



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:41 PM GMT

PDB ID : 1GTM  
Title : STRUCTURE OF GLUTAMATE DEHYDROGENASE  
Authors : Yip, K.S.P.; Stillman, T.J.; Britton, K.L.; Pasquo, A.; Rice, D.W.  
Deposited on : 1996-08-22  
Resolution : 2.20 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

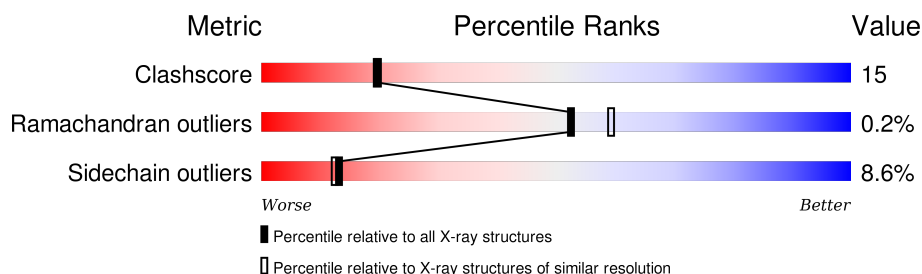
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	419	
1	B	419	
1	C	419	

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	SO4	A	421	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	420	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10224 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 GLUTAMATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3292	2107	554	618	13			
1	B	417	Total	C	N	O	S	0	0	0
			3292	2107	554	618	13			
1	C	417	Total	C	N	O	S	0	0	0
			3292	2107	554	618	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	GLN	CONFLICT	UNP P80319
B	3	ALA	GLN	CONFLICT	UNP P80319
C	3	ALA	GLN	CONFLICT	UNP P80319

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

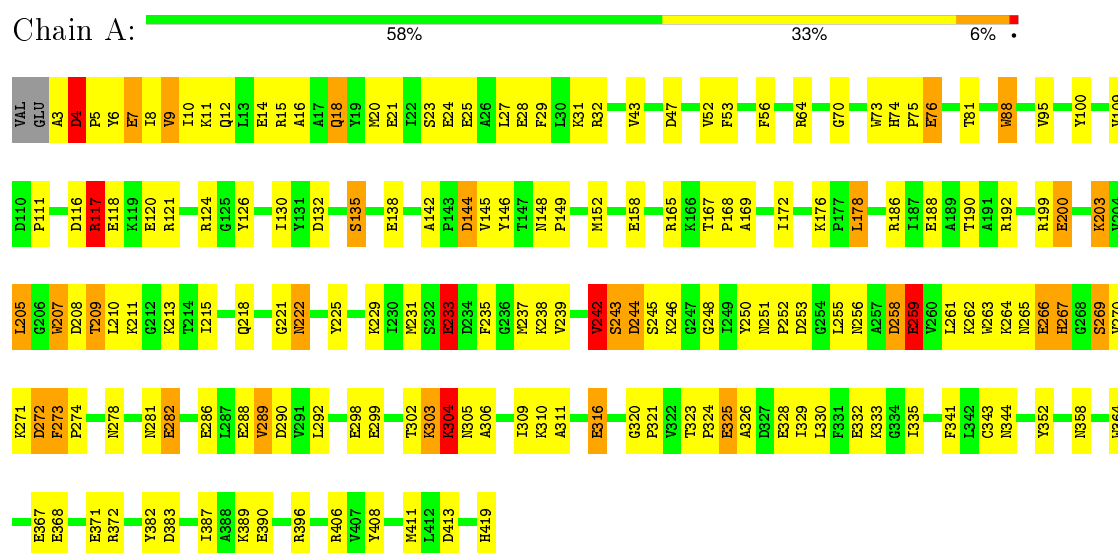
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	107	Total O 107 107	0	0
3	B	112	Total O 112 112	0	0
3	C	99	Total O 99 99	0	0

### 3 Residue-property plots

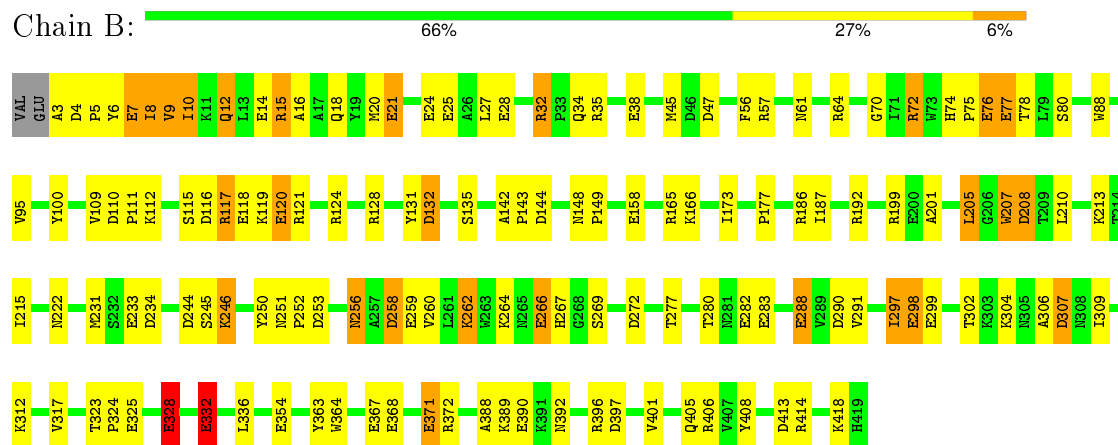
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

#### • Molecule 1: GLUTAMATE DEHYDROGENASE



#### • Molecule 1: GLUTAMATE DEHYDROGENASE



#### • Molecule 1: GLUTAMATE DEHYDROGENASE



VAL	GLU	A3	D4	P5	Y6	E7	I8	V9	I10	K11	Q12	L13	E14	R15		Q18	Y19	M20	E21	E24	E25	E28		R32	E38		D47		F56		R64		G69	G70	I71	R72	W73	H74	P75	E76	E77	I78	L79		K83		W88		V95	W96	D97		G103		K112																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
S115	D116	R117	E118	K119	E120	R121		R128		S135	P136	Y137	E138		A142	P143	D144	W145	Y146	T147	N148	P149	M156	D157	E158	Y159	E160		R165		A169		I172		I180		R186		E200		L205	G206	W207	D208	T209	L210	K211		I215	A216	I217	W222	A223		M231	S232	E233																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
D234	F235	Y242	S243	D244	S245	K246		Y250	N251	P252	D253		N256	A257	D258	E259		E266		S269		D272		I279	T280	N281	E282	E283		E286	L287	E288		V291		P294		I297	E298	E299	V300		K303	K304	N305	A306	D307		K310		A315	E316		P321	W322	T323	P324	E325																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
A326	D327	E328		E332	I338	P339	D340		C343		T349		Y363	W364	T365	I366	E367	E368		E371	R372		M377		Y385	N386	I387	A388	K389	E390		R396	D397	Y400		Q405	R406		D413		K418	H419																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				</

