



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:38 PM UTC

PDB ID : 4KBP / pdb_00004kbp
Title : KIDNEY BEAN PURPLE ACID PHOSPHATASE
Authors : Klabunde, T.; Strater, N.; Krebs, B.
Deposited on : 1995-10-02
Resolution : 2.70 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

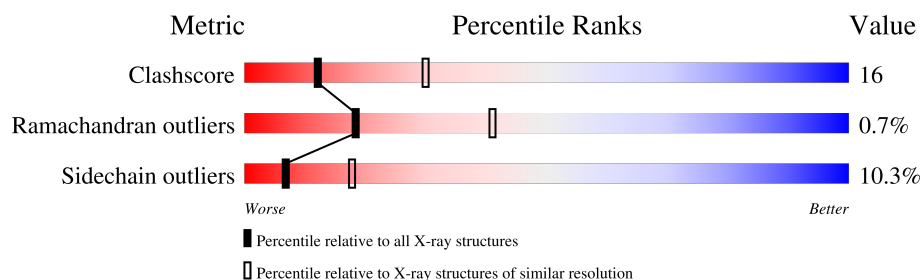
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	432	
1	B	432	
1	C	432	
1	D	432	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14340 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 PURPLE ACID PHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3494	2243	605	636	10			
1	B	424	Total	C	N	O	S	0	0	0
			3494	2243	605	636	10			
1	C	424	Total	C	N	O	S	0	0	0
			3494	2243	605	636	10			
1	D	424	Total	C	N	O	S	0	0	0
			3494	2243	605	636	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	253	TYR	HIS	conflict	UNP P80366
A	254	SER	ILE	conflict	UNP P80366
B	253	TYR	HIS	conflict	UNP P80366
B	254	SER	ILE	conflict	UNP P80366
C	253	TYR	HIS	conflict	UNP P80366
C	254	SER	ILE	conflict	UNP P80366
D	253	TYR	HIS	conflict	UNP P80366
D	254	SER	ILE	conflict	UNP P80366

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

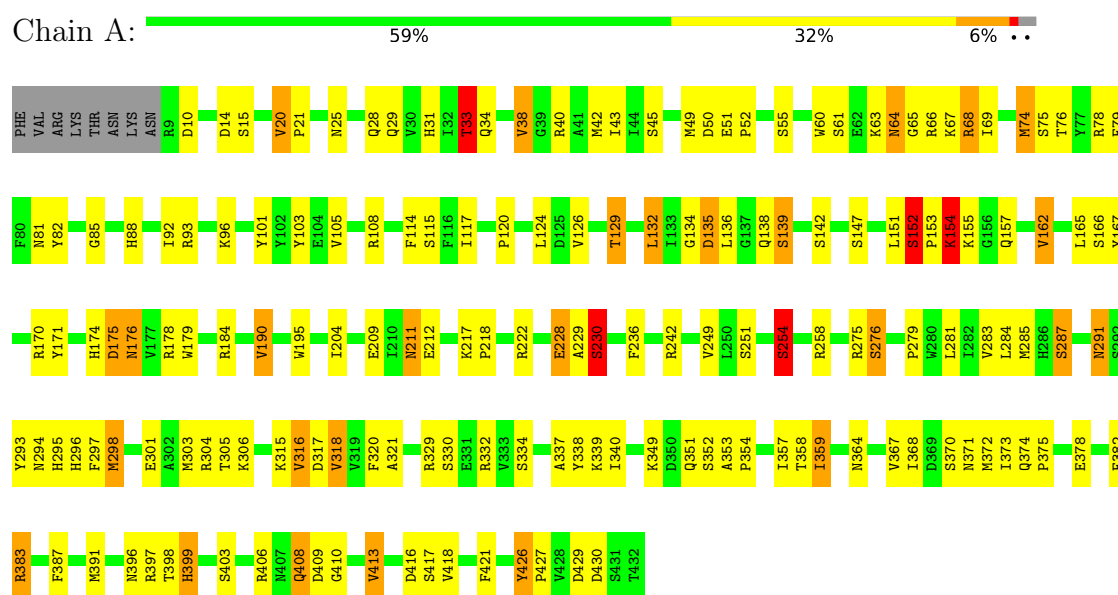
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total	O	0	0
			16	16		
6	B	13	Total	O	0	0
			13	13		
6	C	14	Total	O	0	0
			14	14		
6	D	13	Total	O	0	0
			13	13		

3 Residue-property plots [i](#)

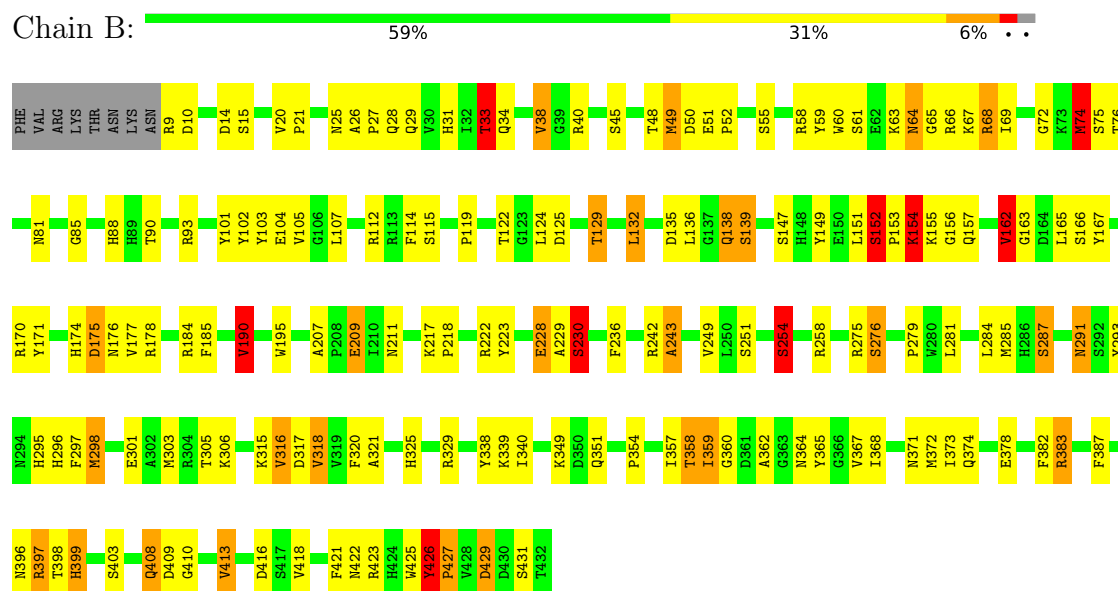
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

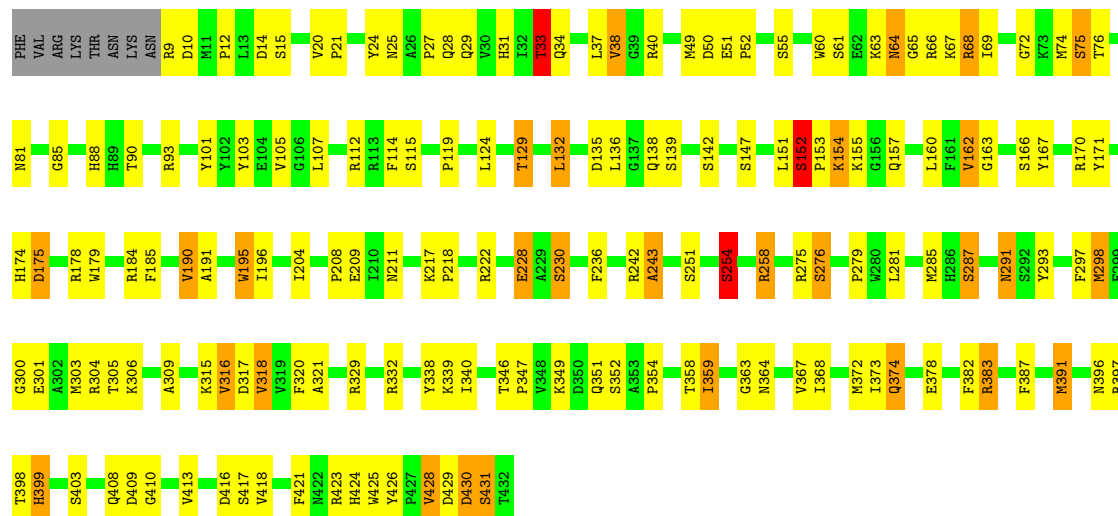


• Molecule 1: PURPLE ACID PHOSPHATASE



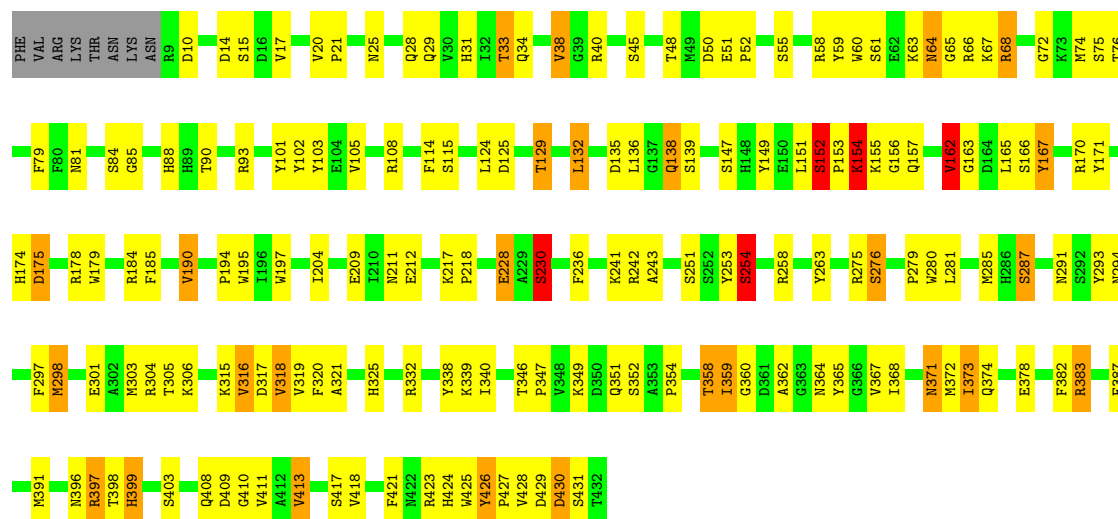
● Molecule 1: PURPLE ACID PHOSPHATASE

Chain C:  60% 31% 7% ..



