



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:21 AM GMT

PDB ID : 3ECA  
Title : CRYSTAL STRUCTURE OF ESCHERICHIA COLI L-ASPARAGINASE,  
AN ENZYME USED IN CANCER THERAPY  
Authors : Swain, A.L.; Jaskolski, M.; Housset, D.; Rao, J.K.M.; Wlodawer, A.  
Deposited on : 1993-07-02  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

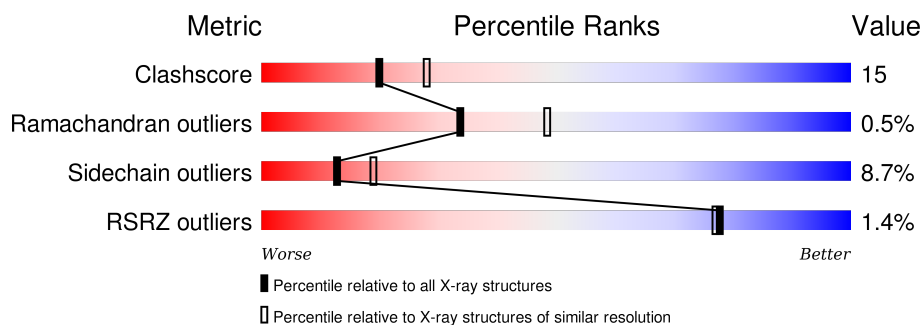
# 1 Overall quality at a glance

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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	326	
1	B	326	
1	C	326	
1	D	326	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ASP	D	327	-	-	X	-

## 2 Entry composition [i](#)

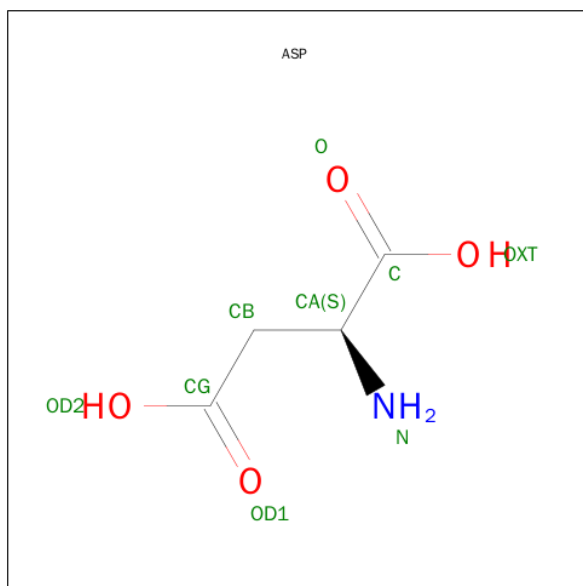
There are 3 unique types of molecules in this entry. The entry contains 10170 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ASPARAGINASE TYPE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2431	1517	415	491	8			
1	B	326	Total	C	N	O	S	0	0	0
			2431	1517	415	491	8			
1	C	326	Total	C	N	O	S	0	0	0
			2431	1517	415	491	8			
1	D	326	Total	C	N	O	S	0	0	0
			2431	1517	415	491	8			

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	1	4		
2	B	1	Total	C	N	O	0	0
			9	4	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			9	4	1	4		
2	D	1	Total	C	N	O	0	0
			9	4	1	4		

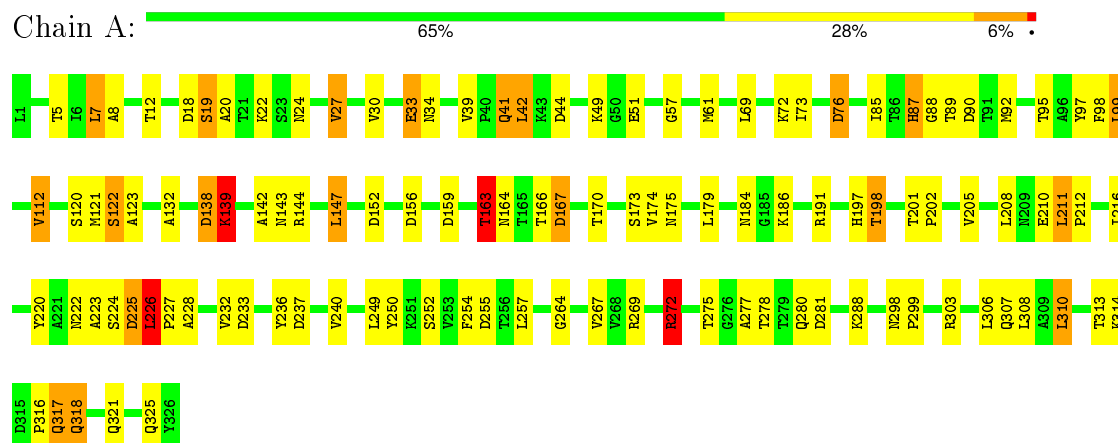
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	97	Total	O	0	0
			97	97		
3	B	100	Total	O	0	0
			100	100		
3	C	103	Total	O	0	0
			103	103		
3	D	110	Total	O	0	0
			110	110		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