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.20 Å   167.20 Å   172.90 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	93.2 (10.00-2.20)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10224	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.99	25/3365 (0.7%)	1.65	53/4560 (1.2%)
1	B	0.99	26/3365 (0.8%)	1.71	73/4560 (1.6%)
1	C	1.00	26/3365 (0.8%)	1.69	58/4560 (1.3%)
All	All	0.99	77/10095 (0.8%)	1.68	184/13680 (1.3%)

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	282	GLU	CD-OE2	8.64	1.35	1.25
1	A	282	GLU	CD-OE1	8.25	1.34	1.25
1	B	7	GLU	CD-OE2	8.24	1.34	1.25
1	B	282	GLU	CD-OE1	7.84	1.34	1.25
1	C	371	GLU	CD-OE2	7.78	1.34	1.25
1	C	266	GLU	CD-OE1	7.70	1.34	1.25
1	C	325	GLU	CD-OE2	7.62	1.34	1.25
1	C	328	GLU	CD-OE1	7.61	1.34	1.25
1	C	7	GLU	CD-OE1	7.46	1.33	1.25
1	C	14	GLU	CD-OE2	7.29	1.33	1.25
1	A	14	GLU	CD-OE1	7.27	1.33	1.25
1	B	371	GLU	CD-OE2	7.26	1.33	1.25
1	C	390	GLU	CD-OE1	7.24	1.33	1.25
1	A	266	GLU	CD-OE1	7.21	1.33	1.25
1	B	259	GLU	CD-OE1	7.18	1.33	1.25
1	B	21	GLU	CD-OE1	6.96	1.33	1.25
1	A	328	GLU	CD-OE1	6.92	1.33	1.25
1	A	259	GLU	CD-OE1	6.84	1.33	1.25
1	A	24	GLU	CD-OE1	6.78	1.33	1.25
1	A	288	GLU	CD-OE2	6.69	1.33	1.25
1	C	367	GLU	CD-OE2	6.68	1.32	1.25
1	B	233	GLU	CD-OE2	6.66	1.32	1.25
1	A	299	GLU	CD-OE1	6.63	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	390	GLU	CD-OE2	6.59	1.32	1.25
1	C	233	GLU	CD-OE2	6.54	1.32	1.25
1	C	283	GLU	CD-OE1	6.51	1.32	1.25
1	B	14	GLU	CD-OE1	6.49	1.32	1.25
1	B	24	GLU	CD-OE2	6.45	1.32	1.25
1	A	325	GLU	CD-OE2	6.43	1.32	1.25
1	A	7	GLU	CD-OE1	6.41	1.32	1.25
1	A	233	GLU	CD-OE2	6.35	1.32	1.25
1	B	328	GLU	CD-OE1	6.30	1.32	1.25
1	C	286	GLU	CD-OE1	6.29	1.32	1.25
1	B	332	GLU	CD-OE2	6.28	1.32	1.25
1	C	158	GLU	CD-OE2	6.28	1.32	1.25
1	B	76	GLU	CD-OE2	6.25	1.32	1.25
1	C	298	GLU	CD-OE1	6.18	1.32	1.25
1	A	368	GLU	CD-OE1	6.14	1.32	1.25
1	B	38	GLU	CD-OE2	6.12	1.32	1.25
1	A	76	GLU	CD-OE2	6.11	1.32	1.25
1	B	28	GLU	CD-OE1	6.10	1.32	1.25
1	B	354	GLU	CD-OE1	6.09	1.32	1.25
1	C	332	GLU	CD-OE2	6.08	1.32	1.25
1	C	288	GLU	CD-OE2	6.07	1.32	1.25
1	C	259	GLU	CD-OE2	6.06	1.32	1.25
1	C	21	GLU	CD-OE1	6.04	1.32	1.25
1	A	332	GLU	CD-OE1	5.99	1.32	1.25
1	C	368	GLU	CD-OE1	5.99	1.32	1.25
1	B	299	GLU	CD-OE1	5.94	1.32	1.25
1	C	24	GLU	CD-OE1	5.78	1.32	1.25
1	B	266	GLU	CD-OE1	5.74	1.31	1.25
1	A	371	GLU	CD-OE1	5.63	1.31	1.25
1	B	298	GLU	CD-OE2	5.62	1.31	1.25
1	B	368	GLU	CD-OE1	5.57	1.31	1.25
1	A	200	GLU	CD-OE1	5.54	1.31	1.25
1	B	325	GLU	CD-OE2	5.52	1.31	1.25
1	B	120	GLU	CD-OE2	-5.49	1.19	1.25
1	B	158	GLU	CD-OE2	5.48	1.31	1.25
1	C	76	GLU	CD-OE2	5.45	1.31	1.25
1	A	367	GLU	CD-OE2	5.43	1.31	1.25
1	B	288	GLU	CD-OE1	5.43	1.31	1.25
1	C	77	GLU	CD-OE1	5.40	1.31	1.25
1	A	188	GLU	CD-OE1	5.38	1.31	1.25
1	B	77	GLU	CD-OE2	5.37	1.31	1.25
1	C	200	GLU	CD-OE1	5.33	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	390	GLU	CD-OE1	5.30	1.31	1.25
1	C	38	GLU	CD-OE2	5.28	1.31	1.25
1	B	367	GLU	CD-OE2	5.23	1.31	1.25
1	A	158	GLU	CD-OE1	-5.22	1.20	1.25
1	C	28	GLU	CD-OE1	5.21	1.31	1.25
1	C	160	GLU	CD-OE2	5.18	1.31	1.25
1	B	118	GLU	CD-OE1	5.16	1.31	1.25
1	A	298	GLU	CD-OE2	5.16	1.31	1.25
1	A	21	GLU	CD-OE2	5.12	1.31	1.25
1	A	158	GLU	CD-OE2	5.10	1.31	1.25
1	A	316	GLU	CD-OE1	5.04	1.31	1.25
1	A	28	GLU	CD-OE1	5.02	1.31	1.25

