



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:03 AM UTC

PDB ID : 3XIM / pdb_00003xim
Title : ARGININE RESIDUES AS STABILIZING ELEMENTS IN PROTEINS
Authors : Mrabet, N.T.; Van Denbroek, A.; Van Den Brande, I.; Stanssens, P.; Laroche, Y.; Lambeir, A.-M.; Matthyssens, G.; Jenkins, J.; Chiadmi, M.; Vantilbeurgh, H.; Rey, F.; Janin, J.; Quax, W.J.; Lasters, I.; Demaeyer, M.; Wodak, S.J.
Deposited on : 1991-05-29
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

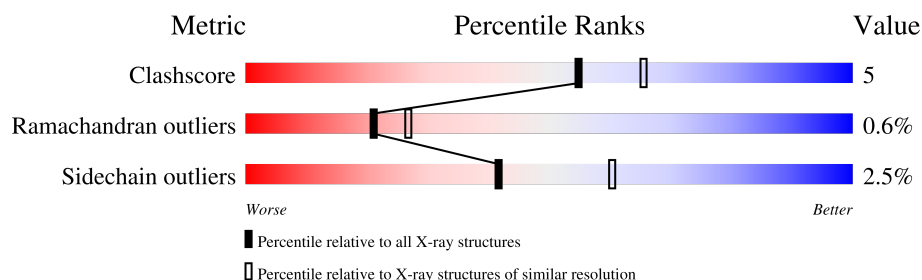
1 Overall quality at a glance

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	
1	B	393	
1	C	393	
1	D	393	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13147 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.

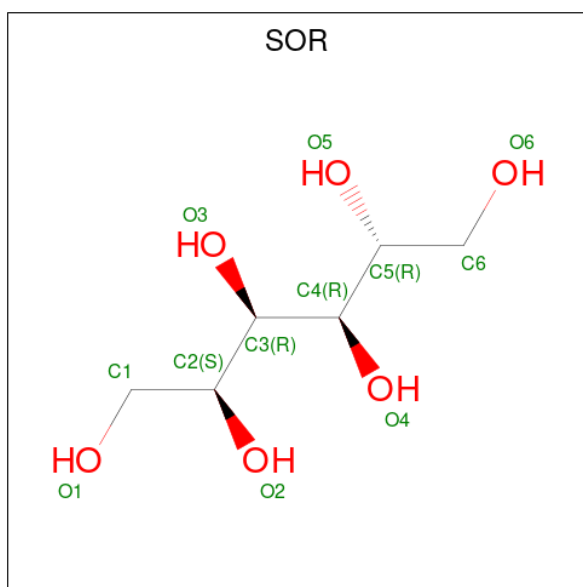
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3052	1934	537	577	4			
1	B	392	Total	C	N	O	S	0	0	0
			3059	1939	538	578	4			
1	C	390	Total	C	N	O	S	0	0	0
			3047	1931	536	576	4			
1	D	392	Total	C	N	O	S	0	0	0
			3062	1940	538	580	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	ARG	LYS	conflict	UNP P12851
A	319	ARG	LYS	conflict	UNP P12851
A	323	ARG	LYS	conflict	UNP P12851
B	309	ARG	LYS	conflict	UNP P12851
B	319	ARG	LYS	conflict	UNP P12851
B	323	ARG	LYS	conflict	UNP P12851
C	309	ARG	LYS	conflict	UNP P12851
C	319	ARG	LYS	conflict	UNP P12851
C	323	ARG	LYS	conflict	UNP P12851
D	309	ARG	LYS	conflict	UNP P12851
D	319	ARG	LYS	conflict	UNP P12851
D	323	ARG	LYS	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	222	Total	O	0	0
			222	222		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	206	Total 206	O 206	0	0
4	C	232	Total 232	O 232	0	0
4	D	211	Total 211	O 211	0	0

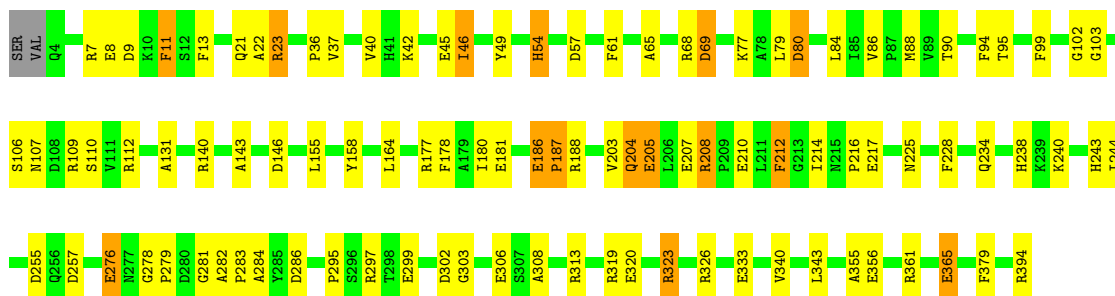
3 Residue-property plots

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.