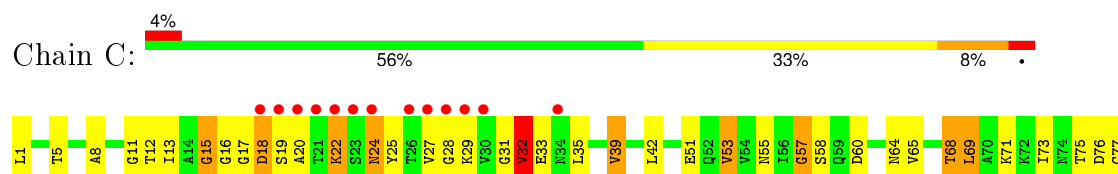
#### • Molecule 1: ASPARAGINASE TYPE II

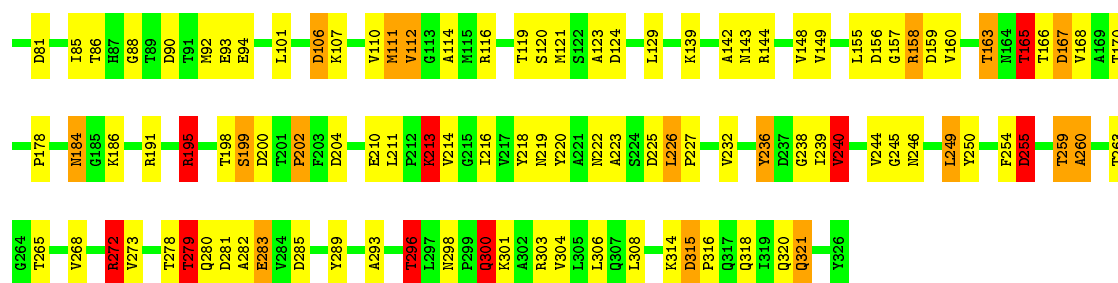


#### • Molecule 1: ASPARAGINASE TYPE II

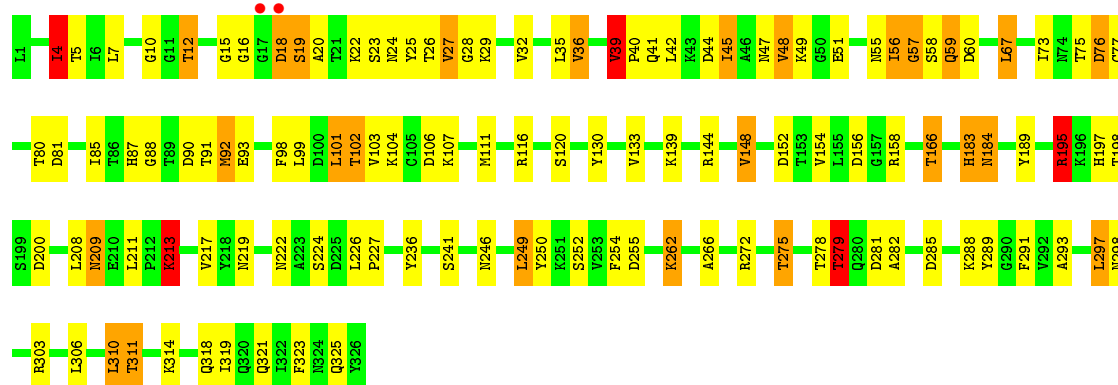


#### • Molecule 1: ASPARAGINASE TYPE II





• Molecule 1: ASPARAGINASE TYPE II



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.70Å 96.10Å 111.30Å 90.00° 97.10° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40 9.99 – 2.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40) 81.3 (9.99-2.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.149 , (Not available) 0.134 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 74.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 56390 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10170	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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	1.07	2/2468 (0.1%)	1.98	64/3361 (1.9%)
1	B	1.12	5/2468 (0.2%)	2.16	80/3361 (2.4%)
1	C	1.13	6/2468 (0.2%)	2.21	87/3361 (2.6%)
1	D	1.13	3/2468 (0.1%)	2.26	82/3361 (2.4%)
All	All	1.11	16/9872 (0.2%)	2.16	313/13444 (2.3%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	272	ARG	CD-NE	-10.22	1.29	1.46
1	B	272	ARG	CD-NE	-8.61	1.31	1.46
1	D	272	ARG	CG-CD	-7.78	1.32	1.51
1	C	283	GLU	CD-OE2	-6.60	1.18	1.25
1	C	272	ARG	CD-NE	-6.57	1.35	1.46
1	B	272	ARG	CG-CD	-6.40	1.35	1.51
1	C	195	ARG	CD-NE	-6.24	1.35	1.46
1	C	94	GLU	CG-CD	-5.95	1.43	1.51
1	C	195	ARG	NE-CZ	-5.88	1.25	1.33
1	A	272	ARG	CD-NE	-5.86	1.36	1.46
1	B	122	SER	CA-CB	-5.68	1.44	1.52
1	B	122	SER	N-CA	5.42	1.57	1.46
1	D	144	ARG	CD-NE	-5.39	1.37	1.46
1	A	173	SER	CB-OG	5.36	1.49	1.42
1	C	300	GLN	CB-CG	-5.26	1.38	1.52
1	B	121	MET	C-O	5.20	1.33	1.23

