



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:17 PM GMT

PDB ID : 1EUZ  
Title : GLUTAMATE DEHYDROGENASE FROM THERMOCOCCUS PROFUNDUS IN THE UNLIGATED STATE  
Authors : Nakasako, M.  
Deposited on : 2000-04-19  
Resolution : 2.25 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

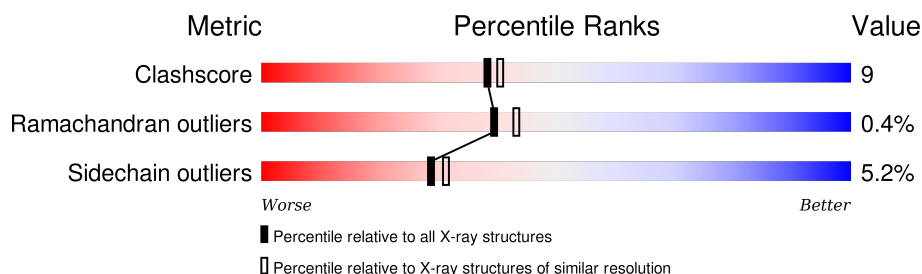
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)

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	 74% 23% ..
1	B	419	 73% 24% ..
1	C	419	 80% 17% ..
1	D	419	 72% 26% ..
1	E	419	 76% 20% ..
1	F	419	 70% 26% ..

## 2 Entry composition [i](#)

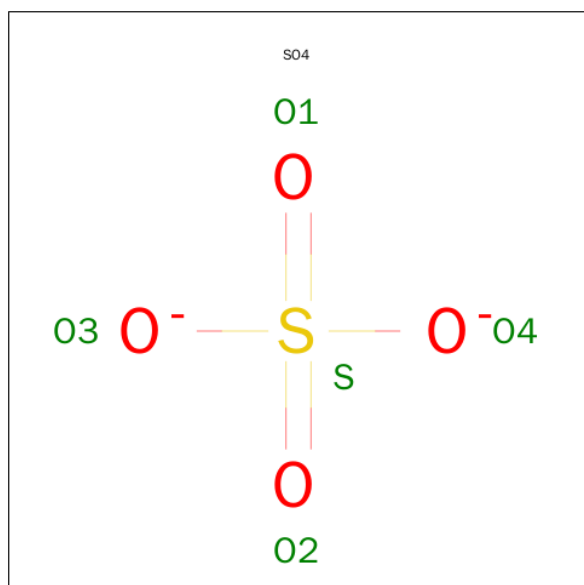
There are 2 unique types of molecules in this entry. The entry contains 19422 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	416	Total	C	N	O	S	0	0	0
			3226	2062	546	604	14			
1	B	416	Total	C	N	O	S	0	0	0
			3205	2050	543	598	14			
1	C	416	Total	C	N	O	S	0	0	0
			3225	2063	550	598	14			
1	D	416	Total	C	N	O	S	0	0	0
			3215	2054	551	596	14			
1	E	416	Total	C	N	O	S	0	0	0
			3258	2080	556	608	14			
1	F	417	Total	C	N	O	S	0	0	0
			3208	2047	542	605	14			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



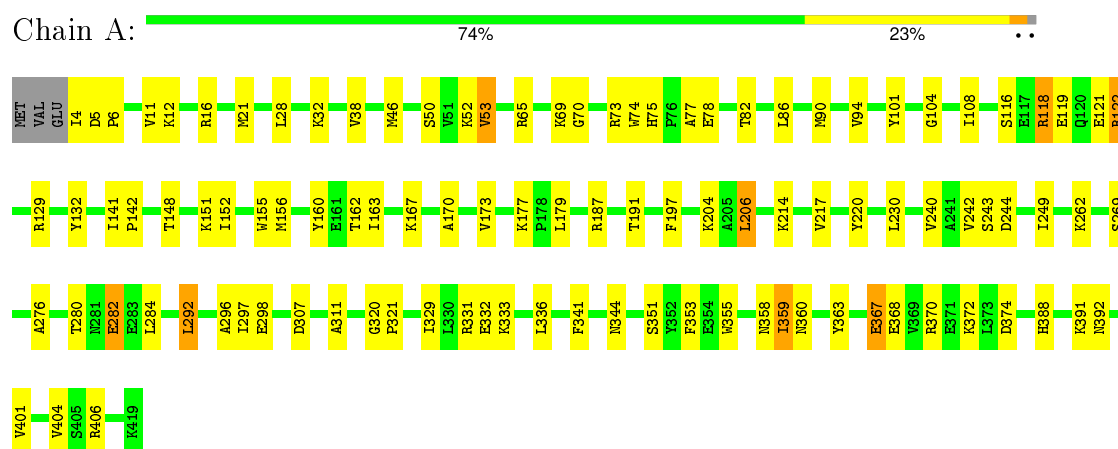
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0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

### 3 Residue-property plots

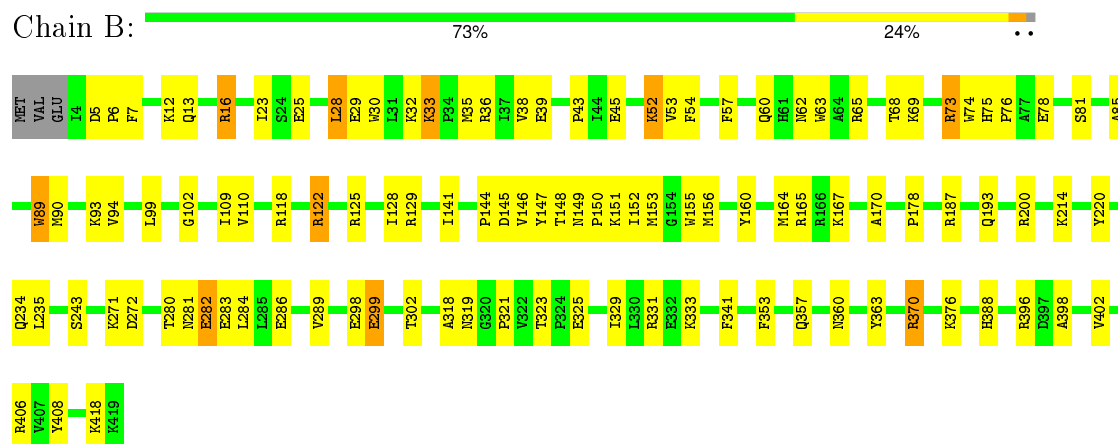
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