● Molecule 1: PURPLE ACID PHOSPHATASE

Chain D:  58% 33% 6% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	132.70Å 347.30Å 128.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70	Depositor
% Data completeness (in resolution range)	72.4 (10.00-2.70)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.192 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14340	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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: NAG, ZN, PO4, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.17	10/3613 (0.3%)	1.33	43/4912 (0.9%)
1	B	1.05	2/3613 (0.1%)	1.32	40/4912 (0.8%)
1	C	1.12	5/3613 (0.1%)	1.33	41/4912 (0.8%)
1	D	1.10	2/3613 (0.1%)	1.31	43/4912 (0.9%)
All	All	1.11	19/14452 (0.1%)	1.32	167/19648 (0.8%)

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	B	0	2
1	D	0	2
All	All	0	4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	49	MET	SD-CE	6.98	1.97	1.79
1	C	49	MET	SD-CE	6.34	1.95	1.79
1	A	204	ILE	CA-CB	-6.33	1.47	1.54
1	A	74	MET	SD-CE	-6.19	1.64	1.79
1	A	117	ILE	CA-CB	-6.15	1.47	1.54
1	A	92	ILE	CA-CB	-6.14	1.47	1.54
1	C	204	ILE	CA-CB	-5.86	1.47	1.54
1	D	319	VAL	CA-CB	-5.73	1.46	1.54
1	A	20	VAL	CA-C	-5.58	1.47	1.52
1	B	74	MET	SD-CE	-5.39	1.66	1.79
1	C	391	MET	SD-CE	-5.38	1.66	1.79
1	D	194	PRO	CA-C	-5.32	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	ALA	CA-C	-5.29	1.46	1.53
1	A	43	ILE	CA-CB	-5.22	1.47	1.54
1	A	42	MET	SD-CE	-5.13	1.66	1.79
1	A	337	ALA	CA-CB	-5.08	1.46	1.54
1	C	196	ILE	CA-CB	-5.08	1.48	1.54
1	C	309	ALA	CA-CB	-5.05	1.45	1.53
1	A	283	VAL	CA-CB	-5.04	1.47	1.54

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	230	SER	N-CA-C	-14.42	91.93	110.53
1	D	230	SER	N-CA-C	-13.47	91.76	110.35
1	A	230	SER	N-CA-C	-13.46	91.77	110.35
1	B	230	SER	N-CA-C	-13.34	91.94	110.35
1	C	38	VAL	N-CA-C	10.62	123.40	113.10
1	A	154	LYS	N-CA-C	-10.58	91.38	108.41
1	A	38	VAL	N-CA-C	10.46	123.25	113.10
1	D	38	VAL	N-CA-C	10.11	121.73	112.43
1	B	38	VAL	N-CA-C	10.04	122.84	113.10
1	D	154	LYS	N-CA-C	-9.21	93.58	108.41
1	B	287	SER	CA-C-N	9.17	128.93	119.76
1	B	287	SER	C-N-CA	9.17	128.93	119.76
1	C	397	ARG	N-CA-C	-9.09	102.19	113.28
1	A	287	SER	CA-C-N	8.69	129.02	119.90
1	A	287	SER	C-N-CA	8.69	129.02	119.90
1	C	287	SER	CA-C-N	8.44	128.77	119.90
1	C	287	SER	C-N-CA	8.44	128.77	119.90
1	A	162	VAL	N-CA-CB	-8.42	102.54	112.39
1	B	154	LYS	N-CA-C	-8.27	93.43	107.99
1	D	287	SER	CA-C-N	8.23	128.54	119.90
1	D	287	SER	C-N-CA	8.23	128.54	119.90
1	C	21	PRO	CA-C-N	8.09	128.02	119.85
1	C	21	PRO	C-N-CA	8.09	128.02	119.85
1	C	154	LYS	N-CA-C	-7.85	94.17	107.99
1	C	230	SER	CA-C-N	-7.78	110.04	122.95
1	C	230	SER	C-N-CA	-7.78	110.04	122.95
1	D	152	SER	CA-C-N	7.75	127.81	119.28
1	D	152	SER	C-N-CA	7.75	127.81	119.28
1	B	163	GLY	N-CA-C	7.69	119.25	111.95
1	B	152	SER	CA-C-N	7.53	127.57	119.28
1	B	152	SER	C-N-CA	7.53	127.57	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	162	VAL	N-CA-CB	-7.46	103.66	112.39
1	D	162	VAL	N-CA-C	7.45	118.54	111.91
1	C	136	LEU	N-CA-C	7.43	120.09	111.02
1	A	426	TYR	CA-C-N	7.42	129.11	119.84
1	A	426	TYR	C-N-CA	7.42	129.11	119.84
1	C	135	ASP	N-CA-CB	-7.40	101.05	112.30
1	C	430	ASP	N-CA-C	-7.39	104.41	113.50
1	D	81	ASN	N-CA-C	-7.34	103.90	112.92
1	A	230	SER	CA-C-N	-7.31	109.61	122.62
1	A	230	SER	C-N-CA	-7.31	109.61	122.62
1	D	397	ARG	N-CA-C	-7.23	104.45	113.28
1	B	397	ARG	N-CA-C	-7.22	104.44	113.18
1	B	81	ASN	N-CA-C	-7.13	104.59	112.72
1	B	85	GLY	N-CA-C	-7.12	100.38	112.77
1	D	85	GLY	N-CA-C	-7.07	100.47	112.77
1	B	162	VAL	N-CA-CB	-6.95	104.26	112.39
1	C	317	ASP	N-CA-C	6.95	118.54	110.97
1	A	136	LEU	N-CA-C	6.91	118.50	110.97
1	B	230	SER	CA-C-N	-6.91	110.32	122.62
1	B	230	SER	C-N-CA	-6.91	110.32	122.62
1	B	135	ASP	N-CA-CB	-6.88	101.74	112.13
1	C	163	GLY	N-CA-C	6.83	118.44	111.95
1	A	85	GLY	N-CA-C	-6.82	100.91	112.77
1	C	298	MET	N-CA-C	6.77	121.49	113.23
1	D	135	ASP	N-CA-CB	-6.75	101.93	112.13
1	C	81	ASN	N-CA-C	-6.71	104.67	112.92
1	B	162	VAL	N-CA-C	6.68	117.86	111.91
1	C	152	SER	CA-C-N	6.66	126.60	119.28
1	C	152	SER	C-N-CA	6.66	126.60	119.28
1	A	317	ASP	N-CA-C	6.63	118.30	111.14
1	B	317	ASP	N-CA-C	6.60	118.36	111.03
1	C	254	SER	N-CA-C	-6.57	99.63	109.94
1	A	276	SER	N-CA-C	-6.56	104.53	112.54
1	B	21	PRO	CA-C-N	6.54	126.46	119.85
1	B	21	PRO	C-N-CA	6.54	126.46	119.85
1	A	397	ARG	N-CA-C	-6.52	105.29	113.18
1	A	162	VAL	N-CA-C	6.52	117.71	111.91
1	D	410	GLY	N-CA-C	-6.49	102.41	112.85
1	D	230	SER	CA-C-N	-6.47	112.21	122.95
1	D	230	SER	C-N-CA	-6.47	112.21	122.95
1	A	81	ASN	N-CA-C	-6.46	104.97	112.92
1	B	136	LEU	N-CA-C	6.44	117.99	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	135	ASP	N-CA-C	6.42	120.45	112.24
1	D	21	PRO	CA-C-N	6.35	126.26	119.85
1	D	21	PRO	C-N-CA	6.35	126.26	119.85
1	A	410	GLY	N-CA-C	-6.34	104.07	112.82
1	A	135	ASP	N-CA-CB	-6.28	102.65	112.13
1	A	332	ARG	N-CA-C	-6.23	100.17	109.15
1	D	276	SER	N-CA-C	-6.20	104.98	112.54
1	B	276	SER	N-CA-C	-6.18	105.22	112.89
1	C	332	ARG	N-CA-C	-6.18	100.50	109.59
1	D	430	ASP	N-CA-C	-6.15	105.81	113.38
1	C	107	LEU	N-CA-C	6.11	117.94	111.28
1	A	152	SER	CA-C-N	6.08	125.97	119.28
1	A	152	SER	C-N-CA	6.08	125.97	119.28
1	B	254	SER	N-CA-C	-6.07	100.45	109.86
1	A	190	VAL	CB-CA-C	-6.01	100.31	111.79
1	D	136	LEU	N-CA-C	5.98	117.49	110.97
1	B	318	VAL	CB-CA-C	-5.94	101.52	110.55
1	C	33	THR	CB-CA-C	-5.94	99.52	111.17
1	C	399	HIS	N-CA-C	5.94	119.08	109.40
1	A	21	PRO	CA-C-N	5.91	125.81	119.85
1	A	21	PRO	C-N-CA	5.91	125.81	119.85
1	A	211	ASN	N-CA-C	5.88	120.03	112.86
1	D	413	VAL	N-CA-C	5.86	116.12	107.15
1	C	410	GLY	N-CA-C	-5.77	104.85	112.82
1	C	191	ALA	N-CA-C	-5.71	106.27	113.18
1	A	179	TRP	N-CA-C	-5.71	105.42	112.90
1	C	190	VAL	CB-CA-C	-5.70	100.90	111.79
1	C	318	VAL	CB-CA-C	-5.69	101.89	110.55
1	D	163	GLY	N-CA-C	5.67	117.33	111.95
1	B	426	TYR	CA-C-N	5.67	126.92	119.84
1	B	426	TYR	C-N-CA	5.67	126.92	119.84
1	B	429	ASP	CA-C-N	5.64	129.55	121.71
1	B	429	ASP	C-N-CA	5.64	129.55	121.71
1	A	254	SER	N-CA-C	-5.63	101.13	109.86
1	D	426	TYR	CA-C-N	5.60	126.84	119.84
1	D	426	TYR	C-N-CA	5.60	126.84	119.84
1	A	413	VAL	N-CA-C	5.59	115.71	107.15
1	A	33	THR	CB-CA-C	-5.59	100.22	111.17
1	C	222	ARG	N-CA-C	5.58	118.56	111.69
1	A	135	ASP	N-CA-C	5.57	119.25	111.74
1	A	162	VAL	CB-CA-C	5.55	118.58	112.19
1	D	317	ASP	N-CA-C	5.54	117.18	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	GLY	N-CA-C	-5.53	105.18	112.82
1	D	179	TRP	N-CA-C	-5.52	104.90	111.69
1	D	298	MET	N-CA-C	5.51	119.95	113.23
1	A	298	MET	N-CA-C	5.51	119.95	113.23
1	C	85	GLY	N-CA-C	-5.50	102.14	112.64
1	B	190	VAL	N-CA-C	5.49	119.80	111.89
1	B	33	THR	CB-CA-C	-5.49	100.41	111.17
1	B	399	HIS	N-CA-C	5.47	118.31	109.40
1	D	204	ILE	CB-CA-C	-5.47	104.97	111.97
1	C	160	LEU	N-CA-C	-5.44	98.89	108.20
1	D	243	ALA	CB-CA-C	-5.43	109.84	117.23
1	C	37	LEU	N-CA-C	5.43	118.12	111.82
1	D	254	SER	N-CA-C	-5.42	101.46	109.86
1	C	276	SER	N-CA-C	-5.40	105.96	112.54
1	C	243	ALA	CB-CA-C	-5.39	109.90	117.23
1	C	69	ILE	N-CA-C	5.39	115.65	108.11
1	C	179	TRP	N-CA-C	-5.38	105.45	112.23
1	B	413	VAL	N-CA-C	5.37	116.10	107.73
1	D	318	VAL	CB-CA-C	-5.35	101.25	110.30
1	B	48	THR	N-CA-C	-5.34	100.69	109.40
1	D	241	LYS	N-CA-C	-5.34	100.99	109.59
1	D	431	SER	N-CA-C	5.32	117.88	109.96
1	A	318	VAL	CB-CA-C	-5.30	101.34	110.30
1	B	177	VAL	N-CA-C	-5.29	105.38	110.72
1	A	222	ARG	N-CA-C	5.27	118.87	112.23
1	D	352	SER	N-CA-C	-5.27	107.23	113.97
1	A	352	SER	N-CA-C	-5.26	106.88	113.72
1	A	96	LYS	N-CA-C	-5.26	101.95	110.32
1	B	298	MET	N-CA-C	5.21	119.58	113.23
1	B	138	GLN	N-CA-C	5.18	117.09	110.61
1	B	139	SER	N-CA-C	-5.16	103.11	110.59
1	C	204	ILE	CB-CA-C	-5.16	105.37	111.97
1	A	139	SER	N-CA-C	-5.15	103.12	110.59
1	D	135	ASP	CB-CG-OD1	-5.15	106.56	118.40
1	B	243	ALA	CB-CA-C	-5.14	110.24	117.23
1	D	411	VAL	N-CA-C	5.12	118.24	111.17
1	B	107	LEU	N-CA-C	5.12	117.59	111.71
1	D	280	TRP	N-CA-C	5.11	117.09	108.96
1	A	330	SER	N-CA-C	5.05	116.97	109.69
1	C	195	TRP	N-CA-C	-5.05	100.67	108.90
1	D	197	TRP	N-CA-C	5.04	118.44	109.96
1	A	399	HIS	N-CA-C	5.04	117.62	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	ARG	N-CA-C	5.03	119.09	112.25
1	A	166	SER	N-CA-C	5.02	121.10	114.12
1	D	138	GLN	N-CA-C	5.02	116.89	110.61
1	D	399	HIS	N-CA-C	5.02	117.58	109.40
1	D	40	ARG	N-CA-C	5.02	119.53	111.81
1	A	135	ASP	CB-CG-OD1	-5.01	106.87	118.40
1	A	40	ARG	N-CA-C	5.01	119.06	112.25
1	B	40	ARG	N-CA-C	5.01	119.06	112.25
1	C	352	SER	N-CA-C	-5.00	107.22	113.72
1	D	332	ARG	N-CA-C	-5.00	100.15	110.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	223	TYR	Sidechain
1	B	426	TYR	Sidechain
1	D	167	TYR	Sidechain
1	D	253	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3494	0	3306	100	0
1	B	3494	0	3305	113	0
1	C	3494	0	3305	109	0
1	D	3494	0	3306	112	0
2	A	70	0	65	2	0
2	B	70	0	65	1	0
2	C	70	0	65	1	0
2	D	70	0	65	1	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	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	A	16	0	0	0	0
6	B	13	0	0	4	0
6	C	14	0	0	2	0
6	D	13	0	0	2	0
All	All	14340	0	13482	433	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 16.