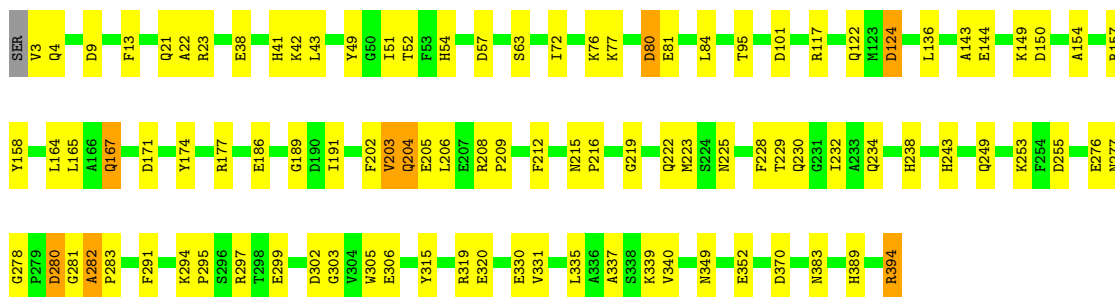
• Molecule 1: D-XYLOSE ISOMERASE

Chain A: 



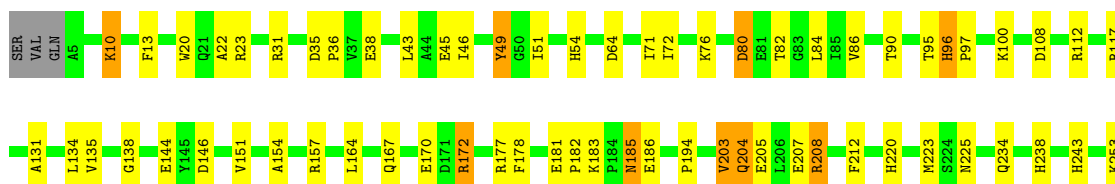
• Molecule 1: D-XYLOSE ISOMERASE

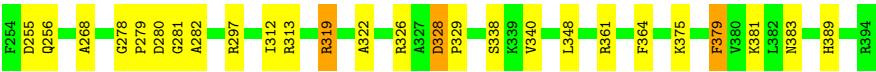
Chain B: 



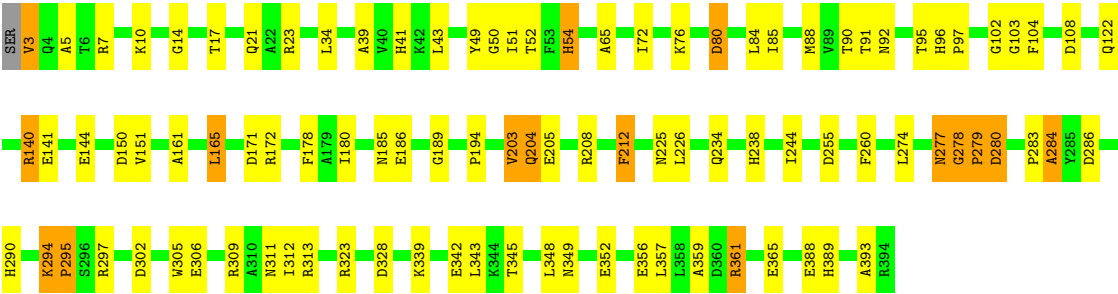
• Molecule 1: D-XYLOSE ISOMERASE

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}	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13147	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.98	0/3124	2.06	96/4232 (2.3%)
1	B	0.96	0/3131	1.96	78/4242 (1.8%)
1	C	0.97	0/3119	1.90	72/4225 (1.7%)
1	D	0.98	1/3134 (0.0%)	1.98	72/4246 (1.7%)
All	All	0.97	1/12508 (0.0%)	1.98	318/16945 (1.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	103	GLY	N-CA	6.57	1.50	1.45