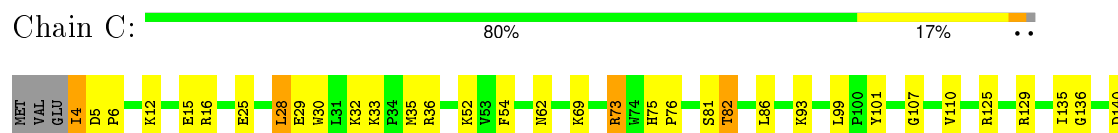
#### • Molecule 1: GLUTAMATE DEHYDROGENASE

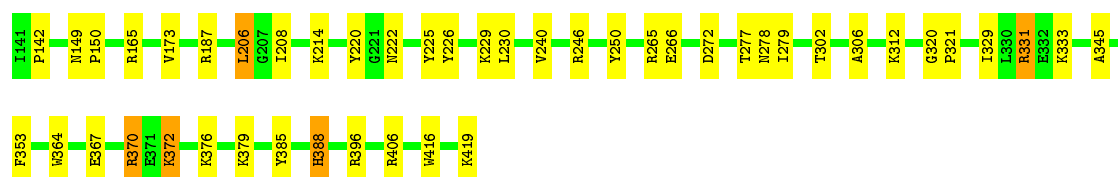


#### • Molecule 1: GLUTAMATE DEHYDROGENASE



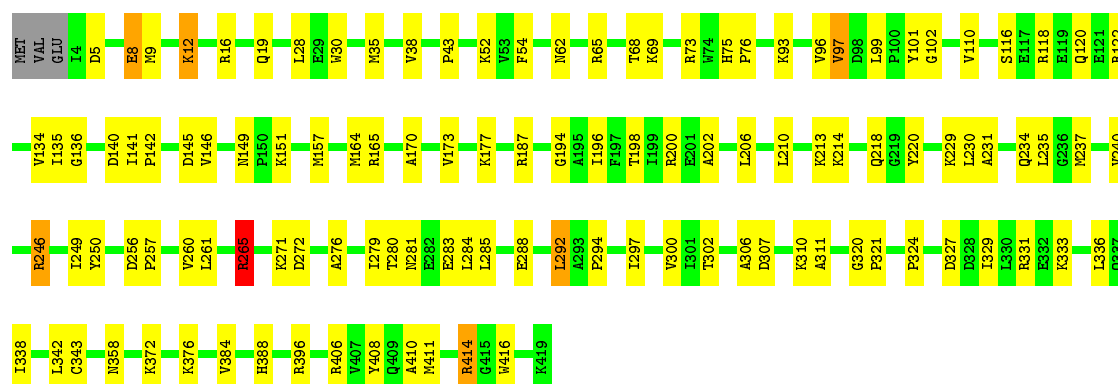
#### • Molecule 1: GLUTAMATE DEHYDROGENASE





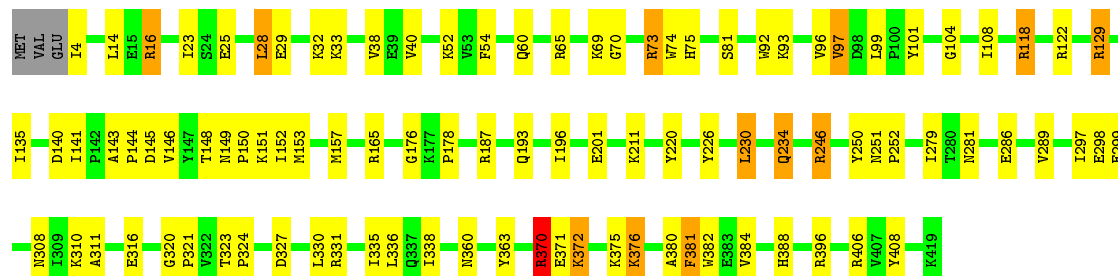
• Molecule 1: GLUTAMATE DEHYDROGENASE

Chain D: 72% 26% ..



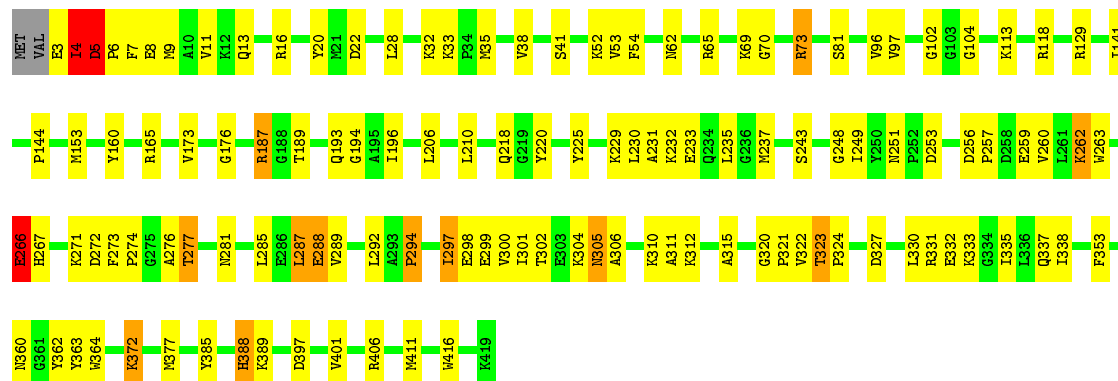
• Molecule 1: GLUTAMATE DEHYDROGENASE

Chain E: 76% 20% ..



• Molecule 1: GLUTAMATE DEHYDROGENASE

Chain F: 70% 26% ..