All (433) 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:372:MET:HE2	1:B:383:ARG:HD3	1.44	0.98
1:D:398:THR:HG22	1:D:426:TYR:HB2	1.59	0.82
1:D:368:ILE:HG12	1:D:387:PHE:CZ	2.19	0.78
1:C:33:THR:HG23	1:C:195:TRP:O	1.87	0.75
1:B:426:TYR:N	1:B:427:PRO:HD3	2.01	0.75
1:C:63:LYS:HZ3	1:C:64:ASN:HB3	1.53	0.74
1:B:275:ARG:NH2	1:B:315:LYS:O	2.21	0.73
1:D:63:LYS:HZ3	1:D:64:ASN:HB3	1.52	0.73
1:B:368:ILE:HG12	1:B:387:PHE:CZ	2.23	0.73
1:C:28:GLN:NE2	1:C:184:ARG:HE	1.87	0.73
1:A:398:THR:HG22	1:A:426:TYR:HB2	1.70	0.73
1:A:368:ILE:HG12	1:A:387:PHE:CZ	2.25	0.72
1:D:421:PHE:CD2	1:D:428:VAL:HG23	2.25	0.71
1:B:33:THR:HG23	1:B:195:TRP:O	1.90	0.71
1:C:217:LYS:HB3	1:C:218:PRO:HD3	1.74	0.70
1:D:275:ARG:NH2	1:D:315:LYS:O	2.24	0.69
1:B:63:LYS:HZ3	1:B:64:ASN:HB3	1.57	0.69
1:D:258:ARG:HG3	1:D:258:ARG:HH11	1.56	0.69
1:C:374:GLN:NE2	1:C:383:ARG:HH12	1.89	0.69
1:B:258:ARG:HG3	1:B:258:ARG:HH11	1.57	0.69
1:A:33:THR:HG23	1:A:195:TRP:O	1.93	0.69
1:B:359:ILE:N	1:B:359:ILE:HD13	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:GLN:NE2	1:D:178:ARG:HH11	1.91	0.69
1:C:359:ILE:HD13	1:C:359:ILE:N	2.08	0.68
1:C:138:GLN:NE2	1:C:178:ARG:HH11	1.92	0.68
1:A:258:ARG:HH11	1:A:258:ARG:HG3	1.58	0.67
1:C:258:ARG:HG3	1:C:258:ARG:HH11	1.58	0.67
1:B:63:LYS:NZ	1:B:64:ASN:HB3	2.10	0.67
1:D:409:ASP:HB3	1:D:413:VAL:HB	1.75	0.67
1:A:275:ARG:NH2	1:A:315:LYS:O	2.26	0.67
1:A:359:ILE:HD13	1:A:359:ILE:N	2.09	0.67
1:B:338:TYR:CZ	1:B:340:ILE:HA	2.30	0.67
1:D:359:ILE:HD13	1:D:359:ILE:N	2.10	0.67
1:A:28:GLN:NE2	1:A:184:ARG:HE	1.92	0.67
1:A:338:TYR:CZ	1:A:340:ILE:HA	2.30	0.67
1:A:409:ASP:HB3	1:A:413:VAL:HB	1.77	0.66
1:A:228:GLU:CD	1:A:228:GLU:H	2.03	0.66
1:B:138:GLN:NE2	1:B:178:ARG:HH11	1.94	0.66
1:C:338:TYR:CZ	1:C:340:ILE:HA	2.30	0.66
1:C:368:ILE:HG12	1:C:387:PHE:CZ	2.31	0.66
1:A:63:LYS:HZ3	1:A:64:ASN:HB3	1.60	0.65
1:B:316:VAL:O	1:B:354:PRO:HB3	1.96	0.65
1:B:217:LYS:HB3	1:B:218:PRO:HD3	1.78	0.65
1:C:275:ARG:NH2	1:C:315:LYS:O	2.27	0.65
1:B:28:GLN:NE2	1:B:184:ARG:HE	1.94	0.64
1:B:409:ASP:HB3	1:B:413:VAL:HB	1.79	0.64
1:A:55:SER:OG	1:A:88:HIS:HD2	1.79	0.64
1:A:217:LYS:HB3	1:A:218:PRO:HD3	1.79	0.64
1:A:10:ASP:HA	1:A:139:SER:HA	1.80	0.63
1:B:285:MET:SD	1:B:303:MET:HE3	2.39	0.63
1:A:138:GLN:NE2	1:A:178:ARG:HH11	1.97	0.63
1:D:129:THR:H	1:D:157:GLN:HE21	1.47	0.63
1:D:33:THR:HG23	1:D:195:TRP:O	1.99	0.63
1:C:374:GLN:HE22	1:C:383:ARG:HH12	1.45	0.62
1:D:63:LYS:NZ	1:D:64:ASN:HB3	2.14	0.62
1:D:338:TYR:CZ	1:D:340:ILE:HA	2.33	0.62
1:B:228:GLU:H	1:B:228:GLU:CD	2.08	0.62
1:D:55:SER:OG	1:D:88:HIS:HD2	1.83	0.62
1:B:55:SER:OG	1:B:88:HIS:HD2	1.82	0.62
1:A:129:THR:H	1:A:157:GLN:HE21	1.47	0.61
1:C:396:ASN:HB3	1:C:398:THR:H	1.66	0.61
1:B:362:ALA:HB2	6:B:443:HOH:O	2.01	0.61
1:C:129:THR:H	1:C:157:GLN:HE21	1.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:LYS:NZ	1:C:64:ASN:HB3	2.15	0.61
1:D:25:ASN:ND2	1:D:51:GLU:H	1.98	0.60
1:C:316:VAL:O	1:C:354:PRO:HB3	2.01	0.60
1:C:34:GLN:NE2	1:C:242:ARG:HE	2.00	0.60
1:B:33:THR:HG21	6:B:448:HOH:O	2.01	0.60
1:C:66:ARG:NH2	1:C:68:ARG:HG2	2.17	0.60
1:A:34:GLN:HE22	1:A:242:ARG:HE	1.48	0.60
1:D:217:LYS:HB3	1:D:218:PRO:HD3	1.84	0.60
1:C:34:GLN:HE22	1:C:242:ARG:HE	1.49	0.60
1:C:66:ARG:CZ	1:C:68:ARG:HG2	2.32	0.59
1:D:138:GLN:HE21	1:D:178:ARG:HH11	1.51	0.59
1:A:421:PHE:CD2	1:A:430:ASP:HB3	2.38	0.59
1:C:29:GLN:O	1:C:31:HIS:HD2	1.85	0.59
1:A:63:LYS:NZ	1:A:64:ASN:HB3	2.17	0.58
1:C:421:PHE:CD1	1:C:426:TYR:HE2	2.21	0.58
1:D:28:GLN:NE2	1:D:184:ARG:HE	2.00	0.58
1:C:228:GLU:CD	1:C:228:GLU:H	2.11	0.58
1:A:61:SER:H	1:A:68:ARG:NH2	2.01	0.58
1:B:66:ARG:NH2	1:B:68:ARG:HG2	2.19	0.58
1:C:351:GLN:OE1	1:C:429:ASP:HA	2.04	0.58
1:A:25:ASN:ND2	1:A:51:GLU:H	2.01	0.58
1:B:74:MET:HE3	1:B:76:THR:HG23	1.86	0.58
1:C:33:THR:HG21	6:C:449:HOH:O	2.04	0.58
1:B:29:GLN:O	1:B:31:HIS:HD2	1.87	0.58
1:A:34:GLN:NE2	1:A:242:ARG:HE	2.02	0.57
1:B:33:THR:HG22	1:B:34:GLN:H	1.70	0.57
1:D:129:THR:HG23	1:D:157:GLN:HE21	1.70	0.57
1:B:149:TYR:OH	1:B:156:GLY:HA3	2.05	0.57
1:D:228:GLU:CD	1:D:228:GLU:H	2.12	0.57
1:B:61:SER:H	1:B:68:ARG:NH2	2.03	0.56
1:C:285:MET:SD	1:C:303:MET:HE3	2.45	0.56
1:A:66:ARG:NH2	1:A:68:ARG:HG2	2.21	0.56
1:A:174:HIS:O	1:A:175:ASP:C	2.48	0.56
1:C:174:HIS:O	1:C:175:ASP:C	2.48	0.56
1:C:291:ASN:HD21	1:C:293:TYR:HB2	1.71	0.56
1:D:29:GLN:O	1:D:31:HIS:HD2	1.87	0.56
1:D:351:GLN:OE1	1:D:429:ASP:HA	2.05	0.56
1:B:174:HIS:O	1:B:175:ASP:C	2.48	0.56
1:C:138:GLN:HE21	1:C:178:ARG:HH11	1.51	0.56
1:B:25:ASN:ND2	1:B:51:GLU:H	2.02	0.56
1:D:374:GLN:NE2	1:D:374:GLN:HA	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:MET:SD	1:A:303:MET:HE3	2.46	0.56
1:A:167:TYR:HD2	1:A:170:ARG:HD2	1.71	0.56
1:A:382:PHE:CD1	1:A:382:PHE:C	2.84	0.56
1:B:72:GLY:HA3	1:B:90:THR:OG1	2.06	0.56
1:B:138:GLN:HE21	1:B:178:ARG:HH11	1.54	0.56