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	ARG	NE-CZ-NH1	16.34	128.47	120.30
1	A	64	ARG	NE-CZ-NH2	-15.60	112.50	120.30
1	B	64	ARG	NE-CZ-NH2	-15.24	112.68	120.30
1	C	406	ARG	NE-CZ-NH1	13.17	126.89	120.30
1	B	64	ARG	NE-CZ-NH1	12.90	126.75	120.30
1	C	157	ASP	CB-CG-OD2	12.46	129.51	118.30
1	C	64	ARG	NE-CZ-NH2	-11.98	114.31	120.30
1	A	165	ARG	NE-CZ-NH1	-11.74	114.43	120.30
1	C	64	ARG	NE-CZ-NH1	11.70	126.15	120.30
1	A	406	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	B	186	ARG	NE-CZ-NH2	-11.20	114.70	120.30
1	C	208	ASP	CB-CG-OD1	11.13	128.32	118.30
1	A	121	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	B	144	ASP	CB-CG-OD1	11.00	128.20	118.30
1	B	208	ASP	CB-CG-OD1	10.99	128.19	118.30
1	B	132	ASP	CB-CG-OD1	-10.50	108.85	118.30
1	C	406	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	A	32	ARG	NE-CZ-NH1	10.39	125.49	120.30
1	B	186	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	A	406	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	C	396	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	C	121	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	B	121	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	B	372	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	C	157	ASP	CB-CG-OD1	-9.72	109.55	118.30
1	B	132	ASP	CB-CG-OD2	9.65	126.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	ARG	NE-CZ-NH1	9.43	125.01	120.30
1	C	413	ASP	CB-CG-OD2	9.38	126.74	118.30
1	A	186	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	C	186	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	B	363	TYR	CB-CG-CD2	-8.70	115.78	121.00
1	C	244	ASP	CB-CG-OD1	-8.70	110.47	118.30
1	B	18	GLN	CB-CA-C	-8.66	93.08	110.40
1	B	165	ARG	NE-CZ-NH1	-8.63	115.99	120.30
1	C	128	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	C	4	ASP	CB-CG-OD1	8.38	125.84	118.30
1	C	116	ASP	CB-CG-OD1	-8.32	110.81	118.30
1	C	253	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	A	47	ASP	CB-CG-OD1	-8.26	110.87	118.30
1	B	406	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	B	414	ARG	NE-CZ-NH1	-8.03	116.28	120.30
1	B	244	ASP	CB-CG-OD1	-8.02	111.08	118.30
1	C	128	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	C	307	ASP	CB-CG-OD1	7.96	125.47	118.30
1	A	117	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	A	186	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	C	397	ASP	CB-CG-OD1	-7.89	111.20	118.30
1	C	307	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	A	244	ASP	CB-CG-OD1	-7.70	111.37	118.30
1	C	121	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	B	72	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	B	72	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	C	272	ASP	CB-CG-OD1	7.57	125.12	118.30
1	B	208	ASP	CB-CG-OD2	-7.56	111.49	118.30
1	A	408	TYR	CB-CG-CD1	7.41	125.44	121.00
1	B	32	ARG	CD-NE-CZ	7.41	133.97	123.60
1	A	267	HIS	CA-CB-CG	-7.39	101.04	113.60
1	B	144	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	B	290	ASP	CB-CG-OD1	-7.34	111.69	118.30
1	B	57	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	C	72	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	B	199	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	C	413	ASP	CB-CG-OD1	-7.21	111.81	118.30
1	C	4	ASP	CB-CG-OD2	-7.16	111.85	118.30
1	B	290	ASP	CB-CG-OD2	7.14	124.72	118.30
1	A	253	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	C	21	GLU	N-CA-CB	7.02	123.23	110.60
1	B	372	ARG	NE-CZ-NH2	-6.86	116.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ASP	CB-CG-OD1	-6.84	112.14	118.30
1	C	116	ASP	CB-CG-OD2	6.83	124.45	118.30
1	C	327	ASP	CB-CG-OD2	6.80	124.42	118.30
1	B	307	ASP	CB-CG-OD1	-6.79	112.19	118.30
1	C	144	ASP	CB-CG-OD1	6.77	124.40	118.30
1	B	406	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	253	ASP	CB-CG-OD2	6.67	124.31	118.30
1	A	64	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	A	20	MET	CG-SD-CE	-6.63	89.59	100.20
1	C	15	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	B	15	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	272	ASP	CB-CG-OD1	6.54	124.18	118.30
1	C	47	ASP	CB-CG-OD1	-6.49	112.46	118.30
1	B	272	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	B	253	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	B	397	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	16	ALA	CB-CA-C	-6.37	100.55	110.10
1	A	209	THR	N-CA-CB	6.31	122.28	110.30
1	A	383	ASP	CB-CG-OD1	-6.30	112.63	118.30
1	B	413	ASP	CB-CG-OD1	-6.26	112.67	118.30
1	A	135	SER	N-CA-CB	6.24	119.86	110.50
1	B	234	ASP	CB-CG-OD2	6.24	123.92	118.30
1	C	282	GLU	CB-CA-C	6.23	122.86	110.40
1	B	397	ASP	CB-CG-OD1	-6.23	112.70	118.30
1	A	152	MET	CG-SD-CE	6.23	110.16	100.20
1	B	131	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	B	372	ARG	CA-CB-CG	-6.17	99.82	113.40
1	B	7	GLU	CB-CA-C	-6.13	98.13	110.40
1	B	332	GLU	CB-CA-C	-6.10	98.20	110.40
1	C	327	ASP	CB-CG-OD1	-6.06	112.84	118.30
1	C	6	TYR	CB-CG-CD2	6.03	124.62	121.00
1	B	396	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	C	208	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	C	258	ASP	CB-CG-OD1	-5.95	112.94	118.30
1	C	147	THR	CA-CB-CG2	-5.95	104.08	112.40
1	A	190	THR	CA-CB-CG2	-5.93	104.09	112.40
1	B	317	VAL	CA-CB-CG2	-5.92	102.03	110.90
1	C	234	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	207	TRP	O-C-N	5.91	132.15	122.70
1	B	207	TRP	N-CA-CB	5.89	121.20	110.60
1	C	371	GLU	N-CA-CB	5.88	121.18	110.60
1	C	97	ASP	CB-CG-OD2	5.86	123.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	ARG	NE-CZ-NH2	5.85	123.23	120.30
1	B	272	ASP	CB-CG-OD1	5.85	123.56	118.30
1	B	207	TRP	CA-C-N	-5.84	104.34	117.20
1	C	32	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	118	GLU	CG-CD-OE2	5.80	129.90	118.30
1	B	258	ASP	CB-CG-OD2	5.79	123.51	118.30
1	C	244	ASP	CB-CG-OD2	5.77	123.49	118.30
1	B	408	TYR	CB-CG-CD1	5.76	124.45	121.00
1	A	273	PHE	CB-CG-CD1	-5.76	116.77	120.80
1	B	298	GLU	CB-CG-CD	-5.74	98.71	114.20
1	C	400	TYR	CB-CG-CD1	-5.71	117.58	121.00
1	C	207	TRP	N-CA-CB	5.67	120.81	110.60
1	A	116	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	C	332	GLU	CA-CB-CG	-5.66	100.96	113.40
1	C	258	ASP	CB-CG-OD2	5.65	123.39	118.30
1	C	272	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	B	35	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	C	244	ASP	CB-CA-C	5.61	121.62	110.40
1	A	413	ASP	CB-CG-OD2	5.56	123.30	118.30
1	C	298	GLU	CA-C-N	-5.55	104.99	117.20
1	A	408	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	B	7	GLU	C-N-CA	-5.54	107.86	121.70
1	A	382	TYR	CA-CB-CG	-5.51	102.93	113.40
1	A	52	VAL	CA-CB-CG2	-5.50	102.65	110.90
1	A	269	SER	N-CA-CB	5.49	118.74	110.50
1	A	192	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	100	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	B	131	TYR	CB-CG-CD1	5.44	124.26	121.00
1	C	372	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	14	GLU	CA-CB-CG	-5.38	101.56	113.40
1	A	244	ASP	N-CA-CB	5.38	120.29	110.60
1	B	332	GLU	CB-CG-CD	-5.36	99.72	114.20
1	B	277	THR	CA-CB-CG2	-5.35	104.91	112.40
1	B	128	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	192	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	124	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	116	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	4	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	117	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	207	TRP	N-CA-CB	5.28	120.11	110.60
1	A	258	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	C	137	TYR	CB-CG-CD1	-5.28	117.83	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	138	GLU	CG-CD-OE2	5.25	128.80	118.30
1	B	124	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	100	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	A	178	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	C	47	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	266	GLU	CB-CG-CD	-5.23	100.08	114.20
1	A	124	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	121	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	56	PHE	CB-CA-C	-5.20	100.00	110.40
1	B	165	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	C	377	MET	CG-SD-CE	5.19	108.51	100.20
1	A	9	VAL	N-CA-CB	-5.18	100.10	111.50
1	C	349	THR	CA-CB-CG2	-5.18	105.14	112.40
1	B	124	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	32	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	B	32	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
1	A	352	TYR	CB-CG-CD2	5.09	124.06	121.00
1	C	396	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	233	GLU	C-N-CA	-5.08	109.00	121.70
1	B	177	PRO	N-CA-CB	5.08	109.39	103.30
1	B	234	ASP	N-CA-CB	5.07	119.73	110.60
1	B	128	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	144	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	396	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	B	187	ILE	CG1-CB-CG2	-5.04	100.30	111.40
1	B	78	THR	CA-CB-CG2	-5.04	105.35	112.40
1	C	9	VAL	N-CA-CB	-5.04	100.42	111.50
1	A	242	VAL	N-CA-CB	5.03	122.57	111.50
1	C	253	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	4	ASP	CB-CG-OD1	-5.02	113.78	118.30
1	A	81	THR	CA-CB-CG2	-5.01	105.39	112.40