All (313) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	272	ARG	CD-NE-CZ	40.16	179.83	123.60
1	C	195	ARG	CD-NE-CZ	35.26	172.97	123.60
1	B	195	ARG	CD-NE-CZ	29.69	165.16	123.60
1	D	272	ARG	CG-CD-NE	28.41	171.46	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	ARG	CD-NE-CZ	26.88	161.23	123.60
1	D	144	ARG	CD-NE-CZ	25.93	159.91	123.60
1	C	272	ARG	NE-CZ-NH2	-25.85	107.37	120.30
1	B	272	ARG	CD-NE-CZ	25.68	159.56	123.60
1	C	272	ARG	NE-CZ-NH1	24.96	132.78	120.30
1	A	272	ARG	NE-CZ-NH2	-18.19	111.21	120.30
1	A	191	ARG	NE-CZ-NH2	-15.54	112.53	120.30
1	B	269	ARG	NE-CZ-NH1	13.97	127.29	120.30
1	C	200	ASP	CB-CG-OD1	-13.58	106.08	118.30
1	D	272	ARG	NE-CZ-NH1	-13.49	113.56	120.30
1	D	272	ARG	NE-CZ-NH2	13.36	126.98	120.30
1	D	144	ARG	NE-CZ-NH1	12.85	126.72	120.30
1	B	272	ARG	CG-CD-NE	12.51	138.07	111.80
1	B	191	ARG	NE-CZ-NH2	-12.27	114.17	120.30
1	B	272	ARG	NE-CZ-NH1	-12.02	114.29	120.30
1	A	159	ASP	CB-CG-OD2	11.85	128.97	118.30
1	B	272	ARG	CB-CG-CD	11.85	142.41	111.60
1	B	51	GLU	OE1-CD-OE2	11.24	136.79	123.30
1	C	116	ARG	NE-CZ-NH2	11.14	125.87	120.30
1	A	269	ARG	CD-NE-CZ	11.12	139.18	123.60
1	D	272	ARG	CB-CG-CD	11.12	140.52	111.60
1	B	195	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	D	303	ARG	NE-CZ-NH1	-10.62	114.99	120.30
1	D	144	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	B	225	ASP	CB-CG-OD2	-10.51	108.84	118.30
1	B	269	ARG	CD-NE-CZ	10.22	137.90	123.60
1	D	116	ARG	NE-CZ-NH2	10.15	125.37	120.30
1	C	218	TYR	CB-CG-CD2	10.04	127.02	121.00
1	C	272	ARG	CD-NE-CZ	9.97	137.55	123.60
1	C	315	ASP	CB-CG-OD1	9.83	127.15	118.30
1	B	63	ASP	CB-CG-OD2	-9.78	109.50	118.30
1	A	163	THR	CA-CB-CG2	9.60	125.83	112.40
1	A	272	ARG	CB-CG-CD	9.48	136.24	111.60
1	B	63	ASP	CB-CG-OD1	9.18	126.56	118.30
1	C	106	ASP	CB-CG-OD2	-9.07	110.14	118.30
1	B	167	ASP	CB-CG-OD1	9.00	126.40	118.30
1	C	106	ASP	CB-CG-OD1	8.93	126.33	118.30
1	B	281	ASP	CB-CG-OD2	-8.90	110.29	118.30
1	A	76	ASP	CB-CG-OD1	8.88	126.29	118.30
1	C	191	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	D	255	ASP	CB-CG-OD2	-8.84	110.34	118.30
1	A	303	ARG	NE-CZ-NH1	8.84	124.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	92	MET	CG-SD-CE	8.65	114.04	100.20
1	C	218	TYR	CB-CG-CD1	-8.64	115.82	121.00
1	C	255	ASP	CB-CG-OD1	-8.62	110.54	118.30
1	D	39	VAL	CB-CA-C	8.56	127.66	111.40
1	B	4	ILE	CA-CB-CG2	8.52	127.93	110.90
1	A	250	TYR	CB-CG-CD1	-8.51	115.90	121.00
1	B	272	ARG	NE-CZ-NH2	8.45	124.52	120.30
1	C	191	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	B	158	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	B	204	ASP	CB-CG-OD2	-8.24	110.88	118.30
1	B	282	ALA	CB-CA-C	8.18	122.37	110.10
1	C	60	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	B	296	THR	CA-CB-CG2	8.15	123.81	112.40
1	C	159	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	D	166	THR	CA-CB-CG2	8.10	123.74	112.40
1	C	279	THR	N-CA-CB	-8.05	95.00	110.30
1	A	138	ASP	CB-CG-OD1	8.05	125.54	118.30
1	D	158	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	C	249	LEU	CA-CB-CG	7.99	133.69	115.30
1	A	122	SER	O-C-N	-7.98	109.93	122.70
1	D	130	TYR	CB-CG-CD2	-7.89	116.27	121.00
1	C	112	VAL	CB-CA-C	-7.86	96.47	111.40
1	A	18	ASP	CB-CG-OD1	-7.84	111.25	118.30
1	C	303	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	B	218	TYR	CB-CG-CD2	7.82	125.69	121.00
1	D	213	LYS	CB-CA-C	7.79	125.98	110.40
1	B	303	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	B	195	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	C	296	THR	CA-CB-CG2	7.72	123.21	112.40
1	A	272	ARG	CD-NE-CZ	7.71	134.39	123.60
1	C	39	VAL	CB-CA-C	7.68	125.99	111.40
1	A	122	SER	C-N-CA	7.67	140.87	121.70
1	B	225	ASP	CB-CG-OD1	7.65	125.19	118.30
1	A	272	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	D	44	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	B	244	VAL	N-CA-CB	-7.55	94.89	111.50
1	C	18	ASP	CB-CA-C	7.51	125.43	110.40
1	B	210	GLU	OE1-CD-OE2	7.44	132.22	123.30
1	D	217	VAL	CA-CB-CG1	7.43	122.05	110.90
1	D	45	ILE	CA-CB-CG2	7.38	125.65	110.90
1	C	300	GLN	CA-CB-CG	7.37	129.61	113.40
1	D	56	ILE	N-CA-CB	-7.33	93.95	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	D	152	ASP	CB-CG-OD1	7.28	124.85	118.30
1	C	296	THR	N-CA-CB	-7.28	96.47	110.30
1	B	205	VAL	N-CA-CB	-7.25	95.55	111.50
1	C	158	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	A	272	ARG	CG-CD-NE	7.22	126.97	111.80
1	B	244	VAL	CB-CA-C	7.22	125.12	111.40
1	A	191	ARG	CD-NE-CZ	7.21	133.69	123.60
1	A	92	MET	CA-CB-CG	-7.21	101.05	113.30
1	B	92	MET	CG-SD-CE	7.10	111.56	100.20
1	A	303	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	317	GLN	N-CA-CB	7.06	123.32	110.60
1	A	225	ASP	CB-CG-OD1	7.05	124.64	118.30
1	D	56	ILE	CA-CB-CG1	7.04	124.38	111.00
1	B	158	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	D	275	THR	N-CA-CB	-7.01	96.98	110.30
1	A	237	ASP	CB-CG-OD2	6.99	124.59	118.30
1	B	76	ASP	CB-CG-OD2	6.98	124.59	118.30
1	B	152	ASP	CB-CG-OD1	6.98	124.58	118.30
1	D	166	THR	N-CA-CB	-6.96	97.07	110.30
1	C	144	ARG	CD-NE-CZ	6.95	133.34	123.60
1	C	156	ASP	CB-CG-OD1	6.95	124.56	118.30
1	C	314	LYS	CA-CB-CG	6.91	128.59	113.40
1	A	233	ASP	CB-CG-OD1	6.90	124.51	118.30
1	D	148	VAL	CA-CB-CG1	6.90	121.25	110.90
1	C	225	ASP	CB-CG-OD1	6.87	124.49	118.30
1	B	69	LEU	N-CA-CB	-6.85	96.70	110.40
1	D	184	ASN	OD1-CG-ND2	6.84	137.63	121.90
1	C	289	TYR	CB-CG-CD1	-6.83	116.91	121.00
1	C	139	LYS	CB-CA-C	6.78	123.96	110.40
1	B	99	LEU	CB-CG-CD1	6.77	122.51	111.00
1	D	213	LYS	CG-CD-CE	6.76	132.19	111.90
1	C	60	ASP	CB-CG-OD1	6.71	124.33	118.30
1	A	156	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	167	ASP	CB-CG-OD1	6.70	124.33	118.30
1	B	81	ASP	CB-CG-OD1	6.64	124.28	118.30
1	C	240	VAL	N-CA-CB	6.63	126.10	111.50
1	A	152	ASP	CB-CG-OD1	6.63	124.27	118.30
1	B	296	THR	N-CA-CB	-6.60	97.76	110.30
1	C	300	GLN	CB-CA-C	-6.60	97.20	110.40
1	A	211	LEU	CB-CA-C	6.60	122.73	110.20
1	D	279	THR	N-CA-CB	-6.58	97.80	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	298	ASN	CB-CA-C	6.57	123.54	110.40
1	B	220	TYR	CB-CG-CD2	6.56	124.93	121.00
1	C	263	THR	CA-CB-CG2	6.55	121.58	112.40
1	A	147	LEU	N-CA-CB	-6.55	97.31	110.40
1	C	167	ASP	CB-CG-OD1	6.49	124.14	118.30
1	D	282	ALA	CB-CA-C	6.46	119.79	110.10
1	A	211	LEU	N-CA-CB	-6.46	97.49	110.40
1	C	303	ARG	CD-NE-CZ	6.45	132.63	123.60
1	C	163	THR	N-CA-CB	-6.44	98.07	110.30
1	B	191	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	D	154	VAL	CG1-CB-CG2	6.43	121.19	110.90
1	D	262	LYS	CB-CG-CD	6.42	128.29	111.60
1	C	204	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	B	7	LEU	CA-CB-CG	6.36	129.93	115.30
1	A	87	HIS	N-CA-CB	-6.35	99.17	110.60
1	C	202	PRO	N-CA-CB	-6.32	95.65	102.60
1	D	106	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	B	51	GLU	CG-CD-OE2	-6.28	105.75	118.30
1	B	87	HIS	N-CA-CB	-6.26	99.33	110.60
1	C	285	ASP	CB-CG-OD1	6.26	123.94	118.30
1	C	300	GLN	CB-CG-CD	6.26	127.86	111.60
1	D	298	ASN	CB-CA-C	6.24	122.88	110.40
1	B	92	MET	CA-CB-CG	-6.22	102.72	113.30
1	B	312	GLN	CB-CA-C	-6.22	97.95	110.40