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.48Å 163.12Å 132.19Å 90.00° 113.20° 90.00°	Depositor
Resolution (Å)	8.00 – 2.25	Depositor
% Data completeness (in resolution range)	88.8 (8.00-2.25)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.187 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19422	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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	0.52	0/3299	0.79	13/4479 (0.3%)
1	B	0.49	0/3278	0.80	21/4453 (0.5%)
1	C	0.53	0/3298	0.78	16/4476 (0.4%)
1	D	0.49	0/3288	0.74	16/4465 (0.4%)
1	E	0.56	0/3331	0.79	18/4514 (0.4%)
1	F	0.53	2/3280 (0.1%)	0.72	10/4459 (0.2%)
All	All	0.52	2/19774 (0.0%)	0.77	94/26846 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	D	0	3
1	E	0	4
1	F	0	6
All	All	0	19

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	266	GLU	CD-OE2	6.98	1.33	1.25
1	F	266	GLU	CD-OE1	5.48	1.31	1.25

All (94) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	ARG	NE-CZ-NH2	-15.66	112.47	120.30
1	F	406	ARG	NE-CZ-NH1	12.43	126.52	120.30
1	C	331	ARG	NE-CZ-NH2	-11.86	114.37	120.30
1	B	122	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	A	406	ARG	NE-CZ-NH1	11.39	125.99	120.30
1	E	187	ARG	NE-CZ-NH1	10.61	125.60	120.30
1	B	16	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	B	165	ARG	NE-CZ-NH2	-9.96	115.32	120.30
1	E	246	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	C	331	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	B	16	ARG	NE-CZ-NH2	-9.67	115.47	120.30
1	B	73	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	F	73	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	B	122	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	C	165	ARG	NE-CZ-NH2	-8.85	115.87	120.30
1	A	73	ARG	NE-CZ-NH2	-8.79	115.90	120.30
1	E	65	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	A	122	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	B	129	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	E	165	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	D	122	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	E	331	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	200	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	C	406	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	E	73	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	C	187	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	A	118	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	B	187	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	E	370	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	118	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	370	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	F	331	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	C	265	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	B	370	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	D	246	ARG	NE-CZ-NH2	7.21	123.91	120.30
1	D	265	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	A	122	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	C	129	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	D	331	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	C	165	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	C	246	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	E	65	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	B	65	ARG	NE-CZ-NH2	-6.91	116.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	396	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	D	165	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	F	406	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	65	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	B	406	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	D	396	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	D	65	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	C	73	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	D	200	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	E	406	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	406	ARG	CG-CD-NE	-6.36	98.44	111.80
1	C	125	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	200	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	D	73	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	C	396	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	E	16	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	D	396	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	F	16	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	E	187	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	187	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	E	165	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	65	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	E	16	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	F	165	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	D	414	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	C	396	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	16	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	36	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	E	73	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	36	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	D	406	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	F	187	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	406	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	E	396	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	F	129	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	D	414	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	73	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	125	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	331	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	125	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	F	118	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	C	129	ARG	NE-CZ-NH2	-5.19	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	129	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	D	187	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	C	16	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	F	65	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	E	406	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	E	122	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	396	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	16	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	D	200	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	TYR	Sidechain
1	A	341	PHE	Sidechain
1	A	363	TYR	Sidechain
1	B	160	TYR	Sidechain
1	B	363	TYR	Sidechain
1	B	370	ARG	Sidechain
1	D	101	TYR	Sidechain
1	D	265	ARG	Sidechain
1	D	408	TYR	Sidechain
1	E	246	ARG	Sidechain
1	E	363	TYR	Sidechain
1	E	381	PHE	Sidechain
1	E	408	TYR	Sidechain
1	F	20	TYR	Sidechain
1	F	225	TYR	Sidechain
1	F	362	TYR	Sidechain
1	F	363	TYR	Sidechain
1	F	4	ILE	Mainchain
1	F	5	ASP	Peptide

## 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	3226	0	3192	55	0
1	B	3205	0	3160	63	0
1	C	3225	0	3204	42	0
1	D	3215	0	3178	66	0
1	E	3258	0	3255	54	0
1	F	3208	0	3141	82	0
2	A	25	0	0	1	0
2	B	15	0	0	1	0
2	C	10	0	0	0	0
2	D	5	0	0	0	0
2	E	20	0	0	2	0
2	F	10	0	0	0	0
All	All	19422	0	19130	351	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 9.