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	3292	0	3290	109	0
1	B	3292	0	3290	89	0
1	C	3292	0	3290	97	0
2	A	10	0	0	3	0
2	B	10	0	0	0	0
2	C	10	0	0	3	0
3	A	107	0	0	0	0
3	B	112	0	0	0	0
3	C	99	0	0	0	0
All	All	10224	0	9870	294	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 (294) 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:8:ILE:CD1	1:B:9:VAL:N	1.99	1.25
1:B:8:ILE:HD12	1:B:9:VAL:N	1.52	1.23
1:B:8:ILE:HD13	1:B:8:ILE:C	1.55	1.19
1:B:8:ILE:CD1	1:B:8:ILE:C	2.03	1.18
1:A:25:GLU:OE1	1:A:419:HIS:HD2	1.28	1.16
1:A:3:ALA:O	1:A:5:PRO:HD2	1.52	1.07
1:B:3:ALA:O	1:B:7:GLU:N	1.93	1.00
1:C:4:ASP:O	1:C:7:GLU:HB3	1.62	0.99
1:A:256:ASN:ND2	1:A:259:GLU:H	1.61	0.98
1:C:10:ILE:HD13	1:C:10:ILE:H	1.30	0.94
1:A:323:THR:HB	1:A:324:PRO:HD2	1.51	0.93
1:A:25:GLU:OE1	1:A:419:HIS:CD2	2.21	0.93
1:B:8:ILE:HD12	1:B:9:VAL:H	1.34	0.92
1:B:12:GLN:HE21	1:B:12:GLN:HA	1.32	0.92
1:A:148:ASN:HB2	1:A:149:PRO:HD2	1.53	0.90
1:A:286:GLU:O	1:A:310:LYS:NZ	2.05	0.90
1:A:256:ASN:HD22	1:A:259:GLU:HB2	1.37	0.90
1:C:10:ILE:HD13	1:C:10:ILE:N	1.86	0.90
1:C:250:TYR:CZ	1:C:252:PRO:HG3	2.08	0.89
1:C:385:TYR:OH	1:C:389:LYS:HE3	1.73	0.89
1:C:3:ALA:O	1:C:4:ASP:C	2.11	0.88
1:B:117:ARG:HA	1:B:117:ARG:NE	1.89	0.88
1:B:258:ASP:O	1:B:262:LYS:HG3	1.73	0.87
1:C:8:ILE:HG22	1:C:9:VAL:N	1.88	0.87
1:C:4:ASP:HB3	1:C:5:PRO:HD3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:THR:HB	1:B:324:PRO:HD2	1.59	0.84
1:B:8:ILE:HD13	1:B:9:VAL:N	1.77	0.84
1:C:5:PRO:O	1:C:8:ILE:HB	1.78	0.83
1:B:3:ALA:O	1:B:6:TYR:N	2.13	0.82
1:C:10:ILE:CD1	1:C:10:ILE:N	2.41	0.82
1:B:4:ASP:O	1:B:8:ILE:HG23	1.79	0.82
1:A:3:ALA:O	1:A:5:PRO:CD	2.27	0.81
1:A:326:ALA:O	1:A:330:LEU:HG	1.81	0.81
1:A:243:SER:OG	1:A:281:ASN:ND2	2.13	0.80
1:A:272:ASP:O	1:A:273:PHE:C	2.21	0.77
1:C:9:VAL:HG12	1:C:10:ILE:CD1	2.16	0.76
1:B:12:GLN:NE2	1:B:12:GLN:HA	2.00	0.76
1:C:117:ARG:HA	1:C:117:ARG:NE	2.00	0.76
1:C:148:ASN:HB2	1:C:149:PRO:HD2	1.66	0.76
1:C:79:LEU:O	1:C:83:LYS:HG3	1.86	0.75
1:B:245:SER:OG	1:B:246:LYS:HE3	1.86	0.75
1:C:3:ALA:C	1:C:5:PRO:HD2	2.06	0.75
1:A:256:ASN:ND2	1:A:259:GLU:HB2	2.01	0.75
1:B:12:GLN:HE21	1:B:12:GLN:CA	1.98	0.75
1:A:256:ASN:HD22	1:A:259:GLU:H	1.31	0.75
1:C:25:GLU:OE2	1:C:419:HIS:ND1	2.19	0.73
1:C:3:ALA:O	1:C:5:PRO:N	2.21	0.73
1:B:148:ASN:HB2	1:B:149:PRO:HD2	1.71	0.73
1:A:4:ASP:HB3	1:A:5:PRO:HD3	1.70	0.73
1:A:329:ILE:O	1:A:333:LYS:HG3	1.89	0.73
1:A:229:LYS:O	1:A:233:GLU:HG3	1.89	0.73
1:C:117:ARG:HA	1:C:117:ARG:HE	1.53	0.72
1:B:8:ILE:C	1:B:8:ILE:HD12	1.89	0.72
1:C:368:GLU:O	1:C:372:ARG:HG3	1.89	0.72
1:A:221:GLY:HA3	2:A:421:SO4:O2	1.90	0.71
1:A:316:GLU:O	1:A:343:CYS:HB3	1.90	0.71
1:B:148:ASN:HB2	1:B:149:PRO:CD	2.20	0.71
1:A:9:VAL:HG12	1:A:10:ILE:N	2.04	0.71
1:A:6:TYR:O	1:A:10:ILE:HD12	1.92	0.69
1:C:148:ASN:HB2	1:C:149:PRO:CD	2.21	0.69
1:B:250:TYR:CE2	1:B:252:PRO:HG3	2.27	0.69
1:C:3:ALA:O	1:C:6:TYR:N	2.26	0.69
1:C:9:VAL:HG12	1:C:10:ILE:HD13	1.75	0.68
1:A:244:ASP:OD2	1:A:270:VAL:HG22	1.93	0.68
1:A:323:THR:HB	1:A:324:PRO:CD	2.22	0.67
1:A:148:ASN:HB2	1:A:149:PRO:CD	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LYS:HG3	1:A:278:ASN:HD21	1.59	0.67
1:B:74:HIS:HE1	1:B:76:GLU:HB2	1.60	0.67
1:C:3:ALA:O	1:C:5:PRO:HD2	1.95	0.67
1:B:74:HIS:CE1	1:B:76:GLU:HB2	2.30	0.67
1:C:280:THR:HB	1:C:282:GLU:HG2	1.77	0.67
1:C:3:ALA:O	1:C:5:PRO:CD	2.42	0.66
1:B:74:HIS:CD2	1:B:75:PRO:HD2	2.31	0.66
1:C:3:ALA:HB3	1:C:6:TYR:HB3	1.76	0.65
1:B:117:ARG:HA	1:B:117:ARG:HE	1.61	0.65
1:C:305:ASN:O	1:C:306:ALA:C	2.34	0.65
1:C:244:ASP:OD2	1:C:269:SER:HA	1.96	0.65
1:C:3:ALA:CB	1:C:6:TYR:HB3	2.27	0.65
1:A:213:LYS:HB3	1:A:290:ASP:OD2	1.97	0.65
1:A:263:TRP:CZ3	1:A:274:PRO:HD3	2.31	0.65
1:A:282:GLU:O	1:A:286:GLU:HG3	1.96	0.64
1:A:258:ASP:O	1:A:261:LEU:HB3	1.98	0.64
1:C:385:TYR:CZ	1:C:389:LYS:HE3	2.33	0.64
1:A:88:TRP:CZ3	1:A:341:PHE:HB3	2.34	0.63
1:A:243:SER:HA	1:A:248:GLY:HA2	1.82	0.62
1:C:223:ALA:N	2:C:420:SO4:O3	2.28	0.62
1:B:8:ILE:O	1:B:8:ILE:HD13	1.97	0.61
1:C:6:TYR:O	1:C:9:VAL:HB	2.00	0.61
1:C:4:ASP:HB3	1:C:5:PRO:CD	2.27	0.61
1:B:266:GLU:HB2	1:B:267:HIS:ND1	2.14	0.61
1:A:289:VAL:O	1:A:311:ALA:HA	2.00	0.61
1:A:305:ASN:O	1:A:309:ILE:HD12	2.01	0.60
1:C:297:ILE:HD12	1:C:298:GLU:O	2.01	0.60
1:B:4:ASP:HB3	1:B:5:PRO:HD3	1.83	0.60
1:A:117:ARG:NE	1:A:117:ARG:HA	2.17	0.60
1:C:316:GLU:HB2	1:C:338:ILE:O	2.01	0.60
1:C:115:SER:O	1:C:119:LYS:HG3	2.02	0.59