1	D	60	ASP	CB-CG-OD1	6.21	123.89	118.30
1	C	195	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	122	SER	CA-C-N	6.20	130.83	117.20
1	C	124	ASP	CB-CG-OD1	6.20	123.88	118.30
1	D	18	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	123	ALA	N-CA-CB	6.18	118.75	110.10
1	D	183	HIS	CA-CB-CG	-6.18	103.09	113.60
1	D	12	THR	CA-CB-CG2	6.17	121.04	112.40
1	A	163	THR	N-CA-CB	-6.17	98.58	110.30
1	B	9	THR	CA-CB-CG2	6.15	121.00	112.40
1	D	57	GLY	N-CA-C	-6.15	97.74	113.10
1	A	19	SER	CA-C-N	-6.14	103.69	117.20
1	B	44	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	B	51	GLU	N-CA-CB	6.11	121.60	110.60
1	D	189	TYR	CB-CG-CD2	6.11	124.67	121.00
1	A	236	TYR	CA-CB-CG	-6.11	101.79	113.40
1	B	278	THR	CA-CB-OG1	-6.09	96.22	109.00
1	A	61	MET	CA-CB-CG	6.08	123.63	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	C	94	GLU	CG-CD-OE2	6.08	130.45	118.30
1	D	209	ASN	N-CA-CB	-6.07	99.67	110.60
1	B	285	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	B	69	LEU	CB-CA-C	6.01	121.61	110.20
1	C	53	VAL	CB-CA-C	5.99	122.77	111.40
1	B	279	THR	O-C-N	5.98	132.27	122.70
1	D	189	TYR	CB-CG-CD1	-5.98	117.41	121.00
1	D	195	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	C	186	LYS	CD-CE-NZ	5.97	125.44	111.70
1	C	76	ASP	CB-CG-OD1	5.96	123.67	118.30
1	D	289	TYR	CB-CG-CD1	-5.96	117.42	121.00
1	C	165	THR	N-CA-CB	-5.93	99.02	110.30
1	C	57	GLY	N-CA-C	-5.93	98.27	113.10
1	C	159	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	147	LEU	CB-CG-CD1	5.92	121.06	111.00
1	D	67	LEU	CB-CA-C	5.92	121.44	110.20
1	B	55	ASN	CB-CG-OD1	5.88	133.36	121.60
1	D	81	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	C	282	ALA	N-CA-CB	5.87	118.32	110.10
1	D	319	ILE	CB-CA-C	5.85	123.30	111.60
1	C	116	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	C	200	ASP	OD1-CG-OD2	5.85	134.41	123.30
1	C	304	VAL	CA-CB-CG1	5.84	119.67	110.90
1	A	317	GLN	O-C-N	5.84	132.05	122.70
1	C	279	THR	CA-CB-CG2	5.83	120.56	112.40
1	A	92	MET	CG-SD-CE	5.83	109.53	100.20
1	B	4	ILE	CB-CA-C	5.82	123.25	111.60
1	D	213	LYS	CB-CG-CD	5.81	126.70	111.60
1	B	136	ALA	N-CA-CB	5.80	118.23	110.10
1	C	81	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	24	ASN	CA-CB-CG	5.78	126.11	113.40
1	D	249	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	264	GLY	N-CA-C	5.76	127.51	113.10
1	D	200	ASP	CA-C-O	-5.76	108.00	120.10
1	D	217	VAL	N-CA-CB	-5.75	98.84	111.50
1	B	130	TYR	N-CA-CB	-5.75	100.25	110.60
1	B	220	TYR	CB-CG-CD1	-5.74	117.56	121.00
1	D	148	VAL	CG1-CB-CG2	5.74	120.08	110.90
1	B	167	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	C	210	GLU	OE1-CD-OE2	5.72	130.16	123.30
1	B	127	PHE	CB-CA-C	5.70	121.79	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	VAL	CG1-CB-CG2	5.67	119.97	110.90
1	D	314	LYS	CA-CB-CG	5.65	125.83	113.40
1	C	226	LEU	CB-CA-C	5.65	120.94	110.20
1	D	217	VAL	CB-CA-C	5.65	122.14	111.40
1	B	232	VAL	CA-CB-CG2	5.64	119.37	110.90
1	D	266	ALA	CB-CA-C	5.61	118.52	110.10
1	A	144	ARG	CG-CD-NE	-5.60	100.05	111.80
1	A	278	THR	N-CA-CB	5.59	120.93	110.30
1	D	76	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	61	MET	CB-CA-C	5.59	121.58	110.40
1	B	258	ALA	CB-CA-C	5.59	118.48	110.10
1	A	255	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	D	87	HIS	N-CA-CB	-5.57	100.57	110.60
1	D	101	LEU	C-N-CA	5.57	135.63	121.70
1	C	93	GLU	CG-CD-OE1	-5.57	107.16	118.30
1	D	236	TYR	CA-CB-CG	-5.57	102.82	113.40
1	C	69	LEU	N-CA-CB	-5.54	99.31	110.40
1	A	281	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	27	VAL	N-CA-CB	-5.52	99.35	111.50
1	A	97	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	B	298	ASN	CB-CA-C	5.51	121.43	110.40
1	A	280	GLN	CB-CA-C	5.50	121.40	110.40
1	A	19	SER	CA-C-O	5.50	131.65	120.10
1	C	260	ALA	N-CA-CB	5.49	117.79	110.10
1	C	272	ARG	CG-CD-NE	5.49	123.33	111.80
1	C	163	THR	CA-CB-CG2	5.49	120.08	112.40
1	A	175	ASN	CB-CG-ND2	5.48	129.86	116.70
1	C	90	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	57	GLY	N-CA-C	-5.47	99.42	113.10
1	D	48	VAL	C-N-CA	5.47	135.38	121.70
1	C	199	SER	CB-CA-C	-5.47	99.71	110.10
1	D	148	VAL	N-CA-CB	5.47	123.53	111.50
1	D	318	GLN	O-C-N	5.46	131.44	122.70
1	B	138	ASP	CB-CG-OD2	5.45	123.20	118.30
1	C	314	LYS	CB-CA-C	5.45	121.29	110.40
1	C	158	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	B	163	THR	CA-CB-CG2	5.41	119.97	112.40
1	D	93	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	A	210	GLU	OE1-CD-OE2	5.39	129.76	123.30
1	C	283	GLU	CA-C-O	-5.37	108.81	120.10
1	B	317	GLN	CA-CB-CG	5.37	125.20	113.40
1	B	278	THR	N-CA-CB	5.36	120.47	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	252	SER	CB-CA-C	5.36	120.28	110.10
1	A	233	ASP	CA-CB-CG	5.35	125.16	113.40
1	B	278	THR	N-CA-C	-5.33	96.61	111.00
1	B	103	VAL	CA-CB-CG1	5.31	118.87	110.90
1	B	172	LYS	O-C-N	5.30	131.19	122.70
1	C	168	VAL	CG1-CB-CG2	5.30	119.37	110.90
1	C	111	MET	CG-SD-CE	5.29	108.67	100.20
1	D	293	ALA	N-CA-CB	5.29	117.50	110.10
1	C	156	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	D	297	LEU	CA-CB-CG	5.28	127.45	115.30
1	B	57	GLY	N-CA-C	-5.28	99.90	113.10
1	A	303	ARG	CD-NE-CZ	5.27	130.98	123.60
1	D	262	LYS	CA-CB-CG	5.27	124.99	113.40
1	A	51	GLU	OE1-CD-OE2	5.25	129.60	123.30
1	A	89	THR	CA-CB-CG2	5.23	119.72	112.40
1	C	18	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	12	THR	CA-CB-OG1	-5.22	98.04	109.00
1	D	111	MET	CG-SD-CE	5.21	108.54	100.20
1	B	138	ASP	CB-CG-OD1	5.21	122.98	118.30
1	C	321	GLN	CA-CB-CG	-5.20	101.96	113.40
1	D	156	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	279	THR	CA-C-N	-5.18	105.81	117.20
1	D	278	THR	N-CA-C	-5.17	97.03	111.00
1	C	236	TYR	CB-CG-CD2	-5.16	117.91	121.00
1	D	278	THR	N-CA-CB	5.16	120.10	110.30
1	C	121	MET	N-CA-C	-5.15	97.10	111.00
1	B	89	THR	CA-CB-CG2	5.14	119.60	112.40
1	C	213	LYS	CG-CD-CE	5.13	127.30	111.90
1	D	24	ASN	O-C-N	5.13	130.91	122.70
1	C	69	LEU	CB-CA-C	5.12	119.94	110.20
1	B	156	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	291	PHE	O-C-N	5.11	130.88	122.70
1	A	8	ALA	CB-CA-C	5.10	117.75	110.10
1	B	241	SER	O-C-N	5.09	130.85	122.70
1	A	226	LEU	CB-CA-C	5.09	119.86	110.20
1	B	244	VAL	CA-CB-CG2	5.09	118.53	110.90
1	B	283	GLU	OE1-CD-OE2	5.08	129.40	123.30
1	A	33	GLU	CG-CD-OE2	-5.08	108.14	118.30
1	A	44	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	D	47	ASN	N-CA-CB	5.08	119.75	110.60
1	C	22	LYS	CA-C-N	-5.08	106.03	117.20
1	D	51	GLU	OE1-CD-OE2	5.07	129.39	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4	ILE	CB-CA-C	5.07	121.73	111.60
1	B	138	ASP	OD1-CG-OD2	-5.06	113.68	123.30
1	A	139	LYS	CG-CD-CE	5.06	127.08	111.90
1	B	76	ASP	O-C-N	5.05	130.79	122.70
1	B	269	ARG	NH1-CZ-NH2	-5.05	113.84	119.40
1	C	278	THR	N-CA-CB	5.05	119.90	110.30
1	C	24	ASN	CB-CA-C	5.05	120.50	110.40
1	B	4	ILE	CB-CG1-CD1	-5.05	99.77	113.90
1	D	87	HIS	CA-CB-CG	5.05	122.18	113.60
1	D	47	ASN	N-CA-C	-5.04	97.40	111.00
1	D	311	THR	N-CA-CB	5.02	119.84	110.30
1	C	184	ASN	C-N-CA	5.01	132.82	122.30
1	D	289	TYR	CA-CB-CG	-5.01	103.88	113.40
1	C	5	THR	CA-C-O	-5.01	109.58	120.10
1	A	152	ASP	OD1-CG-OD2	-5.00	113.80	123.30