All (351) 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:F:5:ASP:HA	1:F:8:GLU:HB2	1.33	1.09
1:F:4:ILE:HA	1:F:81:SER:OG	1.71	0.89
1:B:35:MET:HE3	1:B:62:ASN:HA	1.53	0.89
1:F:249:ILE:HB	1:F:276:ALA:HB1	1.56	0.86
1:B:193:GLN:HE22	1:B:234:GLN:HE22	1.28	0.80
1:E:52:LYS:HD3	1:E:54:PHE:CZ	2.22	0.75
1:C:272:ASP:H	1:C:278:ASN:HD21	1.32	0.74
1:F:189:THR:HG22	1:F:193:GLN:HB2	1.69	0.74
1:A:53:VAL:HG22	1:F:33:LYS:HD2	1.69	0.73
1:C:35:MET:HE2	1:C:62:ASN:HA	1.72	0.72
1:B:329:ILE:O	1:B:333:LYS:HG3	1.90	0.71
1:B:282:GLU:O	1:B:286:GLU:HG3	1.91	0.71
1:E:14:LEU:HD23	1:E:32:LYS:HG2	1.73	0.70
1:F:288:GLU:HA	1:F:310:LYS:HB2	1.73	0.70
1:F:256:ASP:HB3	1:F:259:GLU:HG2	1.73	0.70
1:F:4:ILE:O	1:F:5:ASP:HB3	1.91	0.70
1:F:324:PRO:O	1:F:327:ASP:HB2	1.92	0.70
1:D:288:GLU:HA	1:D:310:LYS:HB3	1.74	0.69
1:F:35:MET:CE	1:F:62:ASN:HA	2.23	0.69
1:C:4:ILE:HA	1:C:81:SER:OG	1.94	0.68
1:B:38:VAL:HG22	1:E:38:VAL:HG22	1.77	0.67
1:E:311:ALA:O	1:E:335:ILE:HG12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:LYS:O	1:F:266:GLU:HB2	1.95	0.66
1:F:297:ILE:HG23	1:F:300:VAL:HG11	1.76	0.66
1:F:301:ILE:HA	1:F:305:ASN:HD21	1.60	0.66
1:F:299:GLU:HG2	1:F:323:THR:HG23	1.79	0.65
1:E:193:GLN:OE1	1:E:370:ARG:NH1	2.30	0.65
1:E:193:GLN:HE22	1:E:234:GLN:HE22	1.44	0.65
1:B:75:HIS:HD2	1:B:146:VAL:HG11	1.62	0.64
1:F:4:ILE:HG23	1:F:5:ASP:H	1.62	0.64
1:A:4:ILE:HG22	1:A:5:ASP:H	1.61	0.64
1:E:28:LEU:O	1:E:32:LYS:HG3	1.98	0.64
1:F:256:ASP:O	1:F:260:VAL:HG23	1.97	0.64
1:F:4:ILE:HA	1:F:81:SER:CB	2.28	0.64
1:A:74:TRP:NE1	1:A:108:ILE:HD12	2.12	0.64
1:E:74:TRP:NE1	1:E:108:ILE:HD12	2.13	0.63
1:E:286:GLU:HG2	1:E:308:ASN:HB3	1.79	0.63
1:F:4:ILE:CG2	1:F:5:ASP:N	2.61	0.63
1:B:299:GLU:HG3	1:B:323:THR:HG22	1.82	0.62
1:E:299:GLU:HG2	1:E:323:THR:HG22	1.82	0.62
1:E:371:GLU:O	1:E:375:LYS:HG3	1.99	0.62
1:C:136:GLY:HA2	1:C:173:VAL:HG23	1.80	0.61
1:E:250:TYR:HB2	1:E:279:ILE:HD13	1.82	0.61
1:A:53:VAL:CG2	1:F:33:LYS:HD2	2.30	0.61
1:A:355:TRP:CE2	1:A:359:ILE:HD12	2.35	0.61
1:A:167:LYS:HA	1:A:167:LYS:HE2	1.83	0.61
1:F:320:GLY:N	1:F:321:PRO:HD3	2.16	0.60
1:F:297:ILE:HG23	1:F:300:VAL:CG1	2.31	0.60
1:A:75:HIS:HB3	1:A:78:GLU:HG2	1.83	0.60
1:F:196:ILE:HG13	1:F:230:LEU:HB2	1.83	0.60
1:F:292:LEU:HG	1:F:294:PRO:HD3	1.84	0.60
1:D:214:LYS:HD3	1:D:240:VAL:HG11	1.83	0.59
1:B:35:MET:HE1	1:B:62:ASN:ND2	2.18	0.59
1:F:273:PHE:HB3	1:F:276:ALA:HB2	1.85	0.59
1:F:35:MET:HE2	1:F:62:ASN:HA	1.84	0.59
1:D:30:TRP:HE1	1:D:35:MET:HE1	1.66	0.59
1:D:307:ASP:HA	1:D:333:LYS:HE2	1.84	0.58
1:F:289:VAL:HG23	1:F:311:ALA:HB2	1.85	0.58
1:E:297:ILE:HG22	1:E:298:GLU:O	2.02	0.58
1:E:73:ARG:HB3	1:E:146:VAL:HB	1.84	0.58
1:C:28:LEU:HD13	1:C:32:LYS:HE3	1.86	0.58
1:D:12:LYS:N	1:D:12:LYS:HD3	2.18	0.58
1:A:292:LEU:HB2	1:A:311:ALA:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:LEU:HB3	1:C:208:ILE:HG13	1.86	0.58
1:E:324:PRO:O	1:E:327:ASP:HB2	2.04	0.57
1:D:16:ARG:O	1:D:19:GLN:HG2	2.03	0.57
1:C:302:THR:O	1:C:306:ALA:HB2	2.04	0.57
1:B:398:ALA:O	1:B:402:VAL:HG23	2.04	0.57
1:B:243:SER:HB3	1:B:284:LEU:HD13	1.85	0.57
1:F:266:GLU:HB3	1:F:267:HIS:ND1	2.20	0.56
1:C:69:LYS:HD3	1:C:101:TYR:CE2	2.40	0.56
1:F:271:LYS:O	1:F:272:ASP:HB2	2.06	0.56
1:F:273:PHE:HB3	1:F:276:ALA:CB	2.35	0.56
1:E:73:ARG:HG2	1:E:145:ASP:OD1	2.06	0.56