1:C:424:HIS:HD2	1:C:425:TRP:CD1	2.23	0.56
1:B:351:GLN:OE1	1:B:429:ASP:HA	2.06	0.55
1:B:66:ARG:CZ	1:B:68:ARG:HG2	2.37	0.55
1:A:74:MET:HE3	1:A:76:THR:HG23	1.88	0.55
1:A:301:GLU:O	1:A:305:THR:HG23	2.06	0.55
1:C:300:GLY:HA2	6:C:447:HOH:O	2.05	0.55
1:B:236:PHE:O	1:B:251:SER:HB2	2.07	0.55
1:C:374:GLN:HE22	1:C:383:ARG:NH1	2.04	0.55
1:C:25:ASN:ND2	1:C:51:GLU:H	2.04	0.55
1:C:409:ASP:HB3	1:C:413:VAL:HB	1.88	0.55
1:A:33:THR:HG22	1:A:34:GLN:H	1.72	0.55
1:B:103:TYR:CZ	1:B:114:PHE:HB2	2.42	0.55
1:C:373:ILE:O	1:C:383:ARG:NH2	2.37	0.55
1:D:382:PHE:CD1	1:D:382:PHE:C	2.83	0.55
1:C:421:PHE:CD2	1:C:430:ASP:HB3	2.41	0.55
1:D:174:HIS:O	1:D:175:ASP:C	2.50	0.55
1:A:25:ASN:HD22	1:A:50:ASP:H	1.54	0.54
1:B:10:ASP:HA	1:B:139:SER:HA	1.89	0.54
1:D:72:GLY:HA3	1:D:90:THR:OG1	2.07	0.54
1:A:60:TRP:HB3	1:A:67:LYS:HA	1.89	0.54
1:A:370:SER:O	1:A:372:MET:HG3	2.07	0.54
1:B:171:TYR:CE2	1:B:178:ARG:HG3	2.42	0.54
1:D:396:ASN:HB3	1:D:398:THR:H	1.72	0.54
1:B:25:ASN:HD22	1:B:50:ASP:H	1.53	0.54
1:A:29:GLN:O	1:A:31:HIS:HD2	1.90	0.54
1:A:66:ARG:CZ	1:A:68:ARG:HG2	2.38	0.54
1:B:34:GLN:NE2	1:B:242:ARG:HE	2.05	0.54
1:C:421:PHE:CD1	1:C:426:TYR:CE2	2.97	0.54
1:B:338:TYR:O	1:B:339:LYS:HD3	2.09	0.53
1:C:61:SER:H	1:C:68:ARG:NH2	2.06	0.53
1:A:351:GLN:OE1	1:A:429:ASP:HA	2.07	0.53
1:C:10:ASP:HA	1:C:139:SER:HA	1.90	0.53
1:C:24:TYR:OH	1:C:51:GLU:HG2	2.08	0.53
1:C:424:HIS:HD2	1:C:425:TRP:NE1	2.07	0.53
1:D:66:ARG:CZ	1:D:68:ARG:HG2	2.38	0.53
1:D:364:ASN:HD21	1:D:367:VAL:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:MET:HE3	1:C:76:THR:HG23	1.91	0.53
1:C:382:PHE:CD1	1:C:382:PHE:C	2.87	0.53
1:D:364:ASN:HD22	1:D:365:TYR:H	1.57	0.53
1:A:396:ASN:HB3	1:A:398:THR:H	1.73	0.53
1:C:398:THR:HG22	1:C:426:TYR:HB2	1.90	0.53
1:D:93:ARG:HG2	1:D:93:ARG:HH11	1.74	0.53
1:B:426:TYR:N	1:B:427:PRO:CD	2.71	0.52
1:D:132:LEU:HD22	1:D:320:PHE:CD1	2.44	0.52
1:C:374:GLN:NE2	1:C:374:GLN:HA	2.25	0.52
1:B:359:ILE:HD13	1:B:359:ILE:H	1.72	0.52
1:C:301:GLU:O	1:C:305:THR:HG23	2.08	0.52
1:D:25:ASN:HD22	1:D:50:ASP:H	1.56	0.52
1:D:251:SER:OG	1:D:254:SER:HB2	2.10	0.52
1:B:396:ASN:HB3	1:B:398:THR:H	1.75	0.52
1:A:285:MET:O	1:A:321:ALA:HA	2.10	0.52
1:D:33:THR:HG22	1:D:34:GLN:H	1.74	0.52
1:A:129:THR:HG23	1:A:157:GLN:HE21	1.75	0.52
1:B:373:ILE:O	1:B:383:ARG:NH2	2.39	0.52
1:A:373:ILE:O	1:A:383:ARG:NH2	2.40	0.52
1:C:281:LEU:HD23	1:C:316:VAL:HA	1.91	0.52
1:B:129:THR:H	1:B:157:GLN:HE21	1.58	0.51
1:B:132:LEU:HD22	1:B:320:PHE:CD1	2.46	0.51
1:B:285:MET:O	1:B:321:ALA:HA	2.10	0.51
1:C:351:GLN:HE22	1:C:431:SER:HB2	1.75	0.51
1:D:171:TYR:CE1	1:D:178:ARG:HG3	2.45	0.51
1:D:190:VAL:HG13	1:D:195:TRP:CD1	2.45	0.51
1:A:132:LEU:HD22	1:A:320:PHE:CD1	2.45	0.51
1:D:34:GLN:NE2	1:D:242:ARG:HE	2.09	0.51
1:D:124:LEU:O	1:D:279:PRO:HG3	2.11	0.51
1:A:316:VAL:O	1:A:354:PRO:HB3	2.11	0.51
1:B:316:VAL:HG22	1:B:354:PRO:HB3	1.93	0.51
1:A:14:ASP:O	1:A:15:SER:C	2.53	0.50
1:B:301:GLU:O	1:B:305:THR:HG23	2.11	0.50
1:D:373:ILE:O	1:D:383:ARG:NH2	2.43	0.50
1:C:33:THR:HG22	1:C:34:GLN:H	1.76	0.50
1:B:124:LEU:HD11	1:B:425:TRP:CZ2	2.46	0.50
1:D:421:PHE:CD2	1:D:430:ASP:HB3	2.47	0.50
1:A:251:SER:OG	1:A:254:SER:HB2	2.12	0.50
1:B:162:VAL:HG11	1:B:321:ALA:C	2.36	0.50
1:A:297:PHE:CE2	1:A:298:MET:HG3	2.46	0.50
1:D:281:LEU:HD23	1:D:316:VAL:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PHE:O	1:A:251:SER:HB2	2.12	0.50
1:B:129:THR:HG23	1:B:157:GLN:HE21	1.75	0.50
1:B:382:PHE:CD1	1:B:382:PHE:C	2.88	0.50
1:C:285:MET:O	1:C:321:ALA:HA	2.11	0.50
1:D:66:ARG:NH2	1:D:68:ARG:HG2	2.26	0.50
1:D:167:TYR:HD2	1:D:170:ARG:HD2	1.77	0.50
1:A:374:GLN:HA	1:A:374:GLN:NE2	2.27	0.50
1:C:396:ASN:HB2	1:C:399:HIS:H	1.77	0.50
1:C:421:PHE:HB3	1:C:426:TYR:CD2	2.46	0.49
1:D:103:TYR:CZ	1:D:114:PHE:HB2	2.47	0.49
1:D:34:GLN:HE22	1:D:242:ARG:HE	1.60	0.49
1:B:28:GLN:HE21	1:B:29:GLN:HE21	1.60	0.49
1:B:408:GLN:NE2	6:B:444:HOH:O	2.45	0.49
1:C:25:ASN:HD22	1:C:50:ASP:H	1.59	0.49
1:A:426:TYR:N	1:A:427:PRO:CD	2.76	0.49
1:C:171:TYR:CE1	1:C:178:ARG:HG3	2.48	0.49
1:B:93:ARG:HG2	1:B:93:ARG:HH11	1.78	0.49
1:B:291:ASN:HD21	1:B:293:TYR:HB2	1.78	0.49
1:B:295:HIS:O	1:B:296:HIS:HB2	2.12	0.49
1:C:60:TRP:HB3	1:C:67:LYS:HA	1.94	0.49
1:B:124:LEU:O	1:B:279:PRO:HG3	2.13	0.49
1:D:14:ASP:O	1:D:15:SER:C	2.56	0.49
1:D:61:SER:H	1:D:68:ARG:NH2	2.10	0.49
1:C:359:ILE:HD13	1:C:359:ILE:H	1.78	0.48
1:C:124:LEU:O	1:C:279:PRO:HG3	2.13	0.48
1:D:285:MET:SD	1:D:303:MET:HE3	2.52	0.48
1:D:358:THR:HG21	6:D:450:HOH:O	2.13	0.48
1:D:60:TRP:HB3	1:D:67:LYS:HA	1.95	0.48
1:D:236:PHE:O	1:D:251:SER:HB2	2.13	0.48
1:A:129:THR:H	1:A:157:GLN:NE2	2.11	0.48
1:B:165:LEU:N	1:B:165:LEU:HD12	2.28	0.48
1:A:211:ASN:OD1	2:A:436(A):NAG:N2	2.46	0.48
1:C:167:TYR:HD2	1:C:170:ARG:HD2	1.78	0.48
1:B:364:ASN:HD22	1:B:365:TYR:H	1.61	0.48