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	2431	0	2424	68	0
1	B	2431	0	2424	85	0
1	C	2431	0	2424	93	0
1	D	2431	0	2424	66	0
2	A	9	0	3	2	0
2	B	9	0	3	3	0
2	C	9	0	3	3	0
2	D	9	0	3	4	0
3	A	97	0	0	1	0
3	B	100	0	0	5	0
3	C	103	0	0	7	0
3	D	110	0	0	2	0
All	All	10170	0	9708	289	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 15.

All (289) 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:74:ASN:HD21	1:B:104:LYS:H	1.08	0.92
1:D:39:VAL:HG22	1:D:42:LEU:HD13	1.51	0.92
1:A:139:LYS:H	1:A:139:LYS:HE3	1.30	0.92
1:D:59:GLN:H	1:D:59:GLN:HE21	1.16	0.91
1:C:16:GLY:HA3	1:C:29:LYS:HD2	1.55	0.88
1:C:92:MET:HE1	1:C:148:VAL:HG13	1.57	0.86
1:A:41:GLN:H	1:A:41:GLN:HE21	1.20	0.85
1:A:164:ASN:HD22	1:A:167:ASP:H	1.19	0.85
1:C:216:ILE:HG12	1:C:240:VAL:HG22	1.58	0.84
1:C:20:ALA:HA	1:C:120:SER:HA	1.59	0.83
1:B:158:ARG:HH12	1:B:296:THR:HG22	1.44	0.83
1:C:293:ALA:H	1:C:320:GLN:HE22	1.23	0.83
1:A:122:SER:HB2	1:B:127:PHE:HB2	1.62	0.81
1:B:74:ASN:ND2	1:B:104:LYS:H	1.80	0.80
1:B:19:SER:HB3	1:B:22:LYS:HB3	1.63	0.80
1:C:163:THR:HB	1:C:170:THR:O	1.83	0.79
1:B:244:VAL:HG13	1:D:90:ASP:HB3	1.66	0.76
1:C:8:ALA:HB2	1:C:32:VAL:HG13	1.66	0.75
1:B:153:THR:HG21	3:B:365:HOH:O	1.84	0.75
1:C:158:ARG:HH12	1:C:296:THR:HG22	1.50	0.74
1:C:92:MET:CE	1:C:148:VAL:HG13	2.20	0.72
1:C:17:GLY:HA2	1:C:25:TYR:CB	2.19	0.72
1:D:226:LEU:HB2	1:D:227:PRO:HD3	1.72	0.72
1:A:41:GLN:NE2	1:A:41:GLN:H	1.87	0.71
1:A:121:MET:HE1	1:B:39:VAL:HG13	1.71	0.71
1:A:277:ALA:O	1:C:165:THR:HG21	1.91	0.71
1:A:163:THR:HB	1:A:170:THR:O	1.91	0.70
1:A:306:LEU:HG	1:A:310:LEU:HD22	1.74	0.70
1:B:164:ASN:HD22	1:D:275:THR:CG2	2.04	0.70
1:D:20:ALA:HA	1:D:120:SER:HA	1.73	0.70
1:B:27:VAL:HG12	1:B:57:GLY:HA2	1.74	0.69
1:C:27:VAL:HG21	2:C:327:ASP:HA	1.72	0.69
1:B:164:ASN:HD22	1:D:275:THR:HG22	1.57	0.69
1:B:296:THR:HG23	3:B:376:HOH:O	1.92	0.69
1:D:59:GLN:H	1:D:59:GLN:NE2	1.91	0.68
1:D:99:LEU:HA	1:D:102:THR:HG22	1.75	0.68
1:B:12:THR:HA	1:B:27:VAL:HG22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LYS:H	1:A:139:LYS:CE	2.06	0.67
1:D:59:GLN:N	1:D:59:GLN:HE21	1.92	0.66
1:C:17:GLY:HA2	1:C:25:TYR:HB2	1.76	0.66
1:B:158:ARG:NH1	1:B:296:THR:HG22	2.11	0.66
1:B:27:VAL:CG1	1:B:57:GLY:HA2	2.26	0.65
1:C:213:LYS:HA	1:C:213:LYS:CE	2.25	0.65
1:D:4:ILE:HD11	1:D:48:VAL:HG22	1.78	0.65
1:C:12:THR:HA	1:C:15:GLY:HA3	1.79	0.63
1:D:75:THR:HG22	1:D:76:ASP:OD1	1.98	0.63
1:C:296:THR:HB	3:C:346:HOH:O	1.98	0.63
1:C:32:VAL:HA	1:C:35:LEU:HD12	1.81	0.63
1:A:138:ASP:HA	1:A:139:LYS:HE3	1.81	0.62
1:A:184:ASN:HB3	1:A:186:LYS:HE2	1.82	0.62
1:C:165:THR:HG23	1:C:166:THR:HG23	1.81	0.62
1:D:197:HIS:HD2	1:D:198:THR:OG1	1.82	0.62
1:C:220:TYR:CZ	1:C:223:ALA:HA	2.35	0.61
1:C:184:ASN:HB2	1:D:23:SER:OG	2.01	0.61
1:B:225:ASP:HB3	1:B:252:SER:HB3	1.83	0.61
1:A:164:ASN:ND2	1:A:167:ASP:H	1.96	0.61
1:B:219:ASN:ND2	1:B:250:TYR:H	1.99	0.61
1:C:244:VAL:HG12	1:C:272:ARG:CZ	2.31	0.61
1:C:219:ASN:ND2	1:C:250:TYR:H	1.99	0.61
1:C:255:ASP:O	1:C:259:THR:HG23	2.01	0.60
1:D:32:VAL:O	1:D:36:VAL:HG13	2.02	0.60
1:C:279:THR:HG23	1:C:280:GLN:O	2.02	0.60
1:B:25:TYR:CE2	1:B:27:VAL:HG23	2.36	0.59
1:A:87:HIS:HD2	1:A:88:GLY:O	1.85	0.59
1:C:142:ALA:O	1:C:143:ASN:HB2	2.01	0.59
1:A:122:SER:HB2	1:B:127:PHE:CB	2.30	0.59
1:D:77:CYS:O	1:D:107:LYS:NZ	2.34	0.59
1:B:95:THR:HG22	1:B:99:LEU:HD22	1.85	0.59
1:C:158:ARG:NH1	1:C:296:THR:HG22	2.17	0.59
1:B:25:TYR:HE2	1:B:27:VAL:HG23	1.68	0.59
1:D:73:ILE:HD11	1:D:85:ILE:HD11	1.85	0.59
1:D:219:ASN:HD22	1:D:250:TYR:H	1.51	0.58
1:D:4:ILE:CD1	1:D:48:VAL:HG22	2.34	0.58
1:C:219:ASN:HD22	1:C:250:TYR:H	1.51	0.58
1:C:28:GLY:C	1:C:55:ASN:HD21	2.07	0.57
1:D:32:VAL:HA	1:D:35:LEU:HD12	1.85	0.57
1:B:163:THR:HB	1:B:170:THR:O	2.04	0.57
1:C:8:ALA:CB	1:C:32:VAL:HG13	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:GLY:CA	1:B:27:VAL:HG13	2.35	0.56
1:C:220:TYR:CE2	1:C:223:ALA:HA	2.39	0.56
1:B:10:GLY:HA2	1:B:55:ASN:OD1	2.05	0.56
1:D:39:VAL:CG2	1:D:42:LEU:HD13	2.31	0.56
1:C:27:VAL:HG11	2:C:327:ASP:OXT	2.05	0.56
1:A:139:LYS:N	1:A:139:LYS:HE3	2.11	0.56
1:B:318:GLN:O	1:B:321:GLN:HB3	2.05	0.56
1:C:17:GLY:HA2	1:C:25:TYR:HB3	1.88	0.56
1:B:163:THR:O	1:D:275:THR:HB	2.06	0.55
1:C:293:ALA:H	1:C:320:GLN:NE2	2.00	0.55
1:B:220:TYR:CZ	1:B:223:ALA:HA	2.42	0.55
1:B:23:SER:O	1:B:25:TYR:HD1	1.90	0.55
1:C:16:GLY:O	1:C:25:TYR:HB2	2.06	0.55
1:B:11:GLY:HA2	1:B:27:VAL:HG13	1.88	0.54
1:C:17:GLY:H	1:C:119:THR:HG23	1.72	0.54
1:B:25:TYR:HE2	1:B:27:VAL:CG2	2.20	0.54
1:C:77:CYS:O	1:C:107:LYS:NZ	2.38	0.54
1:A:73:ILE:HD11	1:A:85:ILE:HD11	1.88	0.54
1:B:163:THR:HG21	1:B:172:LYS:NZ	2.24	0.53
1:C:31:GLY:O	1:C:33:GLU:N	2.41	0.53
1:C:214:VAL:HA	1:C:238:GLY:O	2.09	0.53
1:B:27:VAL:HG21	2:B:327:ASP:HA	1.90	0.53
1:A:19:SER:HB2	1:A:22:LYS:HB3	1.89	0.53
1:C:92:MET:HE3	1:C:111:MET:C	2.30	0.53
1:A:22:LYS:HE2	1:A:24:ASN:OD1	2.09	0.53
1:B:66:TRP:HB3	1:B:98:PHE:CE2	2.44	0.53
1:B:197:HIS:HE1	3:B:403:HOH:O	1.92	0.53
1:C:64:ASN:O	1:C:68:THR:HG23	2.09	0.53
1:D:321:GLN:O	1:D:325:GLN:HG3	2.09	0.53
1:B:164:ASN:ND2	1:D:275:THR:HG22	2.22	0.52
1:D:10:GLY:HA2	1:D:55:ASN:OD1	2.09	0.52
1:A:225:ASP:HB3	1:A:252:SER:HB3	1.90	0.52
1:B:74:ASN:HD21	1:B:104:LYS:N	1.92	0.52
1:D:195:ARG:NH1	1:D:323:PHE:O	2.42	0.52
1:B:135:THR:HA	1:B:187:ILE:HD11	1.91	0.52
1:B:96:ALA:O	1:B:100:ASP:HB2	2.10	0.52
1:A:184:ASN:HD21	1:B:22:LYS:NZ	2.08	0.52
1:B:216:ILE:HG12	1:B:240:VAL:HB	1.92	0.52
1:A:197:HIS:HE1	3:A:399:HOH:O	1.92	0.52
1:A:112:VAL:HG13	1:A:132:ALA:HB2	1.91	0.52
1:C:24:ASN:O	1:C:25:TYR:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ILE:HD12	1:B:4:ILE:C	2.30	0.51
1:B:16:GLY:N	1:B:29:LYS:HD2	2.25	0.51
1:A:227:PRO:HB3	1:C:227:PRO:HB3	1.92	0.51
1:A:174:VAL:HB	1:A:275:THR:HG22	1.91	0.51
1:D:27:VAL:CG1	2:D:327:ASP:HA	2.41	0.51
1:B:226:LEU:HB2	1:B:227:PRO:HD3	1.92	0.51
1:D:39:VAL:O	1:D:42:LEU:HB2	2.10	0.51
1:D:197:HIS:HE1	3:D:413:HOH:O	1.92	0.51
1:C:58:SER:OG	2:C:327:ASP:O	2.25	0.51
1:C:32:VAL:HG21	1:C:51:GLU:C	2.31	0.50
1:B:321:GLN:HG2	1:B:325:GLN:HE21	1.76	0.50
1:C:155:LEU:HD23	1:C:178:PRO:HB3	1.94	0.50
1:A:272:ARG:NH2	1:C:300:GLN:HG3	2.27	0.50
1:C:296:THR:HG23	3:C:418:HOH:O	2.12	0.50
1:B:186:LYS:NZ	1:C:281:ASP:OD2	2.44	0.50
1:A:228:ALA:O	1:A:232:VAL:HG23	2.12	0.49
1:D:59:GLN:HE22	2:D:327:ASP:N	2.10	0.49
1:A:69:LEU:O	1:A:73:ILE:HG13	2.12	0.49
1:A:186:LYS:NZ	1:D:281:ASP:OD2	2.35	0.49
1:D:104:LYS:NZ	1:D:198:THR:O	2.38	0.49
1:B:219:ASN:HD22	1:B:250:TYR:H	1.60	0.49
1:D:76:ASP:O	1:D:80:THR:HG22	2.12	0.49
1:B:183:HIS:CE1	1:C:279:THR:HG23	2.47	0.49
1:D:208:LEU:HD11	1:D:311:THR:HG21	1.94	0.49
1:A:19:SER:HB3	1:A:22:LYS:H	1.78	0.49
1:D:285:ASP:OD2	1:D:288:LYS:HB2	2.12	0.49
1:C:293:ALA:N	1:C:320:GLN:HE22	2.03	0.49
1:B:183:HIS:CE1	1:C:279:THR:CG2	2.96	0.49
1:A:90:ASP:OD1	1:C:245:GLY:HA3	2.12	0.49