1:D:411:MET:HG2	1:D:416:TRP:HE3	1.69	0.55
1:C:353:PHE:CZ	1:C:372:LYS:HB3	2.41	0.55
1:B:144:PRO:HD3	1:B:153:MET:SD	2.46	0.55
1:A:391:LYS:HE3	1:A:401:VAL:HG11	1.87	0.55
1:D:261:LEU:HD21	1:D:265:ARG:NH2	2.22	0.55
1:B:193:GLN:HE22	1:B:234:GLN:NE2	1.99	0.55
1:D:75:HIS:CD2	1:D:76:PRO:HD2	2.42	0.55
1:A:75:HIS:CE1	1:A:77:ALA:HB3	2.42	0.55
1:A:5:ASP:HB3	1:A:6:PRO:HD3	1.89	0.55
1:D:99:LEU:HD23	1:D:376:LYS:HE3	1.88	0.54
1:D:231:ALA:O	1:D:235:LEU:HB2	2.07	0.54
1:C:331:ARG:HG3	1:C:331:ARG:HH11	1.73	0.54
1:F:330:LEU:HD22	1:F:335:ILE:HD12	1.90	0.54
1:C:75:HIS:CD2	1:C:76:PRO:HD2	2.42	0.54
1:A:152:ILE:O	1:A:156:MET:HG3	2.08	0.54
1:A:118:ARG:O	1:A:122:ARG:HG3	2.08	0.54
1:D:410:ALA:O	1:D:414:ARG:HG3	2.08	0.54
1:B:90:MET:O	1:B:94:VAL:HG22	2.08	0.54
1:E:4:ILE:HA	1:E:81:SER:HB2	1.89	0.54
1:C:4:ILE:HA	1:C:81:SER:CB	2.37	0.53
1:F:385:TYR:O	1:F:388:HIS:HD2	1.92	0.53
1:C:52:LYS:HG2	1:C:54:PHE:CE1	2.44	0.53
1:A:21:MET:HE1	1:A:401:VAL:HA	1.88	0.53
1:B:178:PRO:HA	2:B:606:SO4:O3	2.09	0.53
1:D:69:LYS:HD2	1:D:141:ILE:HB	1.91	0.53
1:A:38:VAL:HG22	1:F:38:VAL:HG22	1.89	0.53
1:C:35:MET:HE1	1:C:416:TRP:CZ3	2.44	0.52
1:D:302:THR:O	1:D:306:ALA:HB2	2.08	0.52
1:C:329:ILE:O	1:C:333:LYS:HG3	2.09	0.52
1:E:201:GLU:HB3	1:E:381:PHE:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLU:HG3	1:B:57:PHE:CE1	2.43	0.52
1:C:364:TRP:CZ3	1:C:372:LYS:HE2	2.44	0.52
1:F:4:ILE:HG22	1:F:8:GLU:HG3	1.91	0.52
1:D:5:ASP:O	1:D:9:MET:HG3	2.09	0.52
1:B:75:HIS:ND1	1:B:76:PRO:HD2	2.25	0.52
1:B:25:GLU:O	1:B:29:GLU:HG2	2.10	0.52
1:C:28:LEU:O	1:C:32:LYS:HG3	2.10	0.52
1:B:151:LYS:HD3	1:B:155:TRP:CH2	2.44	0.51
1:F:323:THR:HG22	1:F:324:PRO:HD2	1.92	0.51
1:F:315:ALA:CB	1:F:338:ILE:HD12	2.40	0.51
1:F:231:ALA:O	1:F:235:LEU:HB2	2.10	0.51
1:F:35:MET:HE3	1:F:62:ASN:HA	1.93	0.51
1:A:4:ILE:HG22	1:A:5:ASP:N	2.25	0.51
1:A:148:THR:HA	1:A:152:ILE:HD12	1.93	0.51
1:F:4:ILE:HD13	1:F:7:PHE:HD1	1.75	0.50
1:E:135:ILE:HA	1:E:140:ASP:HB3	1.93	0.50
1:A:329:ILE:O	1:A:333:LYS:HG3	2.11	0.50
1:F:315:ALA:HB2	1:F:338:ILE:HD12	1.94	0.50
1:C:35:MET:CE	1:C:62:ASN:HA	2.41	0.50
1:F:287:LEU:HD12	1:F:288:GLU:N	2.27	0.50
1:E:148:THR:HA	1:E:152:ILE:HD12	1.93	0.50
1:E:371:GLU:HG2	1:E:372:LYS:N	2.27	0.50
1:B:144:PRO:HD3	1:B:153:MET:HG3	1.93	0.50
1:B:353:PHE:O	1:B:357:GLN:HG3	2.11	0.50
1:A:297:ILE:HG22	1:A:298:GLU:N	2.27	0.50
1:D:338:ILE:HG22	1:D:343:CYS:HB2	1.94	0.50
1:A:243:SER:HB3	1:A:284:LEU:HD13	1.93	0.50
1:F:11:VAL:HG13	1:F:32:LYS:HG2	1.94	0.50
1:D:256:ASP:O	1:D:260:VAL:HG23	2.11	0.49
1:B:99:LEU:HD23	1:B:376:LYS:HE3	1.93	0.49
1:B:53:VAL:CG2	1:E:33:LYS:HD2	2.43	0.49
1:F:70:GLY:HA3	1:F:104:GLY:O	2.13	0.49
1:B:6:PRO:HD2	1:B:81:SER:OG	2.12	0.49
1:F:323:THR:HG22	1:F:324:PRO:CD	2.43	0.49
1:B:164:MET:O	1:B:164:MET:HG2	2.12	0.49
1:B:164:MET:HE2	1:B:170:ALA:HB2	1.94	0.49
1:F:353:PHE:CZ	1:F:372:LYS:HB3	2.48	0.49
1:E:178:PRO:HA	2:E:612:SO4:O2	2.13	0.49
1:E:196:ILE:HG12	1:E:230:LEU:HB3	1.93	0.49
1:F:160:TYR:CD1	1:F:173:VAL:HG21	2.48	0.49
1:A:282:GLU:H	1:A:282:GLU:CD	2.17	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLU:H	1:B:325:GLU:CD	2.17	0.48
1:C:69:LYS:HD3	1:C:101:TYR:CZ	2.48	0.48
1:A:21:MET:HE1	1:A:404:VAL:HB	1.94	0.48
1:D:170:ALA:O	1:D:173:VAL:HG12	2.13	0.48
1:F:229:LYS:O	1:F:233:GLU:HG2	2.13	0.48