1:D:28:GLN:HE21	1:D:29:GLN:HE21	1.62	0.48
1:D:151:LEU:O	1:D:152:SER:C	2.56	0.48
1:B:34:GLN:HE22	1:B:242:ARG:HE	1.61	0.47
1:A:151:LEU:O	1:A:152:SER:C	2.56	0.47
1:A:258:ARG:HG3	1:A:258:ARG:NH1	2.27	0.47
1:B:167:TYR:HD2	1:B:170:ARG:HD2	1.78	0.47
1:B:281:LEU:HD23	1:B:316:VAL:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:SER:OG	1:C:254:SER:HB2	2.13	0.47
1:D:74:MET:HE3	1:D:76:THR:HG23	1.96	0.47
1:D:93:ARG:HG2	1:D:93:ARG:NH1	2.29	0.47
1:B:58:ARG:O	1:B:103:TYR:HA	2.14	0.47
1:D:325:HIS:HA	1:D:360:GLY:O	2.14	0.47
1:B:27:PRO:O	1:B:112:ARG:NH1	2.46	0.47
1:A:391:MET:HE3	1:A:391:MET:HB3	1.83	0.47
1:A:359:ILE:HD13	1:A:359:ILE:H	1.80	0.47
1:B:285:MET:SD	1:B:303:MET:CE	3.03	0.47
1:A:398:THR:CG2	1:A:426:TYR:HB2	2.39	0.47
1:B:151:LEU:O	1:B:152:SER:C	2.59	0.46
1:A:294:ASN:HD22	1:A:371:ASN:C	2.23	0.46
1:D:359:ILE:HD13	1:D:359:ILE:H	1.77	0.46
1:A:25:ASN:HD21	1:A:51:GLU:H	1.63	0.46
1:B:222:ARG:HH11	1:B:222:ARG:HG2	1.81	0.46
1:B:258:ARG:HG3	1:B:258:ARG:NH1	2.29	0.46
1:D:25:ASN:HD21	1:D:51:GLU:H	1.64	0.46
1:D:301:GLU:O	1:D:305:THR:HG23	2.15	0.46
1:C:28:GLN:HE22	1:C:184:ARG:HE	1.61	0.46
1:D:152:SER:HB3	1:D:154:LYS:O	2.16	0.46
1:D:338:TYR:O	1:D:339:LYS:HD3	2.15	0.46
1:B:291:ASN:ND2	1:B:293:TYR:H	2.14	0.46
1:A:152:SER:HB3	1:A:154:LYS:O	2.16	0.46
1:C:242:ARG:O	1:C:243:ALA:HB3	2.16	0.46
1:D:294:ASN:HD22	1:D:371:ASN:C	2.23	0.46
1:A:165:LEU:HD12	1:A:165:LEU:N	2.31	0.45
1:B:171:TYR:CD2	1:B:178:ARG:HG3	2.51	0.45
1:B:185:PHE:CD1	1:B:185:PHE:C	2.93	0.45
1:D:258:ARG:HG3	1:D:258:ARG:NH1	2.28	0.45
1:D:258:ARG:HH11	1:D:258:ARG:CG	2.28	0.45
1:D:297:PHE:CD1	1:D:373:ILE:HD11	2.51	0.45
1:B:122:THR:HA	1:B:243:ALA:O	2.16	0.45
1:B:329:ARG:NH1	1:B:416:ASP:OD2	2.50	0.45
1:D:171:TYR:CD1	1:D:178:ARG:HG3	2.51	0.45
1:D:185:PHE:CD1	1:D:185:PHE:C	2.93	0.45
1:A:78:ARG:NH2	1:D:84:SER:O	2.50	0.45
1:A:103:TYR:CZ	1:A:114:PHE:HB2	2.51	0.45
1:A:154:LYS:H	1:A:154:LYS:HG2	1.54	0.45
1:C:14:ASP:O	1:C:15:SER:C	2.58	0.45
1:C:166:SER:O	1:C:167:TYR:HB2	2.16	0.45
1:C:171:TYR:CD1	1:C:178:ARG:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ASN:ND2	1:C:293:TYR:H	2.14	0.45
1:D:58:ARG:O	1:D:103:TYR:HA	2.17	0.45
1:B:421:PHE:HB3	1:B:426:TYR:CD2	2.51	0.45
1:C:28:GLN:HG3	1:C:29:GLN:HG3	1.98	0.45
1:C:316:VAL:HG22	1:C:354:PRO:HB3	1.99	0.45
1:D:362:ALA:HB2	6:D:444:HOH:O	2.17	0.45
1:A:396:ASN:HB2	1:A:399:HIS:H	1.81	0.45
1:B:421:PHE:HB3	1:B:426:TYR:O	2.17	0.45
1:A:316:VAL:HG22	1:A:354:PRO:HB3	1.99	0.44
1:C:129:THR:H	1:C:157:GLN:NE2	2.14	0.44
1:D:129:THR:H	1:D:157:GLN:NE2	2.12	0.44
1:D:374:GLN:HA	1:D:374:GLN:HE21	1.82	0.44
1:D:152:SER:HA	1:D:153:PRO:HD2	1.68	0.44
1:D:211:ASN:OD1	2:D:436(A):NAG:N2	2.51	0.44
1:D:316:VAL:O	1:D:354:PRO:HB3	2.17	0.44
1:A:406:ARG:HB3	1:A:408:GLN:OE1	2.17	0.44
1:B:60:TRP:HB3	1:B:67:LYS:HA	1.98	0.44
1:B:152:SER:HA	1:B:153:PRO:HD2	1.66	0.44
1:C:132:LEU:HD22	1:C:320:PHE:CD1	2.53	0.44
1:A:138:GLN:HE21	1:A:178:ARG:HH11	1.64	0.44
1:A:329:ARG:HG3	1:A:357:ILE:HG12	1.99	0.44
1:B:211:ASN:OD1	2:B:436(A):NAG:N2	2.50	0.44
1:D:48:THR:OG1	1:D:88:HIS:HE1	2.01	0.44
1:A:417:SER:C	1:A:418:VAL:HG23	2.42	0.44
1:B:9:ARG:O	1:B:9:ARG:HG3	2.18	0.44
1:B:154:LYS:H	1:B:154:LYS:HG2	1.53	0.44
1:D:101:TYR:O	1:D:115:SER:HA	2.17	0.44
1:D:132:LEU:CD2	1:D:320:PHE:CD1	3.01	0.44
1:D:162:VAL:HG11	1:D:321:ALA:C	2.43	0.44
1:B:59:TYR:HA	1:B:102:TYR:O	2.18	0.44
1:C:346:THR:HA	1:C:347:PRO:HD3	1.84	0.44
1:A:82:TYR:CG	1:A:176:ASN:HB2	2.53	0.44
1:C:417:SER:C	1:C:418:VAL:HG23	2.43	0.44
1:D:45:SER:HA	1:D:88:HIS:O	2.18	0.44
1:D:190:VAL:HG13	1:D:195:TRP:CG	2.52	0.44
1:D:364:ASN:ND2	1:D:367:VAL:H	2.15	0.44
1:A:103:TYR:CE2	1:A:114:PHE:HB2	2.52	0.44
1:B:26:ALA:HA	1:B:27:PRO:HD3	1.89	0.44
1:B:325:HIS:HA	1:B:360:GLY:O	2.18	0.44
1:B:398:THR:HG22	1:B:426:TYR:HB2	2.00	0.44
1:C:28:GLN:HE21	1:C:29:GLN:HE21	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:HIS:O	1:A:296:HIS:HB2	2.18	0.43
1:A:364:ASN:HD21	1:A:367:VAL:H	1.66	0.43
1:B:101:TYR:O	1:B:115:SER:HA	2.18	0.43
1:C:423:ARG:HA	1:C:423:ARG:NE	2.33	0.43
1:C:55:SER:OG	1:C:88:HIS:HD2	2.01	0.43
1:D:149:TYR:OH	1:D:156:GLY:HA3	2.19	0.43
1:B:25:ASN:ND2	1:B:50:ASP:H	2.16	0.43
1:C:9:ARG:HH11	1:C:9:ARG:HG2	1.83	0.43
1:D:108:ARG:HB3	1:D:108:ARG:NH1	2.33	0.43
1:B:103:TYR:CE2	1:B:114:PHE:HB2	2.52	0.43
1:C:329:ARG:NH1	1:C:416:ASP:OD2	2.50	0.43
1:C:391:MET:HE3	1:C:391:MET:HB3	1.85	0.43
1:A:93:ARG:HH11	1:A:93:ARG:HG2	1.82	0.43
1:A:120:PRO:HB2	1:A:126:VAL:HG11	2.01	0.43
1:A:152:SER:HA	1:A:153:PRO:HD2	1.69	0.43
1:A:339:LYS:C	1:A:340:ILE:HG12	2.42	0.43
1:D:297:PHE:CE2	1:D:298:MET:HG3	2.53	0.43
1:D:396:ASN:HB2	1:D:399:HIS:H	1.83	0.43
1:A:79:PHE:O	1:A:212:GLU:OE2	2.37	0.43
1:B:45:SER:HA	1:B:88:HIS:O	2.18	0.43
1:B:166:SER:O	1:B:167:TYR:HB2	2.19	0.43