1:C:213:LYS:HA	1:C:213:LYS:HE2	1.95	0.49
1:A:72:LYS:NZ	1:A:76:ASP:OD2	2.45	0.49
2:A:327:ASP:N	1:C:283:GLU:OE2	2.46	0.49
1:B:19:SER:HB3	1:B:22:LYS:CB	2.40	0.48
1:B:22:LYS:HE3	1:B:24:ASN:OD1	2.12	0.48
1:B:151:ASN:O	1:B:153:THR:CG2	2.60	0.48
1:D:58:SER:HB2	1:D:91:THR:OG1	2.12	0.48
1:A:197:HIS:HD2	1:A:198:THR:OG1	1.96	0.48
1:A:212:PRO:HG2	1:A:307:GLN:O	2.13	0.48
1:C:28:GLY:CA	1:C:55:ASN:HD21	2.26	0.48
1:D:249:LEU:HD13	1:D:254:PHE:HA	1.95	0.48
1:D:27:VAL:HB	1:D:57:GLY:HA2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ALA:HB1	3:C:367:HOH:O	2.13	0.48
1:C:17:GLY:HA3	1:C:119:THR:OG1	2.14	0.48
1:D:19:SER:OG	1:D:22:LYS:HB3	2.14	0.48
1:A:112:VAL:CG1	1:A:132:ALA:HB2	2.44	0.47
1:D:285:ASP:OD2	1:D:288:LYS:HE3	2.14	0.47
1:B:321:GLN:HG2	1:B:325:GLN:NE2	2.29	0.47
1:D:98:PHE:O	1:D:102:THR:HB	2.15	0.47
1:B:17:GLY:HA3	1:B:119:THR:OG1	2.13	0.47
1:B:17:GLY:HA2	1:B:25:TYR:CB	2.45	0.47
1:B:88:GLY:HA3	2:B:327:ASP:O	2.14	0.47
1:C:65:VAL:O	1:C:69:LEU:HB2	2.15	0.47
1:B:27:VAL:HG11	2:B:327:ASP:O	2.15	0.47
1:D:213:LYS:HA	1:D:213:LYS:CE	2.44	0.47
1:C:12:THR:C	1:C:15:GLY:H	2.18	0.47
1:A:226:LEU:N	1:A:227:PRO:CD	2.78	0.47
1:A:224:SER:HB2	1:C:236:TYR:OH	2.15	0.47
1:A:20:ALA:HA	1:A:120:SER:HA	1.95	0.47
1:A:39:VAL:O	1:A:42:LEU:HB2	2.15	0.47
1:A:30:VAL:CG1	1:A:34:ASN:HB2	2.44	0.47
1:A:27:VAL:HG12	3:C:406:HOH:O	2.15	0.47
1:A:318:GLN:NE2	1:A:318:GLN:HA	2.30	0.47
1:B:150:MET:O	1:B:151:ASN:C	2.52	0.47
1:C:246:ASN:HD21	1:C:279:THR:CG2	2.27	0.47
1:C:268:VAL:HG23	1:C:306:LEU:HD22	1.97	0.47
3:B:350:HOH:O	1:C:195:ARG:HB2	2.14	0.47
1:D:219:ASN:ND2	1:D:250:TYR:H	2.13	0.46
1:A:216:ILE:HA	1:A:240:VAL:O	2.15	0.46
1:D:183:HIS:HB2	3:D:370:HOH:O	2.14	0.46
1:B:4:ILE:HD13	1:B:84:VAL:HG23	1.97	0.46
1:D:59:GLN:NE2	2:D:327:ASP:N	2.64	0.46
1:D:16:GLY:HA3	1:D:29:LYS:HD3	1.97	0.46
1:B:163:THR:HG21	1:B:172:LYS:HZ3	1.81	0.46
1:B:214:VAL:HA	1:B:238:GLY:O	2.16	0.46
1:D:5:THR:HA	1:D:49:LYS:O	2.16	0.46
1:A:142:ALA:O	1:A:143:ASN:HB2	2.16	0.46
1:A:27:VAL:HG21	2:A:327:ASP:HA	1.97	0.46
1:C:232:VAL:HG21	1:C:260:ALA:HB2	1.98	0.45
1:D:306:LEU:HG	1:D:310:LEU:HD22	1.99	0.45
1:C:110:VAL:HG13	1:C:149:VAL:HG23	1.97	0.45
1:B:286:ASP:O	1:B:290:GLY:N	2.49	0.45
1:A:205:VAL:HA	1:A:208:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:TYR:CZ	1:A:223:ALA:HA	2.52	0.45
1:D:12:THR:HG1	1:D:25:TYR:HE2	1.63	0.45
1:C:20:ALA:HA	1:C:120:SER:CA	2.40	0.45
1:B:6:ILE:HA	1:B:84:VAL:O	2.16	0.45
1:A:30:VAL:HG12	1:A:34:ASN:HB2	1.98	0.45
1:B:228:ALA:O	1:B:232:VAL:HG13	2.15	0.45
1:A:33:GLU:CD	1:A:33:GLU:H	2.20	0.45
1:B:89:THR:HB	1:B:171:PHE:CE2	2.52	0.45
1:C:167:ASP:O	1:C:170:THR:HB	2.17	0.45
1:D:103:VAL:O	1:D:198:THR:HA	2.16	0.45
1:B:197:HIS:HD2	1:B:198:THR:OG1	2.00	0.44
1:D:246:ASN:HD21	1:D:279:THR:CG2	2.31	0.44
1:A:98:PHE:CE1	1:A:211:LEU:HD21	2.51	0.44
1:B:11:GLY:C	1:B:27:VAL:HG13	2.38	0.44
1:D:88:GLY:HA3	2:D:327:ASP:OXT	2.17	0.44
1:B:227:PRO:HB3	1:D:227:PRO:HB3	2.00	0.44
1:C:11:GLY:O	1:C:27:VAL:HG13	2.17	0.44
1:C:260:ALA:HB1	1:C:265:THR:HB	1.99	0.44
1:A:5:THR:HG22	1:A:7:LEU:HD13	2.00	0.44
1:A:298:ASN:HB2	1:A:299:PRO:CD	2.48	0.44
1:A:95:THR:HG22	1:A:99:LEU:HD22	2.00	0.44
1:D:39:VAL:HA	1:D:40:PRO:HD2	1.86	0.43
1:C:18:ASP:HB2	1:C:24:ASN:O	2.19	0.43
1:D:45:ILE:HG22	1:D:133:VAL:HG12	2.00	0.43
1:A:164:ASN:ND2	1:A:166:THR:H	2.16	0.43
1:C:20:ALA:CA	1:C:120:SER:HA	2.39	0.43
1:B:12:THR:CA	1:B:27:VAL:HG22	2.47	0.43
1:D:98:PHE:CE2	1:D:102:THR:HG21	2.53	0.43
1:B:182:ILE:HA	1:B:186:LYS:O	2.18	0.43
1:A:317:GLN:O	1:A:321:GLN:HG3	2.19	0.43
1:B:19:SER:OG	1:B:20:ALA:N	2.50	0.43
1:D:15:GLY:HA2	1:D:26:THR:O	2.19	0.43
1:A:139:LYS:CD	1:A:139:LYS:H	2.32	0.43
1:C:15:GLY:HA2	1:C:27:VAL:HA	2.01	0.43
1:C:148:VAL:HG21	1:C:160:VAL:HG11	2.00	0.43
1:B:238:GLY:HA2	1:B:266:ALA:O	2.19	0.43
1:A:314:LYS:O	1:A:316:PRO:HD3	2.18	0.43
1:A:41:GLN:N	1:A:41:GLN:HE21	2.02	0.43
1:A:249:LEU:CD2	1:A:257:LEU:HD12	2.48	0.43
1:C:27:VAL:HG12	1:C:57:GLY:HA2	2.01	0.42
1:B:212:PRO:HG2	1:B:307:GLN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:MET:HE2	1:C:148:VAL:HG22	2.00	0.42
1:D:241:SER:OG	1:D:249:LEU:HD23	2.19	0.42
1:B:247:GLY:HA3	1:B:278:THR:HG23	2.01	0.42
1:D:226:LEU:CB	1:D:227:PRO:HD3	2.46	0.42
1:D:27:VAL:HG21	1:D:57:GLY:HA3	2.02	0.42
1:B:27:VAL:HG12	1:B:57:GLY:CA	2.46	0.42
1:C:315:ASP:HB3	1:C:318:GLN:HB2	2.02	0.42
1:C:296:THR:CG2	3:C:418:HOH:O	2.67	0.42
1:B:236:TYR:OH	1:D:224:SER:HB2	2.19	0.42
1:C:19:SER:N	1:C:22:LYS:HB2	2.34	0.42
1:D:7:LEU:O	1:D:85:ILE:HA	2.19	0.42
1:A:226:LEU:HB2	1:A:227:PRO:HD3	2.02	0.42
1:C:12:THR:HG23	1:C:25:TYR:CE2	2.55	0.41
1:C:11:GLY:C	1:C:27:VAL:HG13	2.40	0.41
1:A:121:MET:HG2	1:B:127:PHE:HB2	2.02	0.41
1:B:151:ASN:O	1:B:153:THR:HG23	2.19	0.41
1:B:207:LYS:HB3	1:B:207:LYS:HE3	1.94	0.41
1:D:41:GLN:CD	1:D:41:GLN:H	2.24	0.41
1:A:5:THR:HA	1:A:49:LYS:O	2.21	0.41
1:B:243:GLY:O	1:B:272:ARG:HG2	2.20	0.41
1:B:310:LEU:CD2	1:B:314:LYS:HD3	2.50	0.41
1:C:106:ASP:OD2	1:C:199:SER:OG	2.24	0.41
1:C:11:GLY:HA2	1:C:88:GLY:HA2	2.02	0.41
1:C:27:VAL:CG1	1:C:57:GLY:HA2	2.50	0.41
1:D:12:THR:C	1:D:15:GLY:H	2.24	0.41
1:A:121:MET:HE1	1:B:41:GLN:OE1	2.20	0.41
1:A:298:ASN:HB2	1:A:299:PRO:HD2	2.02	0.41
1:A:313:THR:OG1	1:A:314:LYS:N	2.54	0.41
1:B:207:LYS:HA	1:B:207:LYS:HD2	1.95	0.41
1:B:309:ALA:HB2	1:B:322:ILE:HG21	2.02	0.41
1:C:71:LYS:O	1:C:75:THR:HG23	2.21	0.41
1:C:12:THR:HB	1:C:114:ALA:O	2.21	0.41
1:B:151:ASN:ND2	3:B:338:HOH:O	2.54	0.41
1:A:310:LEU:HA	1:A:310:LEU:HD12	1.83	0.41
1:C:246:ASN:HD21	1:C:279:THR:HG21	1.86	0.41
1:A:224:SER:OG	1:A:226:LEU:HB2	2.19	0.41
1:C:73:ILE:HD11	1:C:85:ILE:HD11	2.02	0.41
1:D:32:VAL:O	1:D:35:LEU:HB2	2.21	0.40
1:C:157:GLY:O	1:C:301:LYS:NZ	2.54	0.40
1:C:13:ILE:HG13	3:C:401:HOH:O	2.20	0.40
1:C:17:GLY:CA	1:C:25:TYR:HB2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:MET:HE3	1:C:111:MET:CB	2.52	0.40
1:C:8:ALA:HA	1:C:86:THR:OG1	2.22	0.40
1:D:226:LEU:N	1:D:227:PRO:CD	2.84	0.40
1:A:321:GLN:O	1:A:325:GLN:HG3	2.21	0.40
1:B:191:ARG:HG3	3:C:329:HOH:O	2.20	0.40
1:C:19:SER:HB2	1:C:20:ALA:H	1.75	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	324/326 (99%)	314 (97%)	9 (3%)	1 (0%)	46	63
1	B	324/326 (99%)	313 (97%)	10 (3%)	1 (0%)	46	63
1	C	324/326 (99%)	306 (94%)	15 (5%)	3 (1%)	21	30
1	D	324/326 (99%)	314 (97%)	9 (3%)	1 (0%)	46	63
All	All	1296/1304 (99%)	1247 (96%)	43 (3%)	6 (0%)	34	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	32	VAL
1	C	15	GLY
1	C	198	THR
1	A	198	THR
1	B	198	THR
1	D	28	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	266/266 (100%)	246 (92%)	20 (8%)	17	26
1	B	266/266 (100%)	248 (93%)	18 (7%)	20	31
1	C	266/266 (100%)	236 (89%)	30 (11%)	7	10
1	D	266/266 (100%)	241 (91%)	25 (9%)	11	16
All	All	1064/1064 (100%)	971 (91%)	93 (9%)	13	19