All (318) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	ASP	CA-CB-CG	31.55	144.15	112.60
1	D	255	ASP	CA-CB-CG	22.73	135.33	112.60
1	B	255	ASP	CA-CB-CG	21.36	133.96	112.60
1	D	204	GLN	OE1-CD-NE2	-16.26	106.34	122.60
1	A	204	GLN	OE1-CD-NE2	-15.93	106.67	122.60
1	D	255	ASP	CB-CG-OD1	15.84	154.84	118.40
1	B	204	GLN	OE1-CD-NE2	-13.88	108.72	122.60
1	A	255	ASP	CB-CG-OD1	13.39	149.21	118.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	204	GLN	OE1-CD-NE2	-12.48	110.12	122.60
1	A	394	ARG	NH1-CZ-NH2	11.49	134.23	119.30
1	A	107	ASN	CA-CB-CG	11.36	123.96	112.60
1	A	286	ASP	CA-CB-CG	-11.34	101.26	112.60
1	A	80	ASP	CA-CB-CG	-10.71	101.89	112.60
1	A	177	ARG	CA-CB-CG	10.28	134.65	114.10
1	B	255	ASP	CB-CG-OD1	10.20	141.87	118.40
1	A	379	PHE	CA-CB-CG	10.10	123.90	113.80
1	D	255	ASP	CB-CG-OD2	-9.95	95.51	118.40
1	D	279	PRO	CA-C-N	9.40	139.49	121.54
1	D	279	PRO	C-N-CA	9.40	139.49	121.54
1	B	394	ARG	NE-CZ-NH2	-9.14	110.97	119.20
1	B	319	ARG	NE-CZ-NH2	-8.95	111.14	119.20
1	D	122	GLN	OE1-CD-NE2	-8.90	113.70	122.60
1	D	280	ASP	CA-CB-CG	8.84	121.44	112.60
1	C	361	ARG	NE-CZ-NH2	8.83	127.15	119.20
1	B	117	ARG	NE-CZ-NH1	8.68	130.18	121.50
1	C	208	ARG	CD-NE-CZ	-8.35	112.71	124.40
1	A	394	ARG	NE-CZ-NH2	-8.31	111.72	119.20
1	A	255	ASP	CB-CG-OD2	-8.25	99.42	118.40
1	A	79	LEU	CA-C-O	8.09	129.12	120.55
1	A	244	ILE	CA-C-O	-8.02	112.32	120.90
1	C	54	HIS	N-CA-C	-7.91	98.82	110.52
1	B	281	GLY	CA-C-N	7.87	133.61	121.03
1	B	281	GLY	C-N-CA	7.87	133.61	121.03
1	D	54	HIS	N-CA-C	-7.72	97.74	110.17
1	D	80	ASP	CA-CB-CG	-7.71	104.89	112.60
1	B	177	ARG	NE-CZ-NH2	-7.62	112.34	119.20
1	D	172	ARG	CD-NE-CZ	7.57	135.00	124.40
1	A	320	GLU	CB-CG-CD	7.57	125.46	112.60
1	A	216	PRO	CA-C-O	-7.55	112.45	121.67
1	C	225	ASN	OD1-CG-ND2	-7.54	115.06	122.60
1	A	243	HIS	CA-CB-CG	7.48	121.28	113.80
1	A	394	ARG	NE-CZ-NH1	-7.46	114.04	121.50
1	A	95	THR	N-CA-C	7.45	119.29	111.03
1	A	284	ALA	N-CA-C	-7.38	104.08	113.23
1	C	23	ARG	CA-C-O	-7.37	111.94	120.49
1	D	95	THR	N-CA-C	7.26	118.99	111.14
1	B	95	THR	N-CA-C	7.24	120.23	111.40
1	A	13	PHE	CA-C-O	-7.20	112.71	121.06
1	C	255	ASP	OD1-CG-OD2	-7.17	105.69	122.90
1	C	80	ASP	CA-CB-CG	-7.16	105.44	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	PHE	CA-C-O	-7.08	112.62	120.69
1	D	295	PRO	CB-CA-C	7.01	119.95	111.46
1	A	57	ASP	CA-CB-CG	6.96	119.56	112.60
1	D	311	ASN	CA-CB-CG	6.95	119.55	112.60
1	D	313	ARG	NE-CZ-NH2	6.93	125.44	119.20
1	D	286	ASP	CA-CB-CG	-6.93	105.67	112.60
1	C	194	PRO	N-CA-C	6.93	122.52	113.86
1	C	253	LYS	CA-C-O	-6.92	113.71	121.25
1	B	171	ASP	CA-C-O	-6.91	113.10	120.42
1	A	394	ARG	CD-NE-CZ	-6.85	114.81	124.40
1	D	144	GLU	N-CA-C	-6.84	105.21	113.97
1	D	23	ARG	CA-C-O	-6.83	113.28	120.58
1	D	389	HIS	CA-CB-CG	-6.80	107.00	113.80
1	B	41	HIS	CA-CB-CG	-6.74	107.06	113.80
1	B	394	ARG	N-CA-CB	6.73	121.94	110.50
1	A	88	MET	CA-C-O	-6.73	113.46	120.99
1	C	71	ILE	O-C-N	6.68	128.35	121.87
1	A	177	ARG	N-CA-C	-6.63	99.11	109.72
1	D	204	GLN	CB-CG-CD	6.63	123.87	112.60
1	C	328	ASP	CA-C-O	6.62	125.65	119.76
1	C	170	GLU	CA-C-O	-6.62	113.41	120.42
1	B	225	ASN	OD1-CG-ND2	-6.60	116.00	122.60
1	C	64	ASP	CA-CB-CG	-6.57	106.03	112.60
1	B	319	ARG	CA-C-N	6.55	129.06	120.28
1	B	319	ARG	C-N-CA	6.55	129.06	120.28
1	C	134	LEU	CA-C-O	-6.54	113.12	120.32
1	D	52	THR	CA-C-O	-6.54	114.00	121.58
1	C	389	HIS	CA-CB-CG	-6.50	107.30	113.80
1	A	102	GLY	CA-C-O	-6.50	117.62	122.37
1	B	228	PHE	CA-C-O	-6.47	114.20	121.00
1	B	255	ASP	CB-CG-OD2	-6.44	103.59	118.40
1	C	157	ARG	CA-C-O	-6.41	112.59	119.97
1	C	185	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	B	80	ASP	CA-CB-CG	-6.39	106.21	112.60
1	A	286	ASP	CA-C-O	-6.38	112.03	119.05
1	B	80	ASP	O-C-N	6.38	128.66	122.03
1	C	13	PHE	CA-C-O	-6.37	113.67	121.06
1	A	79	LEU	CA-C-N	6.37	129.06	120.65
1	A	79	LEU	C-N-CA	6.37	129.06	120.65
1	C	23	ARG	NE-CZ-NH2	-6.36	113.48	119.20
1	D	10	LYS	CB-CA-C	-6.36	103.34	111.86
1	A	80	ASP	O-C-N	6.34	128.63	122.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	41	HIS	CA-CB-CG	-6.32	107.48	113.80
1	D	203	VAL	CB-CA-C	6.30	120.65	112.14
1	B	158	TYR	N-CA-C	-6.29	104.35	111.14
1	A	69	ASP	CA-CB-CG	-6.29	106.31	112.60
1	D	225	ASN	OD1-CG-ND2	-6.28	116.33	122.60
1	D	7	ARG	CD-NE-CZ	-6.27	115.62	124.40
1	B	389	HIS	CA-CB-CG	-6.25	107.55	113.80
1	C	64	ASP	N-CA-C	-6.24	102.13	110.55
1	B	177	ARG	N-CA-C	-6.21	100.07	109.95
1	C	96	HIS	CA-CB-CG	-6.21	107.59	113.80
1	A	68	ARG	NE-CZ-NH2	6.21	124.79	119.20
1	B	144	GLU	N-CA-C	-6.20	106.25	113.88
1	D	171	ASP	CA-C-O	-6.18	113.86	120.42
1	C	135	VAL	CA-C-O	-6.16	113.69	120.84
1	A	77	LYS	O-C-N	6.15	128.40	122.07
1	C	340	VAL	CB-CA-C	6.12	119.72	111.88
1	D	306	GLU	CB-CA-C	-6.10	101.30	110.88
1	A	365	GLU	CA-C-O	-6.06	114.08	120.63
1	A	45	GLU	CA-C-O	-6.05	114.14	120.55
1	D	349	ASN	CA-CB-CG	-6.04	106.56	112.60
1	B	320	GLU	CB-CG-CD	6.00	122.81	112.60
1	A	158	TYR	CA-C-O	6.00	126.77	120.42
1	A	181	GLU	O-C-N	5.99	127.94	121.12
1	B	150	ASP	CA-CB-CG	-5.99	106.61	112.60
1	C	281	GLY	CA-C-N	5.99	129.78	120.68
1	C	281	GLY	C-N-CA	5.99	129.78	120.68