1:B:302:THR:O	1:B:306:ALA:HB2	2.01	0.59
1:B:4:ASP:N	1:B:5:PRO:HD2	2.18	0.59
1:A:4:ASP:O	1:A:8:ILE:CD1	2.51	0.59
1:B:3:ALA:O	1:B:6:TYR:CA	2.51	0.59
1:B:207:TRP:CD1	1:B:207:TRP:N	2.69	0.58
1:C:8:ILE:O	1:C:11:LYS:HB2	2.04	0.58
1:C:207:TRP:N	1:C:207:TRP:CD1	2.71	0.58
1:B:8:ILE:HD11	1:B:9:VAL:HG23	1.84	0.58
1:A:74:HIS:HE1	1:A:76:GLU:CG	2.16	0.58
1:B:16:ALA:O	1:B:20:MET:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:CG1	1:A:10:ILE:N	2.66	0.58
1:C:74:HIS:CG	1:C:75:PRO:HD2	2.38	0.58
1:C:74:HIS:CE1	1:C:76:GLU:H	2.21	0.58
1:C:206:GLY:O	1:C:207:TRP:C	2.40	0.57
1:B:9:VAL:HG12	1:B:10:ILE:HD12	1.87	0.57
1:B:6:TYR:O	1:B:9:VAL:HB	2.05	0.57
1:A:311:ALA:O	1:A:335:ILE:HG12	2.05	0.57
1:A:244:ASP:CG	1:A:270:VAL:HG22	2.25	0.57
1:A:256:ASN:HD21	1:A:259:GLU:H	1.49	0.57
1:A:74:HIS:CG	1:A:75:PRO:HD2	2.40	0.56
1:B:297:ILE:HD13	1:B:297:ILE:H	1.69	0.56
1:B:10:ILE:CD1	1:B:10:ILE:N	2.69	0.56
1:A:200:GLU:OE2	1:A:203:LYS:NZ	2.38	0.56
1:C:4:ASP:O	1:C:7:GLU:CB	2.46	0.55
1:A:256:ASN:HD22	1:A:259:GLU:N	2.04	0.55
1:C:250:TYR:CE2	1:C:252:PRO:HG3	2.42	0.55
1:B:5:PRO:O	1:B:8:ILE:CD1	2.55	0.55
1:C:169:ALA:O	1:C:172:ILE:HG22	2.07	0.55
1:A:251:ASN:C	1:A:251:ASN:OD1	2.44	0.54
1:B:323:THR:HB	1:B:324:PRO:CD	2.35	0.54
1:A:176:LYS:HZ2	1:A:358:ASN:ND2	2.05	0.54
1:C:73:TRP:O	1:C:146:TYR:HD2	1.90	0.54
1:B:25:GLU:OE2	1:B:418:LYS:N	2.37	0.54
1:A:209:THR:OG1	1:A:210:LEU:N	2.40	0.54
1:B:280:THR:OG1	1:B:283:GLU:HG3	2.08	0.53
1:C:6:TYR:O	1:C:10:ILE:HD13	2.09	0.53
1:A:271:LYS:HG3	1:A:278:ASN:ND2	2.23	0.52
1:A:176:LYS:HZ2	1:A:358:ASN:HD21	1.57	0.52
1:A:207:TRP:N	1:A:207:TRP:CD1	2.77	0.52
1:A:256:ASN:HD22	1:A:259:GLU:CB	2.17	0.52
1:A:305:ASN:O	1:A:309:ILE:CD1	2.57	0.52
1:A:23:SER:OG	1:A:419:HIS:OXT	2.18	0.52
1:B:323:THR:CB	1:B:324:PRO:CD	2.88	0.52
1:C:323:THR:HB	1:C:324:PRO:HD2	1.90	0.52
1:C:9:VAL:O	1:C:10:ILE:C	2.47	0.52
1:A:4:ASP:O	1:A:8:ILE:HD13	2.10	0.52
1:B:10:ILE:HD13	1:B:10:ILE:H	1.76	0.51
1:A:4:ASP:O	1:A:8:ILE:HD12	2.10	0.51
1:A:323:THR:CB	1:A:324:PRO:CD	2.80	0.51
1:B:109:VAL:O	1:B:111:PRO:HD3	2.11	0.51
1:C:215:ILE:HA	1:C:291:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:MET:HE3	1:B:405:GLN:HG3	1.93	0.50
1:A:109:VAL:O	1:A:111:PRO:HD3	2.10	0.50
1:B:166:LYS:NZ	1:C:138:GLU:OE1	2.40	0.50
1:C:246:LYS:HG3	1:C:269:SER:HB2	1.93	0.50
1:A:302:THR:OG1	1:A:304:LYS:HG3	2.11	0.50
1:A:221:GLY:CA	2:A:421:SO4:O2	2.59	0.50
1:A:251:ASN:HB3	1:A:255:LEU:HD21	1.92	0.50
1:B:12:GLN:NE2	1:B:12:GLN:CA	2.67	0.50
1:A:221:GLY:O	1:A:225:TYR:HB3	2.11	0.50
1:B:215:ILE:HA	1:B:291:VAL:O	2.12	0.50
1:B:8:ILE:HD13	1:B:9:VAL:CA	2.40	0.50
1:B:8:ILE:CD1	1:B:9:VAL:CA	2.87	0.49
1:A:320:GLY:N	1:A:321:PRO:CD	2.75	0.49
1:A:218:GLN:HG3	1:A:281:ASN:HD22	1.76	0.49
1:B:364:TRP:N	1:B:364:TRP:CD1	2.80	0.49
1:C:256:ASN:HB3	1:C:259:GLU:CD	2.33	0.49
1:A:117:ARG:HA	1:A:117:ARG:HE	1.77	0.49
1:A:176:LYS:NZ	1:A:358:ASN:HD21	2.10	0.49
1:B:262:LYS:O	1:B:266:GLU:HG3	2.13	0.49
1:B:256:ASN:O	1:B:260:VAL:HG23	2.12	0.49
1:B:9:VAL:O	1:B:10:ILE:C	2.45	0.49
1:C:142:ALA:HB1	1:C:143:PRO:HD2	1.95	0.49
1:A:15:ARG:O	1:A:18:GLN:N	2.36	0.49
1:C:77:GLU:HA	1:C:77:GLU:OE1	2.13	0.48
1:A:74:HIS:CD2	1:A:75:PRO:HD2	2.48	0.48
1:A:344:ASN:C	1:A:344:ASN:OD1	2.51	0.48
1:B:7:GLU:O	1:B:8:ILE:C	2.49	0.48
1:B:110:ASP:OD1	1:B:112:LYS:HG3	2.13	0.48
1:B:4:ASP:N	1:B:5:PRO:CD	2.77	0.47
1:B:5:PRO:O	1:B:8:ILE:HG13	2.14	0.47
1:A:306:ALA:HA	1:A:309:ILE:HD13	1.95	0.47
1:C:390:GLU:HG2	1:C:390:GLU:O	2.14	0.47
1:B:388:ALA:O	1:B:392:ASN:N	2.47	0.47
1:A:271:LYS:O	1:A:272:ASP:HB2	2.14	0.47
1:A:222:ASN:N	2:A:421:SO4:O2	2.47	0.47
1:C:12:GLN:HG2	1:C:13:LEU:N	2.29	0.47
1:B:267:HIS:N	1:B:267:HIS:ND1	2.63	0.47
1:B:210:LEU:HA	1:B:213:LYS:HG3	1.97	0.47
1:B:5:PRO:O	1:B:8:ILE:HD12	2.14	0.47
1:A:250:TYR:CE2	1:A:252:PRO:HG3	2.49	0.47
1:C:70:GLY:HA2	1:C:142:ALA:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LEU:HA	1:B:205:LEU:HD12	1.60	0.47
1:A:167:THR:OG1	1:A:168:PRO:HD2	2.15	0.47
1:A:263:TRP:CH2	1:A:274:PRO:HD3	2.50	0.47
1:A:126:TYR:O	1:A:130:ILE:HG12	2.15	0.47
1:C:222:ASN:N	2:C:420:SO4:O3	2.48	0.47
1:A:251:ASN:HB3	1:A:255:LEU:CD2	2.45	0.47
1:B:72:ARG:NH2	1:B:77:GLU:OE1	2.45	0.47
1:B:250:TYR:CZ	1:B:252:PRO:HG3	2.49	0.46
1:C:256:ASN:CG	1:C:259:GLU:HG3	2.35	0.46
1:C:250:TYR:OH	1:C:252:PRO:HG3	2.13	0.46
1:B:74:HIS:CE1	1:B:76:GLU:H	2.34	0.46