1:C:251:SER:CB	1:C:254:SER:HB2	2.48	0.43
1:D:28:GLN:HG3	1:D:29:GLN:HG3	2.01	0.43
1:D:124:LEU:HD12	1:D:279:PRO:HD3	2.00	0.43
1:A:108:ARG:HB3	1:A:108:ARG:NH1	2.34	0.43
1:C:258:ARG:HG3	1:C:258:ARG:NH1	2.30	0.43
1:D:391:MET:HE3	1:D:391:MET:HB3	1.86	0.43
1:D:424:HIS:HD2	1:D:425:TRP:CD1	2.37	0.43
1:A:211:ASN:OD1	2:A:436(A):NAG:C2	2.67	0.43
1:B:14:ASP:O	1:B:15:SER:C	2.62	0.43
1:D:285:MET:O	1:D:321:ALA:HA	2.19	0.43
1:B:329:ARG:HG3	1:B:357:ILE:HG12	2.01	0.42
1:C:101:TYR:O	1:C:115:SER:HA	2.19	0.42
1:C:162:VAL:HG11	1:C:321:ALA:C	2.44	0.42
1:D:368:ILE:HG12	1:D:387:PHE:CE1	2.52	0.42
1:C:151:LEU:O	1:C:152:SER:C	2.60	0.42
1:C:421:PHE:HB3	1:C:426:TYR:HD2	1.85	0.42
1:A:364:ASN:ND2	1:A:367:VAL:H	2.17	0.42
1:B:229:ALA:C	1:B:230:SER:O	2.60	0.42
1:D:167:TYR:CD2	1:D:170:ARG:HD2	2.54	0.42
1:C:364:ASN:HD21	1:C:367:VAL:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:PHE:CD2	1:C:428:VAL:HG12	2.54	0.42
1:D:125:ASP:OD1	1:D:397:ARG:HB3	2.18	0.42
1:C:301:GLU:OE1	1:C:304:ARG:NH1	2.50	0.42
1:C:339:LYS:C	1:C:340:ILE:HG12	2.43	0.42
1:D:346:THR:HA	1:D:347:PRO:HD3	1.85	0.42
1:A:301:GLU:CD	1:A:304:ARG:NH1	2.78	0.42
1:A:329:ARG:NH1	1:A:416:ASP:OD2	2.52	0.42
1:B:104:GLU:HA	1:B:112:ARG:O	2.20	0.42
1:A:281:LEU:HD23	1:A:316:VAL:HA	2.01	0.42
1:D:10:ASP:HA	1:D:139:SER:HA	2.00	0.42
1:A:421:PHE:HB3	1:A:426:TYR:O	2.20	0.42
1:B:162:VAL:O	1:B:162:VAL:HG13	2.20	0.42
1:A:25:ASN:ND2	1:A:50:ASP:H	2.17	0.42
1:B:207:ALA:HA	1:B:209:GLU:OE2	2.20	0.42
1:C:338:TYR:O	1:C:339:LYS:HD3	2.19	0.42
1:A:167:TYR:CD2	1:A:170:ARG:HD2	2.52	0.42
1:B:93:ARG:HG2	1:B:93:ARG:NH1	2.33	0.42
1:B:251:SER:HB3	1:B:254:SER:HB2	2.02	0.42
1:B:368:ILE:HG12	1:B:387:PHE:CE1	2.54	0.42
1:C:251:SER:HB3	1:C:254:SER:HB2	2.01	0.42
1:C:421:PHE:CG	1:C:426:TYR:CE2	3.08	0.42
1:D:165:LEU:N	1:D:165:LEU:HD12	2.35	0.42
1:D:371:ASN:HD22	1:D:371:ASN:HA	1.67	0.42
1:A:228:GLU:CD	1:A:228:GLU:N	2.76	0.41
1:B:398:THR:OG1	1:B:399:HIS:HD2	2.03	0.41
1:C:211:ASN:OD1	2:C:436(A):NAG:N2	2.53	0.41
1:B:190:VAL:HG13	1:B:195:TRP:CD1	2.54	0.41
1:B:249:VAL:HG22	1:B:284:LEU:HD12	2.03	0.41
1:C:93:ARG:HG2	1:C:93:ARG:HH11	1.85	0.41
1:C:315:LYS:HB3	1:C:423:ARG:HB3	2.03	0.41
1:A:101:TYR:O	1:A:115:SER:HA	2.20	0.41
1:A:251:SER:CB	1:A:254:SER:HB2	2.49	0.41
1:B:125:ASP:OD1	1:B:397:ARG:HB3	2.21	0.41
1:B:423:ARG:NE	1:B:423:ARG:HA	2.34	0.41
1:D:301:GLU:OE2	1:D:304:ARG:NH1	2.52	0.41
1:B:364:ASN:HD21	1:B:367:VAL:H	1.69	0.41
1:C:27:PRO:O	1:C:112:ARG:NH1	2.48	0.41
1:C:103:TYR:CE2	1:C:114:PHE:HB2	2.55	0.41
1:C:363:GLY:O	1:C:364:ASN:C	2.64	0.41
1:A:134:GLY:O	1:A:135:ASP:HB2	2.17	0.41
1:A:229:ALA:C	1:A:230:SER:O	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLU:OE2	1:A:304:ARG:NH1	2.54	0.41
1:B:129:THR:H	1:B:157:GLN:NE2	2.19	0.41
1:C:426:TYR:O	1:C:428:VAL:N	2.52	0.41
1:C:301:GLU:CD	1:C:304:ARG:NH1	2.79	0.41
1:A:45:SER:HA	1:A:88:HIS:O	2.20	0.41
1:B:152:SER:HB3	1:B:154:LYS:O	2.20	0.41
1:D:263:TYR:CD1	1:D:263:TYR:C	2.99	0.41
1:B:364:ASN:ND2	1:B:367:VAL:H	2.19	0.41
1:B:399:HIS:CE1	1:B:421:PHE:HE1	2.38	0.41
1:B:422:ASN:O	1:B:426:TYR:N	2.54	0.41
1:C:185:PHE:CD1	1:C:185:PHE:C	2.98	0.41
1:D:293:TYR:CE2	1:D:372:MET:HE2	2.56	0.41
1:D:316:VAL:HG22	1:D:354:PRO:HB3	2.03	0.41
1:A:93:ARG:HG2	1:A:93:ARG:NH1	2.35	0.41
1:A:124:LEU:O	1:A:279:PRO:HG3	2.20	0.41
1:B:329:ARG:NE	1:B:418:VAL:HG21	2.35	0.41
1:B:358:THR:HG21	6:B:450:HOH:O	2.20	0.41
1:C:103:TYR:CZ	1:C:114:PHE:HB2	2.55	0.41
1:C:217:LYS:O	1:C:218:PRO:C	2.63	0.41
1:C:297:PHE:CE2	1:C:298:MET:HE2	2.55	0.41
1:D:59:TYR:HA	1:D:102:TYR:O	2.21	0.41
1:A:171:TYR:CE2	1:A:178:ARG:HG3	2.55	0.41
1:C:72:GLY:HA3	1:C:90:THR:OG1	2.21	0.41
1:C:285:MET:SD	1:C:303:MET:CE	3.09	0.41
1:D:132:LEU:HD21	1:D:320:PHE:CG	2.56	0.41
1:D:228:GLU:O	1:D:230:SER:O	2.39	0.41
1:D:426:TYR:N	1:D:427:PRO:HD3	2.35	0.41
1:A:171:TYR:CD2	1:A:178:ARG:HG3	2.56	0.40
1:A:249:VAL:HG22	1:A:284:LEU:HD12	2.04	0.40
1:C:364:ASN:ND2	1:C:367:VAL:H	2.19	0.40
1:D:251:SER:CB	1:D:254:SER:HB2	2.51	0.40
1:D:417:SER:C	1:D:418:VAL:HG23	2.46	0.40
1:D:423:ARG:HA	1:D:423:ARG:NE	2.36	0.40
1:B:297:PHE:CE2	1:B:298:MET:HG3	2.57	0.40
1:A:291:ASN:HD21	1:A:293:TYR:HB2	1.86	0.40
1:C:12:PRO:HG2	1:C:15:SER:OG	2.21	0.40
1:D:79:PHE:CZ	1:D:212:GLU:HG3	2.57	0.40
1:D:166:SER:O	1:D:167:TYR:HB2	2.21	0.40
1:A:251:SER:HB3	1:A:254:SER:HB2	2.04	0.40
1:C:74:MET:HG2	1:C:75:SER:N	2.37	0.40
1:C:152:SER:HA	1:C:153:PRO:HD2	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:PHE:O	1:C:251:SER:HB2	2.20	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	422/432 (98%)	386 (92%)	34 (8%)	2 (0%)	24	48
1	B	422/432 (98%)	383 (91%)	34 (8%)	5 (1%)	10	27
1	C	422/432 (98%)	385 (91%)	34 (8%)	3 (1%)	18	41
1	D	422/432 (98%)	384 (91%)	36 (8%)	2 (0%)	24	48
All	All	1688/1728 (98%)	1538 (91%)	138 (8%)	12 (1%)	18	41