1:C:35:MET:CE	1:C:416:TRP:CZ3	2.96	0.48
1:A:11:VAL:HG13	1:A:32:LYS:HD3	1.95	0.48
1:B:281:ASN:O	1:B:284:LEU:HB3	2.13	0.48
1:D:142:PRO:HD2	1:D:173:VAL:O	2.14	0.48
1:B:271:LYS:O	1:B:272:ASP:HB2	2.14	0.48
1:C:222:ASN:HD21	1:C:226:TYR:HE2	1.62	0.48
1:A:206:LEU:HD13	1:A:336:LEU:HD22	1.96	0.48
1:D:411:MET:HG2	1:D:416:TRP:CE3	2.48	0.48
1:C:25:GLU:O	1:C:29:GLU:HG2	2.13	0.48
1:B:7:PHE:HA	1:B:85:ALA:HB2	1.96	0.48
1:D:324:PRO:O	1:D:327:ASP:HB2	2.14	0.48
1:D:218:GLN:HE22	1:D:300:VAL:HG21	1.79	0.48
1:A:177:LYS:NZ	1:A:358:ASN:HD21	2.11	0.47
1:E:69:LYS:HD3	1:E:101:TYR:CE2	2.49	0.47
1:D:229:LYS:HA	1:D:257:PRO:HG2	1.94	0.47
1:D:320:GLY:N	1:D:321:PRO:HD3	2.29	0.47
1:B:30:TRP:HE1	1:B:35:MET:CE	2.27	0.47
1:D:135:ILE:HA	1:D:140:ASP:HB3	1.95	0.47
1:E:226:TYR:O	1:E:230:LEU:HB2	2.14	0.47
1:D:35:MET:CE	1:D:62:ASN:HA	2.45	0.47
1:E:150:PRO:HA	1:E:176:GLY:O	2.14	0.47
1:D:250:TYR:HB2	1:D:279:ILE:HD13	1.97	0.47
1:C:385:TYR:O	1:C:388:HIS:HD2	1.98	0.47
1:E:289:VAL:O	1:E:311:ALA:HA	2.15	0.47
1:D:116:SER:O	1:D:120:GLN:HG3	2.14	0.47
1:C:35:MET:HE1	1:C:416:TRP:HZ3	1.80	0.47
1:E:99:LEU:HD23	1:E:376:LYS:HE3	1.97	0.47
1:B:52:LYS:HD2	1:B:54:PHE:CZ	2.49	0.47
1:E:38:VAL:HG12	1:E:40:VAL:HG13	1.95	0.46
1:D:35:MET:HE1	1:D:416:TRP:CZ3	2.50	0.46
1:E:93:LYS:O	1:E:97:VAL:HG22	2.15	0.46
1:D:249:ILE:HB	1:D:276:ALA:HB1	1.98	0.46
1:D:292:LEU:HB2	1:D:311:ALA:HB2	1.97	0.46
1:F:4:ILE:O	1:F:5:ASP:CB	2.62	0.46
1:F:9:MET:HG2	1:F:13:GLN:NE2	2.30	0.46
1:E:316:GLU:HG3	1:E:338:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:VAL:HG12	1:D:99:LEU:HG	1.95	0.46
1:F:144:PRO:HD3	1:F:153:MET:SD	2.55	0.46
1:B:164:MET:CE	1:B:170:ALA:HB2	2.46	0.46
1:A:170:ALA:O	1:A:173:VAL:HG12	2.15	0.46
1:E:149:ASN:O	1:E:153:MET:HG2	2.15	0.46
1:D:164:MET:O	1:D:164:MET:HG2	2.15	0.46
1:A:244:ASP:HB2	2:A:605:SO4:O4	2.16	0.46
1:B:148:THR:HA	1:B:152:ILE:HD12	1.98	0.46
1:F:231:ALA:HB1	1:F:237:MET:HE3	1.97	0.46
1:A:70:GLY:O	1:A:142:PRO:HA	2.16	0.46
1:F:249:ILE:CB	1:F:276:ALA:HB1	2.38	0.46
1:C:142:PRO:HD2	1:C:173:VAL:O	2.16	0.46
1:E:4:ILE:HA	1:E:81:SER:CB	2.46	0.46
1:D:306:ALA:HB3	1:D:329:ILE:HD12	1.98	0.46
1:A:129:ARG:HG2	1:A:163:ILE:HD11	1.98	0.46
1:A:307:ASP:OD1	1:A:333:LYS:HE3	2.15	0.45
1:F:144:PRO:HD3	1:F:153:MET:HG3	1.97	0.45
1:E:250:TYR:CE2	1:E:252:PRO:HD3	2.51	0.45
1:A:360:ASN:HA	1:B:360:ASN:HD21	1.80	0.45
1:F:52:LYS:HD3	1:F:54:PHE:CZ	2.51	0.45
1:B:78:GLU:HB3	1:B:109:ILE:HG12	1.99	0.45
1:C:99:LEU:HD23	1:C:376:LYS:HE3	1.98	0.45
1:E:157:MET:SD	1:E:157:MET:C	2.95	0.45
1:E:75:HIS:HD2	1:E:146:VAL:HG11	1.81	0.45
1:D:5:ASP:HA	1:D:8:GLU:HB2	1.97	0.45
1:C:5:ASP:N	1:C:6:PRO:CD	2.80	0.45
1:C:225:TYR:OH	1:C:229:LYS:HD2	2.16	0.45
1:F:4:ILE:CG2	1:F:8:GLU:HG3	2.47	0.45
1:B:62:ASN:O	1:B:102:GLY:HA3	2.16	0.45
1:B:60:GLN:HG2	1:B:68:THR:OG1	2.16	0.45
1:E:69:LYS:HD2	1:E:141:ILE:HB	1.98	0.45
1:A:367:GLU:HG2	1:A:368:GLU:N	2.31	0.45
1:B:69:LYS:HD2	1:B:141:ILE:HB	1.98	0.45
1:D:68:THR:HA	1:D:102:GLY:O	2.17	0.45
1:F:4:ILE:HG23	1:F:8:GLU:H	1.81	0.45
1:F:160:TYR:CG	1:F:173:VAL:HG21	2.52	0.45
1:A:70:GLY:HA3	1:A:104:GLY:O	2.17	0.45
1:A:116:SER:OG	1:A:119:GLU:HG3	2.16	0.45
1:A:249:ILE:HB	1:A:276:ALA:HB1	1.99	0.45
1:D:202:ALA:HB1	1:D:336:LEU:HD23	1.97	0.45
1:F:263:TRP:O	1:F:267:HIS:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:PHE:CE2	1:D:110:VAL:HG23	2.52	0.45