1:B:117:ARG:NH2	1:B:120:GLU:OE1	2.48	0.46
1:B:4:ASP:O	1:B:7:GLU:HB2	2.15	0.46
1:C:305:ASN:O	1:C:307:ASP:N	2.49	0.46
1:C:69:GLY:HA3	1:C:103:GLY:O	2.16	0.46
1:C:20:MET:HE3	1:C:405:GLN:HG3	1.98	0.46
1:A:88:TRP:HZ3	1:A:341:PHE:HB3	1.79	0.46
1:A:309:ILE:HD12	1:A:309:ILE:N	2.31	0.46
1:B:297:ILE:HD13	1:B:297:ILE:N	2.30	0.46
1:A:250:TYR:O	1:A:251:ASN:HB2	2.16	0.46
1:C:10:ILE:HG22	1:C:14:GLU:OE2	2.16	0.46
1:A:169:ALA:O	1:A:172:ILE:HG22	2.16	0.46
1:B:309:ILE:N	1:B:309:ILE:HD12	2.31	0.46
1:C:231:MET:O	1:C:235:PHE:HB2	2.16	0.46
1:A:364:TRP:N	1:A:364:TRP:CD1	2.80	0.45
1:C:3:ALA:C	1:C:5:PRO:CD	2.82	0.45
1:C:9:VAL:HG12	1:C:10:ILE:HD12	1.96	0.45
1:C:74:HIS:ND1	1:C:76:GLU:N	2.56	0.45
1:B:10:ILE:CD1	1:B:10:ILE:H	2.29	0.45
1:A:251:ASN:HA	1:A:252:PRO:HD2	1.43	0.45
1:B:201:ALA:HB1	1:B:336:LEU:HD23	1.98	0.45
1:C:298:GLU:O	1:C:299:GLU:HB2	2.17	0.45
1:A:262:LYS:O	1:A:265:ASN:HB2	2.16	0.45
1:B:251:ASN:HA	1:B:252:PRO:HD3	1.55	0.45
1:C:222:ASN:CB	2:C:420:SO4:O3	2.65	0.45
1:A:29:PHE:HB3	1:A:411:MET:HE1	1.99	0.45
1:A:74:HIS:HE1	1:A:76:GLU:HG3	1.82	0.45
1:C:256:ASN:OD1	1:C:256:ASN:C	2.54	0.45
1:A:74:HIS:CE1	1:A:76:GLU:CG	2.97	0.44
1:C:363:TYR:CD1	1:C:363:TYR:N	2.85	0.44
1:A:43:VAL:HB	1:A:53:PHE:HE1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LYS:HG3	1:B:262:LYS:H	1.31	0.44
1:C:251:ASN:C	1:C:251:ASN:OD1	2.55	0.44
1:A:73:TRP:O	1:A:146:TYR:HD2	1.99	0.44
1:A:303:LYS:HE2	1:A:303:LYS:HB3	1.58	0.44
1:B:115:SER:O	1:B:119:LYS:N	2.46	0.44
1:C:366:ILE:O	1:C:366:ILE:HG13	2.17	0.44
1:B:45:MET:HB3	1:B:45:MET:HE3	1.80	0.44
1:A:290:ASP:OD1	1:A:290:ASP:N	2.48	0.44
1:C:32:ARG:NH1	1:C:32:ARG:HG3	2.33	0.43
1:B:70:GLY:HA2	1:B:142:ALA:O	2.18	0.43
1:C:15:ARG:O	1:C:18:GLN:HG2	2.18	0.43
1:C:298:GLU:HA	1:C:321:PRO:HA	1.99	0.43
1:B:280:THR:HG23	1:B:283:GLU:OE1	2.18	0.43
1:A:266:GLU:HB3	1:A:267:HIS:CE1	2.53	0.43
1:A:8:ILE:O	1:A:11:LYS:HB2	2.18	0.43
1:B:8:ILE:N	1:B:8:ILE:HD12	2.31	0.43
1:A:387:ILE:HD12	1:A:387:ILE:HG23	1.65	0.43
1:A:244:ASP:OD2	1:A:264:LYS:HE2	2.18	0.43
1:A:302:THR:O	1:A:306:ALA:N	2.48	0.43
1:A:3:ALA:O	1:A:5:PRO:N	2.51	0.43
1:B:401:VAL:O	1:B:405:GLN:HB2	2.19	0.43
1:C:251:ASN:HA	1:C:252:PRO:HD3	1.48	0.43
1:B:266:GLU:HB2	1:B:267:HIS:CE1	2.54	0.43
1:B:27:LEU:HA	1:B:27:LEU:HD23	1.76	0.43
1:A:205:LEU:HD12	1:A:205:LEU:HA	1.63	0.43
1:B:3:ALA:O	1:B:4:ASP:C	2.57	0.43
1:A:199:ARG:HA	1:A:210:LEU:HD11	1.99	0.43
1:B:3:ALA:O	1:B:6:TYR:C	2.53	0.42
1:C:280:THR:CB	1:C:282:GLU:HG2	2.48	0.42
1:C:387:ILE:HD12	1:C:387:ILE:HG21	1.62	0.42
1:C:305:ASN:C	1:C:307:ASP:N	2.68	0.42
1:A:231:MET:O	1:A:235:PHE:HB2	2.20	0.42
1:C:297:ILE:HD12	1:C:300:VAL:HG13	2.02	0.42
1:A:242:VAL:O	1:A:248:GLY:HA2	2.20	0.42
1:B:142:ALA:HB1	1:B:143:PRO:HD2	2.01	0.42
1:C:210:LEU:HA	1:C:210:LEU:HD23	1.77	0.42
1:C:3:ALA:HB1	1:C:6:TYR:CB	2.50	0.42
1:B:328:GLU:O	1:B:332:GLU:HG2	2.20	0.41
1:C:25:GLU:OE1	1:C:418:LYS:N	2.51	0.41
1:C:159:TYR:CG	1:C:172:ILE:HG12	2.56	0.41
1:A:70:GLY:HA2	1:A:142:ALA:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:PRO:HD2	1:C:315:ALA:O	2.20	0.41
1:A:144:ASP:O	1:A:145:VAL:C	2.56	0.41
1:C:217:ILE:O	1:C:242:VAL:HA	2.21	0.41
1:B:34:GLN:OE1	1:B:61:ASN:HA	2.21	0.41
1:C:156:MET:HE2	1:C:180:ILE:HD12	2.02	0.41
1:C:364:TRP:CD1	1:C:364:TRP:N	2.87	0.41
1:C:156:MET:CE	1:C:180:ILE:HD12	2.50	0.41
1:B:246:LYS:HG3	1:B:269:SER:HB2	2.03	0.41
1:A:239:VAL:O	1:A:255:LEU:HG	2.21	0.41
1:A:29:PHE:CG	1:A:411:MET:HE1	2.56	0.41
1:C:279:ILE:HG21	1:C:279:ILE:HD13	1.77	0.41
1:A:4:ASP:HB3	1:A:5:PRO:CD	2.44	0.40
1:A:148:ASN:CB	1:A:149:PRO:CD	2.88	0.40
1:C:256:ASN:OD1	1:C:259:GLU:HG3	2.21	0.40
1:C:387:ILE:HG23	1:C:387:ILE:HD13	1.75	0.40
1:A:215:ILE:HB	1:A:237:MET:HE1	2.02	0.40
1:A:269:SER:HB3	1:A:271:LYS:HB3	2.03	0.40
1:A:27:LEU:O	1:A:31:LYS:HG3	2.22	0.40
1:A:117:ARG:HH21	1:A:120:GLU:HB2	1.86	0.40
1:C:338:ILE:HG22	1:C:343:CYS:HB2	2.03	0.40
1:C:32:ARG:HH11	1:C:32:ARG:HG3	1.86	0.40
1:C:316:GLU:O	1:C:340:ASP:HA	2.22	0.40
1:B:173:ILE:HD13	1:B:173:ILE:HG21	1.80	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	415/419 (99%)	393 (95%)	20 (5%)	2 (0%)	34 35
1	B	415/419 (99%)	401 (97%)	14 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	415/419 (99%)	396 (95%)	18 (4%)	1 (0%)	52	59
All	All	1245/1257 (99%)	1190 (96%)	52 (4%)	3 (0%)	52	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	C	4	ASP
1	A	304	LYS