1	D	21	GLN	CB-CG-CD	-5.98	102.43	112.60
1	A	204	GLN	CB-CG-CD	5.97	122.76	112.60
1	A	204	GLN	CG-CD-NE2	5.97	125.35	116.40
1	C	223	MET	N-CA-C	-5.96	105.11	112.38
1	D	104	PHE	CA-C-O	-5.95	113.38	120.10
1	B	305	TRP	CA-CB-CG	-5.93	102.33	113.60
1	A	54	HIS	N-CA-C	-5.89	100.69	110.17
1	B	253	LYS	CA-C-O	-5.88	114.87	121.05
1	B	277	ASN	OD1-CG-ND2	5.88	128.48	122.60
1	A	180	ILE	CB-CA-C	-5.87	103.51	111.15
1	B	191	ILE	CA-C-O	-5.86	114.04	121.48
1	B	52	THR	CA-C-O	-5.86	114.78	121.58
1	A	286	ASP	N-CA-C	5.85	121.33	113.72
1	D	339	LYS	CB-CA-C	-5.83	103.45	111.73
1	C	207	GLU	CG-CD-OE2	-5.82	105.01	118.40
1	A	205	GLU	CG-CD-OE2	5.80	131.75	118.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	GLN	OE1-CD-NE2	-5.80	116.80	122.60
1	D	342	GLU	CG-CD-OE2	5.79	131.73	118.40
1	B	319	ARG	NE-CZ-NH1	5.78	127.28	121.50
1	D	260	PHE	CA-C-O	-5.78	114.33	120.92
1	B	291	PHE	CA-CB-CG	-5.78	108.02	113.80
1	C	117	ARG	NE-CZ-NH1	5.75	127.25	121.50
1	A	146	ASP	CA-C-O	-5.74	114.46	120.55
1	C	203	VAL	N-CA-CB	-5.74	100.83	110.65
1	A	42	LYS	CB-CG-CD	-5.74	98.10	111.30
1	C	379	PHE	CA-CB-CG	5.74	119.54	113.80
1	D	80	ASP	O-C-N	5.73	127.97	122.07
1	D	286	ASP	CA-C-O	-5.73	112.72	119.48
1	B	202	PHE	CA-C-N	5.72	128.30	120.46
1	B	202	PHE	C-N-CA	5.72	128.30	120.46
1	D	151	VAL	N-CA-C	5.72	116.46	110.62
1	D	17	THR	CB-CA-C	5.72	120.48	111.39
1	A	355	ALA	CA-C-O	-5.71	114.49	120.55
1	B	299	GLU	N-CA-C	5.70	119.34	110.17
1	B	243	HIS	CA-CB-CG	5.69	119.49	113.80
1	A	333	GLU	CB-CG-CD	5.69	122.27	112.60
1	B	21	GLN	CB-CG-CD	-5.67	102.96	112.60
1	D	357	LEU	O-C-N	5.65	127.89	122.07
1	A	356	GLU	CB-CG-CD	5.65	122.21	112.60
1	A	21	GLN	CB-CG-CD	-5.65	103.00	112.60
1	A	240	LYS	CA-C-O	-5.64	112.82	119.48
1	B	394	ARG	CD-NE-CZ	-5.64	116.50	124.40
1	B	54	HIS	N-CA-C	-5.64	101.09	110.17
1	A	109	ARG	NH1-CZ-NH2	5.62	126.61	119.30
1	C	146	ASP	CA-C-O	-5.62	114.59	120.55
1	A	8	GLU	CA-CB-CG	-5.62	102.86	114.10
1	C	95	THR	N-CA-C	5.61	118.25	111.40
1	B	57	ASP	CA-CB-CG	5.60	118.20	112.60
1	D	284	ALA	N-CA-C	-5.59	106.47	113.28
1	C	80	ASP	N-CA-CB	-5.58	101.62	109.94
1	C	319	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	D	165	LEU	CA-C-O	-5.57	114.64	120.55
1	D	54	HIS	N-CA-CB	5.57	119.71	110.63
1	A	225	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	B	13	PHE	CA-CB-CG	5.57	119.37	113.80
1	B	202	PHE	CA-C-O	5.57	126.66	120.82
1	D	277	ASN	CA-C-N	5.56	130.60	121.87
1	D	277	ASN	C-N-CA	5.56	130.60	121.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	GLN	CA-C-N	5.56	127.67	120.44
1	B	167	GLN	C-N-CA	5.56	127.67	120.44
1	A	207	GLU	CA-C-O	-5.56	114.53	120.42
1	D	255	ASP	OD1-CG-OD2	-5.56	109.56	122.90
1	C	100	LYS	CA-C-O	-5.55	113.82	120.10
1	C	328	ASP	CB-CA-C	5.55	118.41	109.41
1	A	394	ARG	CG-CD-NE	-5.55	99.78	112.00
1	C	82	THR	CA-CB-OG1	-5.54	101.30	109.60
1	A	102	GLY	O-C-N	5.53	129.01	123.48
1	D	255	ASP	CA-C-O	-5.53	114.05	120.62
1	A	295	PRO	CA-C-O	-5.52	114.73	121.03
1	C	203	VAL	CB-CA-C	5.52	120.71	112.16
1	D	294	LYS	O-C-N	5.51	126.67	121.38
1	C	23	ARG	N-CA-C	-5.50	100.83	109.25
1	B	9	ASP	N-CA-C	-5.50	106.07	112.89
1	A	61	PHE	CA-C-O	-5.50	114.97	120.96
1	D	313	ARG	N-CA-CB	5.49	117.98	110.01
1	A	110	SER	O-C-N	5.49	127.94	122.12
1	D	345	THR	CA-C-O	-5.49	115.16	119.66
1	C	256	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	D	14	GLY	N-CA-C	-5.48	102.74	112.54
1	A	212	PHE	N-CA-C	5.46	118.29	109.40
1	A	313	ARG	NE-CZ-NH1	5.46	126.96	121.50
1	A	257	ASP	CA-CB-CG	5.45	118.05	112.60
1	D	361	ARG	CA-CB-CG	5.45	125.01	114.10
1	A	109	ARG	NE-CZ-NH1	-5.44	116.06	121.50
1	C	23	ARG	CD-NE-CZ	5.44	132.01	124.40
1	A	281	GLY	CA-C-N	5.44	128.94	120.68
1	A	281	GLY	C-N-CA	5.44	128.94	120.68
1	C	45	GLU	CA-CB-CG	5.43	124.97	114.10
1	B	295	PRO	CA-C-O	-5.43	114.84	121.03
1	D	226	LEU	O-C-N	5.43	129.02	122.94
1	A	276	GLU	N-CA-C	5.41	119.99	112.90
1	A	217	GLU	CG-CD-OE1	-5.40	105.97	118.40
1	D	328	ASP	CB-CA-C	5.40	117.16	109.38
1	B	337	ALA	CA-C-O	-5.40	114.00	120.10
1	B	149	LYS	CA-C-O	-5.39	113.62	120.20
1	D	283	PRO	N-CA-CB	5.39	108.11	103.31
1	B	177	ARG	CA-C-O	-5.39	115.07	121.16
1	C	313	ARG	NH1-CZ-NH2	-5.38	112.30	119.30
1	D	91	THR	CA-CB-OG1	-5.38	101.53	109.60
1	A	188	ARG	CA-C-O	-5.38	115.47	121.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	TYR	CA-C-N	5.37	127.42	120.44
1	A	158	TYR	C-N-CA	5.37	127.42	120.44
1	B	340	VAL	CB-CA-C	5.36	118.75	111.88
1	C	108	ASP	CA-CB-CG	-5.36	107.24	112.60
1	A	103	GLY	CA-C-N	5.36	127.99	120.28
1	A	103	GLY	C-N-CA	5.36	127.99	120.28
1	C	313	ARG	CB-CA-C	5.35	119.28	110.88
1	A	306	GLU	CB-CA-C	-5.35	102.48	110.88
1	C	312	ILE	O-C-N	5.35	127.06	121.87
1	A	295	PRO	N-CA-C	-5.35	102.72	110.80
1	C	177	ARG	N-CA-C	-5.35	101.45	109.95
1	C	328	ASP	CA-C-N	5.34	124.97	119.05
1	C	328	ASP	C-N-CA	5.34	124.97	119.05
1	C	135	VAL	O-C-N	5.32	128.57	122.93
1	B	63	SER	O-C-N	5.32	129.42	123.19
1	B	339	LYS	CA-CB-CG	-5.32	103.46	114.10
1	D	342	GLU	CB-CG-CD	5.32	121.64	112.60
1	B	330	GLU	CG-CD-OE2	-5.31	106.18	118.40
1	C	383	ASN	CA-CB-CG	-5.31	107.29	112.60