1:F:299:GLU:HA	1:F:321:PRO:O	2.17	0.45
1:B:118:ARG:O	1:B:122:ARG:HG3	2.17	0.45
1:C:149:ASN:HB2	1:C:150:PRO:CD	2.47	0.44
1:C:30:TRP:CH2	1:D:43:PRO:HG3	2.52	0.44
1:F:5:ASP:O	1:F:9:MET:HB2	2.17	0.44
1:A:46:MET:HE2	1:A:52:LYS:HB2	1.98	0.44
1:E:52:LYS:HD3	1:E:54:PHE:CE2	2.51	0.44
1:B:28:LEU:O	1:B:32:LYS:HG3	2.17	0.44
1:B:298:GLU:N	1:B:298:GLU:CD	2.71	0.44
1:C:73:ARG:O	1:C:107:GLY:HA2	2.18	0.44
1:C:135:ILE:HA	1:C:140:ASP:HB3	1.98	0.44
1:F:13:GLN:H	1:F:13:GLN:HG2	1.66	0.44
1:E:330:LEU:HD23	1:E:330:LEU:HA	1.82	0.44
1:B:144:PRO:HD3	1:B:153:MET:CG	2.48	0.44
1:D:210:LEU:HD22	1:D:237:MET:HE3	1.99	0.44
1:B:89:TRP:CH2	1:B:341:PHE:HB3	2.53	0.44
1:C:12:LYS:HD3	1:C:15:GLU:OE2	2.18	0.43
1:A:320:GLY:N	1:A:321:PRO:CD	2.81	0.43
1:D:271:LYS:O	1:D:272:ASP:HB2	2.18	0.43
1:B:298:GLU:HG3	1:B:319:ASN:O	2.17	0.43
1:F:302:THR:O	1:F:306:ALA:HB2	2.19	0.43
1:F:4:ILE:CG2	1:F:5:ASP:H	2.22	0.43
1:A:214:LYS:HG2	1:A:240:VAL:HG11	1.99	0.43
1:F:41:SER:HB3	1:F:53:VAL:HG13	2.00	0.43
1:D:177:LYS:NZ	1:D:358:ASN:HD21	2.15	0.43
1:A:151:LYS:HE3	1:A:155:TRP:CH2	2.53	0.43
1:E:380:ALA:O	1:E:384:VAL:HG23	2.19	0.43
1:F:218:GLN:HB3	1:F:294:PRO:HA	1.99	0.43
1:D:218:GLN:HB3	1:D:294:PRO:HA	1.99	0.43
1:D:38:VAL:HG21	1:D:134:VAL:HG21	2.01	0.43
1:F:251:ASN:O	1:F:253:ASP:N	2.51	0.43
1:A:217:VAL:O	1:A:242:VAL:HA	2.19	0.43
1:F:411:MET:HG2	1:F:416:TRP:CE3	2.54	0.43
1:F:322:VAL:HG11	1:F:337:GLN:NE2	2.34	0.43
1:B:193:GLN:NE2	1:B:234:GLN:HE22	2.07	0.43
1:C:214:LYS:HE2	1:C:240:VAL:HG11	1.99	0.43
1:C:250:TYR:HB2	1:C:279:ILE:HD13	2.01	0.43
1:C:370:ARG:HB3	1:C:370:ARG:NH1	2.34	0.43
1:D:234:GLN:HE21	1:D:234:GLN:HB3	1.63	0.43
1:E:360:ASN:HA	1:F:360:ASN:HD21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:330:LEU:CD2	1:F:335:ILE:HD12	2.48	0.43
1:E:320:GLY:N	1:E:321:PRO:CD	2.82	0.43
1:D:284:LEU:C	1:D:284:LEU:HD23	2.39	0.43
1:F:364:TRP:CD1	1:F:364:TRP:N	2.86	0.43
1:F:297:ILE:HG13	1:F:298:GLU:N	2.33	0.43
1:D:342:LEU:HD22	1:D:384:VAL:HG21	2.01	0.43
1:B:149:ASN:HB2	1:B:150:PRO:HD2	2.01	0.43
1:B:35:MET:HB3	1:B:63:TRP:CZ3	2.54	0.42
1:F:176:GLY:HA2	1:F:187:ARG:HD3	2.01	0.42
1:C:54:PHE:CE2	1:C:110:VAL:HG23	2.55	0.42
1:D:136:GLY:HA2	1:D:173:VAL:HG23	2.01	0.42
1:A:177:LYS:HB2	1:A:177:LYS:HE2	1.76	0.42
1:F:69:LYS:HD2	1:F:141:ILE:HB	2.00	0.42
1:D:213:LYS:HD3	1:D:213:LYS:HA	1.84	0.42
1:A:82:THR:O	1:A:86:LEU:HG	2.19	0.42
1:B:54:PHE:CE2	1:B:110:VAL:HG23	2.55	0.42
1:C:93:LYS:HE2	1:C:345:ALA:HA	2.01	0.42
1:E:118:ARG:HA	1:E:118:ARG:HH11	1.83	0.42
1:D:297:ILE:HG13	1:D:300:VAL:CG1	2.49	0.42
1:A:69:LYS:HD2	1:A:141:ILE:HB	2.00	0.42
1:D:194:GLY:O	1:D:198:THR:HG23	2.19	0.42
1:D:196:ILE:HG13	1:D:230:LEU:HB2	2.01	0.42
1:A:191:THR:HG23	1:A:344:ASN:HB2	2.01	0.42
1:F:4:ILE:HG12	1:F:7:PHE:HB3	2.02	0.42
1:B:318:ALA:O	1:B:321:PRO:HD3	2.19	0.42
1:A:292:LEU:HB2	1:A:311:ALA:CB	2.49	0.42
1:F:194:GLY:HA2	1:F:377:MET:HG3	2.01	0.42
1:B:43:PRO:HB3	1:B:53:VAL:HG12	2.02	0.42
1:F:281:ASN:O	1:F:285:LEU:HG	2.19	0.42
1:C:82:THR:O	1:C:86:LEU:HG	2.20	0.42
1:F:4:ILE:HG22	1:F:5:ASP:N	2.34	0.42
1:E:251:ASN:HA	1:E:252:PRO:HD2	1.84	0.42
1:B:23:ILE:HA	1:B:408:TYR:CE2	2.54	0.42
1:D:261:LEU:HG	1:D:265:ARG:HD2	2.00	0.42
1:D:372:LYS:HE2	1:D:372:LYS:HA	2.02	0.42