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	41	GLN
1	A	42	LEU
1	A	99	LEU
1	A	112	VAL
1	A	139	LYS
1	A	147	LEU
1	A	163	THR
1	A	179	LEU
1	A	201	THR
1	A	202	PRO
1	A	222	ASN
1	A	226	LEU
1	A	254	PHE
1	A	267	VAL
1	A	272	ARG
1	A	288	LYS
1	A	308	LEU
1	A	310	LEU
1	A	318	GLN
1	B	1	LEU
1	B	4	ILE
1	B	7	LEU
1	B	21	THR

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Mol	Chain	Res	Type
1	B	29	LYS
1	B	99	LEU
1	B	133	VAL
1	B	147	LEU
1	B	153	THR
1	B	186	LYS
1	B	205	VAL
1	B	222	ASN
1	B	232	VAL
1	B	244	VAL
1	B	262	LYS
1	B	272	ARG
1	B	296	THR
1	B	306	LEU
1	C	1	LEU
1	C	32	VAL
1	C	39	VAL
1	C	42	LEU
1	C	53	VAL
1	C	68	THR
1	C	101	LEU
1	C	112	VAL
1	C	129	LEU
1	C	165	THR
1	C	195	ARG
1	C	202	PRO
1	C	211	LEU
1	C	213	LYS
1	C	222	ASN
1	C	226	LEU
1	C	239	ILE
1	C	240	VAL
1	C	249	LEU
1	C	254	PHE
1	C	255	ASP
1	C	259	THR
1	C	272	ARG
1	C	273	VAL
1	C	279	THR
1	C	296	THR
1	C	300	GLN
1	C	308	LEU