1	B	383	ASN	CA-CB-CG	-5.30	107.30	112.60
1	B	282	ALA	N-CA-C	5.29	117.83	110.20
1	A	205	GLU	CB-CG-CD	5.29	121.59	112.60
1	B	230	GLN	CA-C-O	-5.28	114.83	120.42
1	A	394	ARG	N-CA-CB	5.28	119.47	110.50
1	C	151	VAL	O-C-N	5.27	126.98	121.87
1	A	244	ILE	O-C-N	5.27	129.20	123.09
1	D	388	GLU	CA-CB-CG	-5.26	103.57	114.10
1	A	308	ALA	N-CA-C	-5.26	105.46	111.14
1	C	243	HIS	CA-CB-CG	5.25	119.05	113.80
1	A	243	HIS	CA-C-N	-5.25	114.01	122.25
1	A	243	HIS	C-N-CA	-5.25	114.01	122.25
1	C	31	ARG	NE-CZ-NH1	5.25	126.75	121.50
1	A	217	GLU	CG-CD-OE2	5.25	130.47	118.40
1	A	340	VAL	CA-C-O	-5.23	115.51	120.95
1	C	255	ASP	CB-CG-OD2	5.23	130.42	118.40
1	D	204	GLN	CG-CD-OE1	5.23	131.25	120.80
1	A	37	VAL	CB-CA-C	5.22	118.66	111.97
1	D	108	ASP	CA-CB-CG	-5.22	107.38	112.60
1	B	370	ASP	CA-C-O	-5.22	115.02	120.55
1	C	185	ASN	O-C-N	5.21	128.50	123.29
1	C	328	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	177	ARG	CB-CG-CD	-5.21	99.31	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ILE	CA-C-N	5.21	129.57	123.16
1	A	214	ILE	C-N-CA	5.21	129.57	123.16
1	B	291	PHE	CA-C-O	-5.21	115.01	120.58
1	B	124	ASP	O-C-N	5.21	127.43	122.07
1	D	150	ASP	CB-CG-OD1	5.21	130.37	118.40
1	B	331	VAL	N-CA-C	-5.20	105.64	110.53
1	A	228	PHE	CB-CA-C	5.20	118.97	110.96
1	A	57	ASP	N-CA-CB	5.20	117.94	110.20
1	B	335	LEU	O-C-N	5.18	127.61	122.12
1	D	297	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	A	187	PRO	N-CA-C	5.17	125.54	112.10
1	C	177	ARG	N-CA-CB	5.17	119.12	110.85
1	B	189	GLY	N-CA-C	-5.16	106.39	112.64
1	C	144	GLU	N-CA-C	-5.16	107.11	113.41
1	D	140	ARG	CA-C-O	-5.16	113.31	119.35
1	D	302	ASP	CA-C-O	-5.16	114.95	120.42
1	D	393	ALA	CA-C-N	5.16	130.98	121.70
1	D	393	ALA	C-N-CA	5.16	130.98	121.70
1	A	46	ILE	CA-C-O	-5.15	112.85	119.39
1	A	143	ALA	N-CA-CB	-5.15	102.92	111.57
1	D	212	PHE	N-CA-C	5.15	117.79	109.40
1	D	65	ALA	CA-C-O	-5.14	114.29	120.10
1	B	229	THR	CA-CB-OG1	-5.13	101.91	109.60
1	D	349	ASN	OD1-CG-ND2	5.12	127.72	122.60
1	A	155	LEU	CB-CA-C	5.11	119.54	110.85
1	C	138	GLY	CA-C-N	5.10	126.52	120.14
1	C	138	GLY	C-N-CA	5.10	126.52	120.14
1	B	204	GLN	CB-CG-CD	5.10	121.27	112.60
1	C	10	LYS	CB-CA-C	-5.10	105.03	111.86
1	C	326	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	A	302	ASP	CA-C-N	5.09	125.64	119.98
1	A	302	ASP	C-N-CA	5.09	125.64	119.98
1	B	157	ARG	NE-CZ-NH1	5.09	126.59	121.50
1	C	167	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	C	90	THR	CA-C-N	5.09	130.57	122.94
1	C	90	THR	C-N-CA	5.09	130.57	122.94
1	C	112	ARG	CG-CD-NE	5.08	123.17	112.00
1	C	268	ALA	N-CA-C	-5.07	105.83	111.36
1	D	189	GLY	N-CA-C	-5.07	106.64	112.83
1	B	117	ARG	NE-CZ-NH2	-5.07	114.64	119.20
1	B	280	ASP	N-CA-C	-5.07	104.31	111.56
1	A	7	ARG	CA-CB-CG	-5.07	103.96	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	ALA	N-CA-CB	-5.07	103.06	111.57
1	B	303	GLY	N-CA-C	-5.06	106.65	112.73
1	B	57	ASP	N-CA-C	-5.06	105.47	111.69
1	D	328	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	215	ASN	O-C-N	5.05	125.92	121.37
1	B	54	HIS	N-CA-CB	5.05	118.86	110.63
1	D	194	PRO	N-CA-C	5.04	120.17	113.57
1	A	99	PHE	CA-CB-CG	5.04	118.84	113.80
1	B	302	ASP	O-C-N	5.03	127.89	122.15
1	D	88	MET	CA-CB-CG	5.03	124.17	114.10
1	A	23	ARG	CA-C-O	-5.03	115.69	120.92
1	B	165	LEU	CA-C-O	-5.03	115.22	120.55
1	C	322	ALA	N-CA-C	-5.03	105.71	111.14
1	C	375	LYS	CB-CG-CD	-5.02	99.75	111.30
1	C	389	HIS	N-CA-CB	5.01	117.58	110.16
1	B	54	HIS	CB-CA-C	-5.01	101.03	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3052	0	2945	29	0
1	B	3059	0	2954	35	0
1	C	3047	0	2943	28	0
1	D	3062	0	2956	36	0
2	A	12	0	13	0	0
2	B	12	0	14	0	0
2	C	12	0	13	0	0
2	D	12	0	14	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	222	0	0	3	0
4	B	206	0	0	2	0
4	C	232	0	0	2	0
4	D	211	0	0	4	0
All	All	13147	0	11852	116	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 (116) 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:D:278:GLY:HA2	4:D:509:HOH:O	1.21	1.26
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.66	1.10
1:A:204:GLN:OE1	1:C:204:GLN:OE1	1.69	1.09
1:D:277:ASN:HD21	1:D:323:ARG:HE	1.12	0.97
1:D:279:PRO:HD3	1:D:284:ALA:HB2	1.55	0.89
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.20	0.89
1:D:278:GLY:HA3	1:D:284:ALA:HB2	1.55	0.89
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.25	0.82
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.28	0.82
1:C:278:GLY:HA3	1:C:282:ALA:O	1.81	0.81
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.30	0.77
1:C:278:GLY:CA	1:C:282:ALA:O	2.36	0.73
1:A:319:ARG:NH1	4:A:565:HOH:O	2.15	0.73
1:A:204:GLN:HG2	4:A:549:HOH:O	1.91	0.71
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.74	0.70
1:A:278:GLY:HA3	1:A:282:ALA:O	1.92	0.70
1:B:3:VAL:HG12	1:B:4:GLN:H	1.56	0.70
1:D:279:PRO:HD3	1:D:284:ALA:CB	2.23	0.68
1:B:278:GLY:CA	1:B:282:ALA:O	2.43	0.67
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.76	0.67
1:A:279:PRO:HG2	4:A:509:HOH:O	1.95	0.66
1:B:278:GLY:HA3	1:B:282:ALA:O	1.96	0.65
1:A:278:GLY:CA	1:A:282:ALA:O	2.46	0.63
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.81	0.62