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ASP
1	B	175	ASP
1	C	175	ASP
1	D	175	ASP
1	C	431	SER
1	A	65	GLY
1	B	431	SER
1	C	65	GLY
1	B	65	GLY
1	B	176	ASN
1	D	65	GLY
1	B	427	PRO

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	373/381 (98%)	334 (90%)	39 (10%)	6	17
1	B	373/381 (98%)	334 (90%)	39 (10%)	6	17
1	C	373/381 (98%)	333 (89%)	40 (11%)	6	16
1	D	373/381 (98%)	337 (90%)	36 (10%)	8	20
All	All	1492/1524 (98%)	1338 (90%)	154 (10%)	7	18

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	33	THR
1	A	38	VAL
1	A	49	MET
1	A	52	PRO
1	A	64	ASN
1	A	68	ARG
1	A	69	ILE
1	A	75	SER
1	A	105	VAL
1	A	129	THR
1	A	132	LEU
1	A	142	SER
1	A	147	SER
1	A	152	SER
1	A	154	LYS
1	A	155	LYS
1	A	162	VAL
1	A	176	ASN
1	A	190	VAL
1	A	209	GLU
1	A	228	GLU
1	A	230	SER
1	A	254	SER

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Mol	Chain	Res	Type
1	A	276	SER
1	A	287	SER
1	A	291	ASN
1	A	306	LYS
1	A	316	VAL
1	A	318	VAL
1	A	334	SER
1	A	349	LYS
1	A	358	THR
1	A	359	ILE
1	A	375	PRO
1	A	378	GLU
1	A	383	ARG
1	A	403	SER
1	A	408	GLN
1	B	20	VAL
1	B	33	THR
1	B	38	VAL
1	B	49	MET
1	B	52	PRO
1	B	64	ASN
1	B	68	ARG
1	B	69	ILE
1	B	74	MET
1	B	75	SER
1	B	105	VAL
1	B	119	PRO
1	B	129	THR
1	B	132	LEU
1	B	147	SER
1	B	152	SER
1	B	154	LYS
1	B	155	LYS
1	B	162	VAL
1	B	190	VAL
1	B	209	GLU
1	B	228	GLU
1	B	230	SER
1	B	254	SER
1	B	276	SER
1	B	287	SER
1	B	291	ASN

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Mol	Chain	Res	Type
1	B	306	LYS
1	B	316	VAL
1	B	318	VAL
1	B	349	LYS
1	B	358	THR
1	B	359	ILE
1	B	371	ASN
1	B	374	GLN
1	B	378	GLU
1	B	383	ARG
1	B	403	SER
1	B	408	GLN
1	C	20	VAL
1	C	33	THR
1	C	38	VAL
1	C	52	PRO
1	C	64	ASN
1	C	68	ARG
1	C	75	SER
1	C	105	VAL
1	C	119	PRO
1	C	129	THR
1	C	132	LEU
1	C	142	SER
1	C	147	SER
1	C	152	SER
1	C	154	LYS
1	C	155	LYS
1	C	162	VAL
1	C	190	VAL
1	C	208	PRO
1	C	209	GLU
1	C	228	GLU
1	C	230	SER
1	C	254	SER
1	C	258	ARG
1	C	276	SER
1	C	287	SER
1	C	291	ASN
1	C	306	LYS
1	C	316	VAL
1	C	318	VAL

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Mol	Chain	Res	Type
1	C	349	LYS
1	C	358	THR
1	C	359	ILE
1	C	372	MET
1	C	374	GLN
1	C	378	GLU
1	C	383	ARG
1	C	403	SER
1	C	408	GLN
1	C	428	VAL
1	D	17	VAL
1	D	20	VAL
1	D	33	THR
1	D	38	VAL
1	D	52	PRO
1	D	64	ASN
1	D	68	ARG
1	D	75	SER
1	D	105	VAL
1	D	129	THR
1	D	132	LEU
1	D	147	SER
1	D	152	SER
1	D	154	LYS
1	D	155	LYS
1	D	162	VAL
1	D	190	VAL
1	D	209	GLU
1	D	228	GLU
1	D	230	SER
1	D	254	SER
1	D	276	SER
1	D	287	SER
1	D	291	ASN
1	D	306	LYS
1	D	316	VAL
1	D	318	VAL
1	D	349	LYS
1	D	358	THR
1	D	359	ILE
1	D	371	ASN
1	D	373	ILE

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Mol	Chain	Res	Type
1	D	378	GLU
1	D	383	ARG
1	D	403	SER
1	D	408	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	28	GLN
1	A	31	HIS
1	A	34	GLN
1	A	88	HIS
1	A	138	GLN
1	A	157	GLN
1	A	176	ASN
1	A	291	ASN
1	A	294	ASN
1	A	364	ASN
1	A	371	ASN
1	A	374	GLN
1	A	389	HIS
1	A	399	HIS
1	A	424	HIS
1	B	25	ASN
1	B	28	GLN
1	B	31	HIS
1	B	34	GLN
1	B	88	HIS
1	B	138	GLN
1	B	157	GLN
1	B	176	ASN
1	B	291	ASN
1	B	364	ASN
1	B	389	HIS
1	B	399	HIS
1	B	424	HIS
1	C	25	ASN
1	C	28	GLN
1	C	31	HIS
1	C	34	GLN
1	C	88	HIS

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Mol	Chain	Res	Type
1	C	138	GLN
1	C	157	GLN
1	C	176	ASN
1	C	193	GLN
1	C	291	ASN
1	C	294	ASN
1	C	364	ASN
1	C	374	GLN
1	C	389	HIS
1	C	399	HIS
1	C	424	HIS
1	D	25	ASN
1	D	28	GLN
1	D	31	HIS
1	D	34	GLN
1	D	88	HIS
1	D	138	GLN
1	D	157	GLN
1	D	176	ASN
1	D	291	ASN
1	D	294	ASN
1	D	364	ASN
1	D	371	ASN
1	D	374	GLN
1	D	389	HIS
1	D	399	HIS
1	D	424	HIS

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 32 ligands modelled in this entry, 8 are monoatomic - leaving 24 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	NAG	B	437(A)	1	14,14,15	0.94	1 (7%)	17,19,21	1.20	2 (11%)
2	NAG	B	436(A)	1	14,14,15	1.60	3 (21%)	17,19,21	1.55	3 (17%)
2	NAG	C	435(A)	1	14,14,15	0.68	0	17,19,21	0.63	0
5	PO4	C	440	4,3	4,4,4	2.72	3 (75%)	6,6,6	0.56	0
2	NAG	C	437(A)	1	14,14,15	0.81	0	17,19,21	1.24	3 (17%)
2	NAG	D	437(A)	1	14,14,15	1.42	2 (14%)	17,19,21	1.47	2 (11%)
2	NAG	D	433(A)	1	14,14,15	0.90	0	17,19,21	1.47	3 (17%)
2	NAG	B	434(A)	1	14,14,15	0.99	0	17,19,21	1.67	3 (17%)
2	NAG	D	435(A)	1	14,14,15	0.66	0	17,19,21	0.91	0
2	NAG	A	436(A)	1	14,14,15	1.36	3 (21%)	17,19,21	1.68	5 (29%)
2	NAG	B	433(A)	1	14,14,15	1.12	2 (14%)	17,19,21	1.33	2 (11%)
2	NAG	C	433(A)	1	14,14,15	1.20	2 (14%)	17,19,21	1.33	3 (17%)
5	PO4	A	440	4,3	4,4,4	3.52	3 (75%)	6,6,6	0.90	0
2	NAG	A	434(A)	1	14,14,15	1.06	1 (7%)	17,19,21	1.79	4 (23%)
2	NAG	C	436(A)	1	14,14,15	1.58	4 (28%)	17,19,21	1.60	4 (23%)
2	NAG	B	435(A)	1	14,14,15	0.67	0	17,19,21	0.69	0
5	PO4	D	440	4,3	4,4,4	2.61	3 (75%)	6,6,6	0.68	0
5	PO4	B	440	4,3	4,4,4	2.27	1 (25%)	6,6,6	0.64	0
2	NAG	D	434(A)	1	14,14,15	1.14	1 (7%)	17,19,21	1.75	3 (17%)
2	NAG	A	437(A)	1	14,14,15	1.18	1 (7%)	17,19,21	1.21	2 (11%)
2	NAG	A	435(A)	1	14,14,15	0.74	0	17,19,21	0.73	0
2	NAG	C	434(A)	1	14,14,15	1.09	1 (7%)	17,19,21	1.83	4 (23%)
2	NAG	A	433(A)	1	14,14,15	1.12	1 (7%)	17,19,21	1.49	2 (11%)
2	NAG	D	436(A)	1	14,14,15	1.45	3 (21%)	17,19,21	1.51	3 (17%)