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Mol	Chain	Res	Type
1	C	316	PRO
1	C	321	GLN
1	D	4	ILE
1	D	18	ASP
1	D	19	SER
1	D	27	VAL
1	D	36	VAL
1	D	39	VAL
1	D	56	ILE
1	D	59	GLN
1	D	67	LEU
1	D	92	MET
1	D	101	LEU
1	D	102	THR
1	D	139	LYS
1	D	148	VAL
1	D	166	THR
1	D	184	ASN
1	D	195	ARG
1	D	209	ASN
1	D	211	LEU
1	D	213	LYS
1	D	222	ASN
1	D	262	LYS
1	D	279	THR
1	D	297	LEU
1	D	310	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	87	HIS
1	A	164	ASN
1	A	184	ASN
1	A	190	GLN
1	A	197	HIS
1	A	209	ASN
1	A	318	GLN
1	B	34	ASN
1	B	64	ASN
1	B	74	ASN

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Mol	Chain	Res	Type
1	B	131	ASN
1	B	151	ASN
1	B	197	HIS
1	B	219	ASN
1	B	248	ASN
1	C	24	ASN
1	C	52	GLN
1	C	55	ASN
1	C	64	ASN
1	C	131	ASN
1	C	219	ASN
1	C	318	GLN
1	C	320	GLN
1	C	324	ASN
1	D	24	ASN
1	D	59	GLN
1	D	131	ASN
1	D	151	ASN
1	D	190	GLN
1	D	197	HIS
1	D	219	ASN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	ASP	A	327	-	2,8,8	0.51	0	0,10,10	0.00	-
2	ASP	B	327	-	2,8,8	0.34	0	0,10,10	0.00	-
2	ASP	C	327	-	2,8,8	0.55	0	0,10,10	0.00	-
2	ASP	D	327	-	2,8,8	0.32	0	0,10,10	0.00	-

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	ASP	A	327	-	-	0/2/8/8	0/0/0/0
2	ASP	B	327	-	-	0/2/8/8	0/0/0/0
2	ASP	C	327	-	-	0/2/8/8	0/0/0/0
2	ASP	D	327	-	-	0/2/8/8	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	327	ASP	2	0
2	B	327	ASP	3	0
2	C	327	ASP	3	0
2	D	327	ASP	4	0

## 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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	326/326 (100%)	-1.02	0 <span>100</span> <span>100</span>	6, 19, 45, 61	0
1	B	326/326 (100%)	-1.06	3 (0%) <span>85</span> <span>85</span>	4, 16, 57, 83	0
1	C	326/326 (100%)	-0.86	13 (3%) <span>42</span> <span>43</span>	5, 18, 81, 105	0
1	D	326/326 (100%)	-1.03	2 (0%) <span>90</span> <span>90</span>	5, 17, 51, 70	0
All	All	1304/1304 (100%)	-0.99	18 (1%) <span>78</span> <span>77</span>	4, 17, 53, 105	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	19	SER	6.3
1	C	18	ASP	5.0
1	B	18	ASP	4.4
1	B	19	SER	4.4
1	C	26	THR	4.3
1	C	22	LYS	4.0
1	C	30	VAL	3.9
1	C	23	SER	3.9
1	C	29	LYS	3.6
1	C	20	ALA	3.4
1	C	21	THR	3.4
1	B	28	GLY	3.3
1	C	24	ASN	3.0
1	D	18	ASP	3.0
1	C	34	ASN	2.9
1	C	28	GLY	2.5
1	D	17	GLY	2.5
1	C	27	VAL	2.1



## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ASP	C	327	9/9	0.92	0.22	1.71	40,43,45,45	0
2	ASP	B	327	9/9	0.98	0.09	0.23	23,26,27,27	0
2	ASP	D	327	9/9	0.98	0.08	0.01	18,18,26,29	0
2	ASP	A	327	9/9	0.98	0.07	-0.04	18,19,21,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.