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.83	0.60
1:B:72:ILE:O	1:B:76:LYS:HG3	2.02	0.60
1:A:65:ALA:O	1:A:69:ASP:HB2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.82	0.59
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.86	0.58
1:D:277:ASN:ND2	1:D:323:ARG:HE	1.92	0.58
1:B:72:ILE:HG22	1:B:76:LYS:HE3	1.85	0.58
1:B:43:LEU:HD12	1:B:51:ILE:HD12	1.87	0.56
1:B:22:ALA:HB1	1:B:297:ARG:HG3	1.86	0.55
1:D:102:GLY:HA2	1:D:140:ARG:HB2	1.89	0.55
1:D:274:LEU:HD12	4:D:509:HOH:O	2.07	0.55
1:D:43:LEU:HD12	1:D:51:ILE:HD12	1.89	0.55
1:D:277:ASN:HD21	1:D:323:ARG:NE	1.95	0.54
1:C:278:GLY:HA2	4:C:510:HOH:O	2.08	0.54
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.91	0.54
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.13	0.53
1:A:208:ARG:NH1	1:A:210:GLU:OE2	2.41	0.53
1:D:72:ILE:O	1:D:76:LYS:HG3	2.08	0.53
1:D:279:PRO:HD3	1:D:284:ALA:CA	2.40	0.52
1:B:282:ALA:HB1	1:B:283:PRO:HD2	1.93	0.51
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.46	0.50
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.95	0.50
1:C:183:LYS:HG3	1:C:220:HIS:CG	2.47	0.50
1:C:86:VAL:O	1:C:131:ALA:HA	2.11	0.50
1:B:203:VAL:HG22	1:B:212:PHE:HB3	1.94	0.50
1:A:164:LEU:HD12	1:C:348:LEU:HD11	1.93	0.50
1:B:278:GLY:HA2	4:B:496:HOH:O	2.10	0.49
1:B:206:LEU:O	1:B:209:PRO:HD3	2.11	0.49
1:A:36:PRO:O	1:A:40:VAL:HG23	2.13	0.49
1:C:164:LEU:C	1:C:164:LEU:HD23	2.38	0.48
1:B:294:LYS:HE2	4:B:583:HOH:O	2.14	0.48
1:D:141:GLU:OE2	4:D:574:HOH:O	2.20	0.47
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.72	0.47
1:A:186:GLU:HA	1:A:187:PRO:HA	1.71	0.46
1:B:124:ASP:OD1	1:B:174:TYR:OH	2.29	0.46
1:B:77:LYS:O	1:B:80:ASP:HB2	2.16	0.46
1:A:164:LEU:C	1:A:164:LEU:HD23	2.41	0.46
1:B:164:LEU:C	1:B:164:LEU:HD23	2.40	0.46
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.50	0.46
1:B:280:ASP:C	1:B:282:ALA:H	2.24	0.46
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.51	0.46
1:D:178:PHE:HB2	1:D:212:PHE:CD2	2.51	0.46
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.99	0.45
1:B:216:PRO:HG2	1:B:232:ILE:HD11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:VAL:HG12	1:B:4:GLN:N	2.28	0.44
1:D:34:LEU:CD2	1:D:39:ALA:HB2	2.47	0.44
1:C:172:ARG:HE	1:C:172:ARG:HB3	1.33	0.44
1:D:3:VAL:HG23	4:D:594:HOH:O	2.17	0.44
1:D:244:ILE:O	1:D:290:HIS:HB3	2.17	0.44
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.87	0.44
1:C:328:ASP:HA	1:C:329:PRO:HD3	1.81	0.44
1:B:219:GLY:O	1:B:223:MET:HG3	2.18	0.43
1:C:10:LYS:HA	1:C:49:TYR:CD1	2.54	0.43
1:D:161:ALA:O	1:D:165:LEU:HG	2.19	0.43
1:C:20:TRP:CE2	1:C:22:ALA:HA	2.53	0.43
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.82	0.43
1:D:305:TRP:O	1:D:309:ARG:HG3	2.19	0.42
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.19	0.42
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.96	0.42
1:D:54:HIS:CD2	1:D:90:THR:HG23	2.54	0.42
1:A:299:GLU:HB3	1:A:303:GLY:HA3	2.01	0.42
1:D:50:GLY:HA2	1:D:85:ILE:O	2.19	0.42
1:C:43:LEU:HD12	1:C:51:ILE:HD12	2.01	0.42
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.95	0.42
1:D:356:GLU:O	1:D:359:ALA:HB3	2.20	0.42
1:A:343:LEU:HD21	1:C:154:ALA:HB2	2.02	0.41
1:B:276:GLU:OE2	1:B:315:TYR:OH	2.34	0.41
1:C:338:SER:HB3	1:C:379:PHE:CE1	2.56	0.41
1:A:178:PHE:HB2	1:A:212:PHE:CD2	2.55	0.41
1:C:319:ARG:NH2	4:C:583:HOH:O	2.53	0.41
1:A:94:PHE:HA	1:A:140:ARG:HG3	2.00	0.41
1:A:326:ARG:HA	1:A:326:ARG:HD3	1.93	0.41
1:D:92:ASN:OD1	1:D:92:ASN:C	2.63	0.41
1:D:352:GLU:HG3	1:D:356:GLU:HB2	2.01	0.41
1:A:23:ARG:HG2	1:B:23:ARG:NH1	2.36	0.41
1:B:167:GLN:OE1	1:B:208:ARG:NH2	2.52	0.41
1:A:276:GLU:HG3	1:A:319:ARG:HG3	2.01	0.41
1:C:181:GLU:HA	1:C:182:PRO:HD3	1.91	0.41
1:B:232:ILE:HD13	1:B:232:ILE:HA	1.89	0.41
1:B:101:ASP:CG	1:B:101:ASP:O	2.63	0.41
1:A:106:SER:O	1:A:112:ARG:HD3	2.21	0.41
1:B:349:ASN:N	1:B:352:GLU:OE1	2.47	0.41
1:D:294:LYS:HA	1:D:295:PRO:HD3	1.87	0.41
1:C:72:ILE:O	1:C:76:LYS:HG3	2.21	0.41
1:D:5:ALA:HB2	1:D:312:ILE:HG21	2.01	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:LEU:HD21	1:D:39:ALA:HB2	2.02	0.40
1:A:86:VAL:O	1:A:131:ALA:HA	2.20	0.40
1:B:42:LYS:HD3	1:B:42:LYS:HA	1.78	0.40
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.21	0.40
1:C:208:ARG:HH11	1:C:208:ARG:HD3	1.43	0.40
1:C:178:PHE:HB2	1:C:212:PHE:CD2	2.57	0.40
1:B:278:GLY:C	1:B:282:ALA:O	2.64	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	389/393 (99%)	374 (96%)	14 (4%)	1 (0%)	36	46
1	B	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	36	46
1	C	388/393 (99%)	370 (95%)	14 (4%)	4 (1%)	12	15
1	D	390/393 (99%)	376 (96%)	11 (3%)	3 (1%)	16	20
All	All	1557/1572 (99%)	1496 (96%)	52 (3%)	9 (1%)	21	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	279	PRO
1	D	278	GLY
1	D	280	ASP
1	C	280	ASP
1	A	186	GLU
1	B	186	GLU
1	C	186	GLU
1	C	364	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	305/310 (98%)	298 (98%)	7 (2%)	44	63
1	B	306/310 (99%)	299 (98%)	7 (2%)	44	63
1	C	305/310 (98%)	297 (97%)	8 (3%)	40	59
1	D	307/310 (99%)	299 (97%)	8 (3%)	40	59
All	All	1223/1240 (99%)	1193 (98%)	30 (2%)	42	60