### 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	343/345 (99%)	314 (92%)	29 (8%)	13	13
1	B	343/345 (99%)	312 (91%)	31 (9%)	12	11
1	C	343/345 (99%)	315 (92%)	28 (8%)	14	13
All	All	1029/1035 (99%)	941 (91%)	88 (9%)	13	12

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	12	GLN
1	A	18	GLN
1	A	56	PHE
1	A	88	TRP
1	A	95	VAL
1	A	117	ARG
1	A	132	ASP
1	A	135	SER
1	A	178	LEU
1	A	203	LYS
1	A	205	LEU

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Mol	Chain	Res	Type
1	A	208	ASP
1	A	211	LYS
1	A	222	ASN
1	A	233	GLU
1	A	238	LYS
1	A	242	VAL
1	A	243	SER
1	A	245	SER
1	A	246	LYS
1	A	259	GLU
1	A	289	VAL
1	A	292	LEU
1	A	303	LYS
1	A	304	LYS
1	A	325	GLU
1	A	372	ARG
1	A	389	LYS
1	B	8	ILE
1	B	9	VAL
1	B	10	ILE
1	B	12	GLN
1	B	15	ARG
1	B	21	GLU
1	B	32	ARG
1	B	80	SER
1	B	88	TRP
1	B	95	VAL
1	B	117	ARG
1	B	132	ASP
1	B	135	SER
1	B	205	LEU
1	B	208	ASP
1	B	222	ASN
1	B	231	MET
1	B	246	LYS
1	B	256	ASN
1	B	262	LYS
1	B	264	LYS
1	B	288	GLU
1	B	297	ILE
1	B	298	GLU
1	B	304	LYS