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	NAG	B	437(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	B	436(A)	1	-	4/6/23/26	0/1/1/1
2	NAG	C	435(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	C	437(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	D	437(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	D	433(A)	1	-	3/6/23/26	0/1/1/1
2	NAG	B	434(A)	1	-	4/6/23/26	0/1/1/1
2	NAG	D	435(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	A	436(A)	1	-	4/6/23/26	0/1/1/1
2	NAG	B	433(A)	1	-	3/6/23/26	0/1/1/1
2	NAG	C	433(A)	1	-	3/6/23/26	0/1/1/1
2	NAG	A	434(A)	1	-	4/6/23/26	0/1/1/1
2	NAG	C	436(A)	1	-	4/6/23/26	0/1/1/1
2	NAG	B	435(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	D	434(A)	1	-	4/6/23/26	0/1/1/1
2	NAG	A	437(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	A	435(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	C	434(A)	1	-	4/6/23/26	0/1/1/1
2	NAG	A	433(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	D	436(A)	1	-	4/6/23/26	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	440	PO4	P-O2	-4.79	1.40	1.54
5	A	440	PO4	P-O4	3.96	1.66	1.54
5	C	440	PO4	P-O2	-3.79	1.43	1.54
5	B	440	PO4	P-O2	-3.78	1.43	1.54
2	B	436(A)	NAG	C1-C2	3.70	1.57	1.52
5	D	440	PO4	P-O2	-3.69	1.43	1.54
2	C	436(A)	NAG	C1-C2	3.57	1.57	1.52
2	A	437(A)	NAG	C1-C2	3.40	1.57	1.52
2	D	437(A)	NAG	C1-C2	3.39	1.57	1.52
5	A	440	PO4	P-O3	-3.13	1.45	1.54
5	C	440	PO4	P-O4	2.74	1.62	1.54
2	D	436(A)	NAG	O5-C5	2.73	1.48	1.43
5	D	440	PO4	P-O4	2.69	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	433(A)	NAG	C1-C2	2.62	1.55	1.52
2	D	436(A)	NAG	C1-C2	2.61	1.55	1.52
2	A	436(A)	NAG	O5-C5	2.57	1.48	1.43
2	C	436(A)	NAG	O5-C5	2.56	1.48	1.43
2	B	436(A)	NAG	O5-C5	2.52	1.48	1.43
2	A	436(A)	NAG	C1-C2	2.47	1.55	1.52
5	C	440	PO4	P-O3	-2.46	1.47	1.54
2	C	433(A)	NAG	C3-C2	2.40	1.57	1.52
5	D	440	PO4	P-O3	-2.39	1.47	1.54
2	D	434(A)	NAG	C3-C2	2.37	1.57	1.52
2	B	436(A)	NAG	C4-C5	2.32	1.58	1.53
2	B	437(A)	NAG	C1-C2	2.30	1.55	1.52
2	A	433(A)	NAG	C1-C2	2.29	1.55	1.52
2	A	436(A)	NAG	C4-C5	2.26	1.57	1.53
2	C	436(A)	NAG	C4-C5	2.23	1.57	1.53
2	C	434(A)	NAG	C3-C2	2.21	1.57	1.52
2	B	433(A)	NAG	C3-C2	2.19	1.57	1.52
2	C	433(A)	NAG	C1-C2	2.18	1.55	1.52
2	D	436(A)	NAG	C4-C5	2.07	1.57	1.53
2	D	437(A)	NAG	C8-C7	2.07	1.54	1.50
2	C	436(A)	NAG	O5-C1	2.03	1.47	1.43
2	A	434(A)	NAG	C3-C2	2.00	1.56	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	434(A)	NAG	C4-C3-C2	-5.26	103.31	111.02
2	C	434(A)	NAG	C4-C3-C2	-5.26	103.31	111.02
2	D	434(A)	NAG	C4-C3-C2	-5.06	103.61	111.02
2	B	434(A)	NAG	C4-C3-C2	-4.96	103.75	111.02
2	A	436(A)	NAG	C4-C3-C2	-3.71	105.58	111.02
2	C	436(A)	NAG	C4-C3-C2	-3.48	105.92	111.02
2	D	436(A)	NAG	C1-O5-C5	3.37	116.70	112.19
2	D	437(A)	NAG	C4-C3-C2	-3.33	106.14	111.02
2	A	436(A)	NAG	C1-O5-C5	3.31	116.63	112.19
2	D	433(A)	NAG	C4-C3-C2	-3.20	106.33	111.02
2	C	436(A)	NAG	C1-O5-C5	3.18	116.45	112.19
2	B	436(A)	NAG	C4-C3-C2	-3.14	106.41	111.02
2	B	436(A)	NAG	C1-O5-C5	3.09	116.32	112.19
2	A	433(A)	NAG	C4-C3-C2	-3.07	106.52	111.02
2	D	436(A)	NAG	C4-C3-C2	-3.02	106.59	111.02
2	B	433(A)	NAG	C4-C3-C2	-2.97	106.67	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	436(A)	NAG	C1-C2-N2	2.83	114.89	110.43
2	D	433(A)	NAG	C2-N2-C7	-2.82	119.12	122.90
2	D	437(A)	NAG	C1-O5-C5	2.81	115.95	112.19
2	C	434(A)	NAG	O5-C1-C2	-2.73	107.07	111.29
2	D	434(A)	NAG	O5-C1-C2	-2.72	107.08	111.29
2	A	433(A)	NAG	C2-N2-C7	-2.64	119.37	122.90
2	B	436(A)	NAG	C1-C2-N2	2.62	114.56	110.43
2	C	437(A)	NAG	C1-O5-C5	2.58	115.65	112.19
2	C	433(A)	NAG	C4-C3-C2	-2.56	107.26	111.02
2	B	437(A)	NAG	C1-O5-C5	2.54	115.59	112.19
2	C	434(A)	NAG	C2-N2-C7	-2.52	119.53	122.90
2	B	434(A)	NAG	O5-C1-C2	-2.44	107.51	111.29
2	A	437(A)	NAG	C1-O5-C5	2.44	115.45	112.19
2	A	437(A)	NAG	C4-C3-C2	-2.41	107.49	111.02
2	A	436(A)	NAG	C1-C2-N2	2.38	114.19	110.43
2	A	434(A)	NAG	O3-C3-C2	2.35	114.29	109.40
2	A	436(A)	NAG	C6-C5-C4	2.31	118.68	113.02
2	A	434(A)	NAG	O5-C1-C2	-2.27	107.78	111.29
2	B	437(A)	NAG	C4-C3-C2	-2.24	107.74	111.02
2	D	433(A)	NAG	C3-C4-C5	-2.21	106.22	110.23
2	C	434(A)	NAG	O3-C3-C2	2.20	113.97	109.40
2	A	434(A)	NAG	C2-N2-C7	-2.15	120.02	122.90
2	C	437(A)	NAG	C3-C4-C5	-2.13	106.37	110.23
2	C	437(A)	NAG	C4-C3-C2	-2.12	107.91	111.02
2	D	436(A)	NAG	C1-C2-N2	2.09	113.73	110.43
2	C	433(A)	NAG	C1-O5-C5	2.08	114.97	112.19
2	C	433(A)	NAG	C3-C4-C5	-2.06	106.50	110.23
2	B	434(A)	NAG	O3-C3-C2	2.04	113.64	109.40
2	C	436(A)	NAG	C6-C5-C4	2.03	118.00	113.02
2	B	433(A)	NAG	C2-N2-C7	-2.02	120.19	122.90
2	A	436(A)	NAG	C8-C7-N2	-2.01	112.78	116.12
2	D	434(A)	NAG	O3-C3-C2	2.00	113.56	109.40

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	436(A)	NAG	O5-C5-C6-O6
2	A	436(A)	NAG	C4-C5-C6-O6
2	C	436(A)	NAG	C4-C5-C6-O6
2	D	436(A)	NAG	C4-C5-C6-O6
2	B	436(A)	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	436(A)	NAG	O5-C5-C6-O6
2	D	436(A)	NAG	O5-C5-C6-O6
2	A	436(A)	NAG	O5-C5-C6-O6
2	D	433(A)	NAG	O5-C5-C6-O6
2	A	434(A)	NAG	O5-C5-C6-O6
2	C	434(A)	NAG	O5-C5-C6-O6
2	D	434(A)	NAG	O5-C5-C6-O6
2	D	434(A)	NAG	C4-C5-C6-O6
2	A	437(A)	NAG	O5-C5-C6-O6
2	B	433(A)	NAG	O5-C5-C6-O6
2	B	434(A)	NAG	O5-C5-C6-O6
2	C	433(A)	NAG	O5-C5-C6-O6
2	C	437(A)	NAG	O5-C5-C6-O6
2	A	434(A)	NAG	C4-C5-C6-O6
2	C	434(A)	NAG	C4-C5-C6-O6
2	A	433(A)	NAG	O5-C5-C6-O6
2	B	437(A)	NAG	O5-C5-C6-O6
2	B	434(A)	NAG	C4-C5-C6-O6
2	A	437(A)	NAG	C4-C5-C6-O6
2	C	437(A)	NAG	C4-C5-C6-O6
2	B	437(A)	NAG	C4-C5-C6-O6
2	D	437(A)	NAG	O5-C5-C6-O6
2	D	437(A)	NAG	C4-C5-C6-O6
2	D	433(A)	NAG	C4-C5-C6-O6
2	C	433(A)	NAG	C4-C5-C6-O6
2	B	433(A)	NAG	C4-C5-C6-O6
2	A	433(A)	NAG	C4-C5-C6-O6
2	A	434(A)	NAG	C1-C2-N2-C7
2	A	436(A)	NAG	C1-C2-N2-C7
2	B	434(A)	NAG	C1-C2-N2-C7
2	D	434(A)	NAG	C1-C2-N2-C7
2	D	436(A)	NAG	C1-C2-N2-C7
2	A	436(A)	NAG	C3-C2-N2-C7
2	B	436(A)	NAG	C3-C2-N2-C7
2	C	434(A)	NAG	C3-C2-N2-C7
2	C	436(A)	NAG	C3-C2-N2-C7
2	D	436(A)	NAG	C3-C2-N2-C7
2	B	433(A)	NAG	C1-C2-N2-C7
2	B	436(A)	NAG	C1-C2-N2-C7
2	C	433(A)	NAG	C1-C2-N2-C7
2	C	434(A)	NAG	C1-C2-N2-C7
2	C	436(A)	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	D	433(A)	NAG	C1-C2-N2-C7
2	A	434(A)	NAG	C3-C2-N2-C7
2	B	434(A)	NAG	C3-C2-N2-C7
2	D	434(A)	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	436(A)	NAG	1	0
2	A	436(A)	NAG	2	0
2	C	436(A)	NAG	1	0
2	D	436(A)	NAG	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.