-C5-O5
2	D	397	XLS	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	169:SER	C	170:GLU	N	1.12

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.