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Mol	Chain	Res	Type
1	B	307	ASP
1	B	312	LYS
1	B	328	GLU
1	B	332	GLU
1	B	371	GLU
1	B	389	LYS
1	C	9	VAL
1	C	10	ILE
1	C	12	GLN
1	C	15	ARG
1	C	32	ARG
1	C	56	PHE
1	C	77	GLU
1	C	88	TRP
1	C	95	VAL
1	C	112	LYS
1	C	117	ARG
1	C	135	SER
1	C	205	LEU
1	C	208	ASP
1	C	211	LYS
1	C	222	ASN
1	C	246	LYS
1	C	259	GLU
1	C	266	GLU
1	C	282	GLU
1	C	298	GLU
1	C	303	LYS
1	C	304	LYS
1	C	307	ASP
1	C	310	LYS
1	C	328	GLU
1	C	366	ILE
1	C	387	ILE

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

Mol	Chain	Res	Type
1	A	18	GLN
1	A	256	ASN
1	A	265	ASN
1	A	278	ASN

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Mol	Chain	Res	Type
1	A	281	ASN
1	A	358	ASN
1	A	386	ASN
1	A	419	HIS
1	B	12	GLN
1	B	222	ASN
1	B	265	ASN
1	B	386	ASN
1	C	265	ASN
1	C	386	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	SO4	A	420	-	4,4,4	1.00	0	6,6,6	0.23	0
2	SO4	A	421	-	4,4,4	1.81	1 (25%)	6,6,6	0.27	0
2	SO4	B	420	-	4,4,4	0.83	0	6,6,6	0.82	0
2	SO4	B	421	-	4,4,4	0.72	0	6,6,6	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	C	420	-	4,4,4	0.91	0	6,6,6	0.28	0
2	SO4	C	421	-	4,4,4	1.18	0	6,6,6	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	420	-	-	0/0/0/0	0/0/0/0
2	SO4	A	421	-	-	0/0/0/0	0/0/0/0
2	SO4	B	420	-	-	0/0/0/0	0/0/0/0
2	SO4	B	421	-	-	0/0/0/0	0/0/0/0
2	SO4	C	420	-	-	0/0/0/0	0/0/0/0
2	SO4	C	421	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	421	SO4	O1-S	2.11	1.54	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	421	SO4	3	0
2	C	420	SO4	3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.