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	49	TYR
1	A	80	ASP
1	A	84	LEU
1	A	203	VAL
1	A	208	ARG
1	A	323	ARG
1	B	38	GLU
1	B	49	TYR
1	B	81	GLU
1	B	84	LEU
1	B	136	LEU
1	B	203	VAL
1	B	394	ARG
1	C	38	GLU
1	C	46	ILE
1	C	49	TYR
1	C	80	ASP
1	C	84	LEU
1	C	172	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	185	ASN
1	C	203	VAL
1	D	3	VAL
1	D	49	TYR
1	D	80	ASP
1	D	84	LEU
1	D	180	ILE
1	D	185	ASN
1	D	203	VAL
1	D	208	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	HIS
1	B	204	GLN
1	B	222	GLN
1	B	230	GLN
1	B	238	HIS
1	C	41	HIS
1	C	204	GLN
1	C	222	GLN
1	C	238	HIS
1	D	41	HIS
1	D	185	ASN
1	D	222	GLN
1	D	238	HIS
1	D	277	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 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	0.95	0	14,14,14	1.55	4 (28%)
2	SOR	D	397	3	11,11,11	1.29	2 (18%)	14,14,14	2.25	7 (50%)
2	SOR	C	397	3	11,11,11	0.95	0	14,14,14	1.26	3 (21%)
2	SOR	B	397	3	11,11,11	1.00	0	14,14,14	1.77	4 (28%)

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	-	1/16/16/16	-
2	SOR	D	397	3	-	4/16/16/16	-
2	SOR	C	397	3	-	3/16/16/16	-
2	SOR	B	397	3	-	3/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	397	SOR	C1-C2	2.63	1.58	1.52
2	D	397	SOR	C6-C5	2.15	1.57	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	SOR	O4-C4-C3	4.50	119.97	109.46
2	D	397	SOR	O6-C6-C5	-3.97	102.81	111.16
2	D	397	SOR	O2-C2-C3	3.46	117.34	109.25
2	D	397	SOR	C1-C2-C3	-3.37	105.30	112.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	397	SOR	O4-C4-C3	2.79	115.99	109.46
2	D	397	SOR	O2-C2-C1	-2.69	102.92	109.03
2	D	397	SOR	O5-C5-C4	2.61	115.36	109.25
2	A	397	SOR	O6-C6-C5	-2.56	105.77	111.16
2	B	397	SOR	C5-C4-C3	2.45	116.24	112.48
2	C	397	SOR	C6-C5-C4	-2.36	107.36	112.17
2	D	397	SOR	O1-C1-C2	-2.27	106.39	111.16
2	D	397	SOR	C6-C5-C4	-2.23	107.62	112.17
2	B	397	SOR	C6-C5-C4	-2.18	107.73	112.17
2	C	397	SOR	O4-C4-C3	2.11	114.39	109.46
2	C	397	SOR	O6-C6-C5	-2.10	106.74	111.16
2	A	397	SOR	C1-C2-C3	-2.06	107.98	112.17
2	A	397	SOR	C2-C3-C4	2.02	115.58	112.48
2	B	397	SOR	O3-C3-C4	2.00	114.14	109.46

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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.