1:C:320:GLY:N	1:C:321:PRO:CD	2.83	0.41
1:A:132:TYR:CE1	1:A:160:TYR:CE1	3.08	0.41
1:B:30:TRP:HE1	1:B:35:MET:HE1	1.85	0.41
1:B:151:LYS:CD	1:B:155:TRP:CH2	3.03	0.41
1:A:173:VAL:O	1:A:173:VAL:HG22	2.20	0.41
1:E:149:ASN:OD1	1:E:151:LYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:LYS:O	1:D:96:VAL:HG12	2.19	0.41
1:E:281:ASN:HB2	2:E:613:SO4:O4	2.20	0.41
1:B:280:THR:OG1	1:B:283:GLU:HG3	2.20	0.41
1:F:243:SER:HA	1:F:248:GLY:HA2	2.02	0.41
1:B:5:ASP:HB3	1:B:6:PRO:HD3	2.01	0.41
1:A:121:GLU:OE1	1:B:418:LYS:NZ	2.52	0.41
1:E:75:HIS:CD2	1:E:146:VAL:HG11	2.54	0.41
1:E:25:GLU:O	1:E:29:GLU:HG2	2.21	0.41
1:D:62:ASN:O	1:D:102:GLY:HA3	2.20	0.41
1:B:302:THR:HG22	1:B:323:THR:HG21	2.01	0.41
1:D:8:GLU:O	1:D:12:LYS:HD3	2.20	0.41
1:B:128:ILE:HG12	1:B:156:MET:HG2	2.01	0.41
1:D:280:THR:OG1	1:D:283:GLU:HG3	2.21	0.41
1:C:149:ASN:HB2	1:C:150:PRO:HD2	2.02	0.41
1:E:382:TRP:CE3	1:E:382:TRP:HA	2.56	0.41
1:A:162:THR:HG21	1:E:129:ARG:CZ	2.51	0.41
1:A:197:PHE:CD2	1:A:374:ASP:HA	2.56	0.41
1:A:355:TRP:CZ2	1:A:359:ILE:HD12	2.56	0.41
1:D:35:MET:CE	1:D:416:TRP:CZ3	3.04	0.41
1:D:324:PRO:HA	1:D:327:ASP:OD2	2.20	0.41
1:D:218:GLN:NE2	1:D:285:LEU:HD21	2.35	0.41
1:E:143:ALA:HB1	1:E:144:PRO:CD	2.51	0.41
1:B:33:LYS:HD2	1:B:33:LYS:N	2.35	0.41
1:D:157:MET:C	1:D:157:MET:SD	2.98	0.41
1:E:14:LEU:HD13	1:E:92:TRP:CZ2	2.56	0.41
1:F:397:ASP:O	1:F:401:VAL:HG23	2.21	0.41
1:B:45:GLU:HG2	1:D:118:ARG:NH2	2.36	0.41
1:F:229:LYS:HA	1:F:257:PRO:HG2	2.03	0.40
1:C:206:LEU:HA	1:C:206:LEU:HD12	1.87	0.40
1:D:218:GLN:HG3	1:D:281:ASN:HD22	1.87	0.40
1:D:52:LYS:HE3	1:D:54:PHE:CE2	2.56	0.40
1:E:70:GLY:HA3	1:E:104:GLY:O	2.21	0.40
1:A:353:PHE:CZ	1:A:372:LYS:HB3	2.56	0.40
1:F:62:ASN:O	1:F:102:GLY:HA3	2.20	0.40
1:A:21:MET:CE	1:A:401:VAL:HA	2.51	0.40
1:A:90:MET:O	1:A:94:VAL:HG22	2.22	0.40
1:D:149:ASN:OD1	1:D:151:LYS:HB3	2.21	0.40
1:F:6:PRO:HD2	1:F:81:SER:OG	2.22	0.40
1:B:299:GLU:HG3	1:B:323:THR:CG2	2.50	0.40
1:A:331:ARG:NH2	1:A:392:ASN:OD1	2.55	0.40
1:B:214:LYS:O	1:B:289:VAL:HB	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:TRP:O	1:B:147:TYR:HD2	2.04	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	414/419 (99%)	395 (95%)	18 (4%)	1 (0%)	52	61
1	B	414/419 (99%)	395 (95%)	19 (5%)	0	100	100
1	C	414/419 (99%)	397 (96%)	17 (4%)	0	100	100
1	D	414/419 (99%)	394 (95%)	19 (5%)	1 (0%)	52	61
1	E	414/419 (99%)	395 (95%)	19 (5%)	0	100	100
1	F	415/419 (99%)	377 (91%)	30 (7%)	8 (2%)	10	5
All	All	2485/2514 (99%)	2353 (95%)	122 (5%)	10 (0%)	39	43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	4	ILE
1	F	5	ASP
1	F	297	ILE
1	F	232	LYS
1	F	274	PRO
1	F	277	THR
1	F	305	ASN
1	F	294	PRO
1	A	296	ALA
1	D	146	VAL

### 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	330/342 (96%)	311 (94%)	19 (6%)	25	25
1	B	325/342 (95%)	309 (95%)	16 (5%)	31	34
1	C	329/342 (96%)	313 (95%)	16 (5%)	31	34
1	D	326/342 (95%)	315 (97%)	11 (3%)	44	54
1	E	337/342 (98%)	320 (95%)	17 (5%)	30	33
1	F	325/342 (95%)	302 (93%)	23 (7%)	18	17
All	All	1972/2052 (96%)	1870 (95%)	102 (5%)	29	31

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	28	LEU
1	A	50	SER
1	A	53	VAL
1	A	179	LEU
1	A	204	LYS
1	A	206	LEU
1	A	220	TYR
1	A	230	LEU
1	A	262	LYS
1	A	269	SER
1	A	280	THR
1	A	282	GLU
1	A	292	LEU
1	A	332	GLU
1	A	351	SER
1	A	359	ILE
1	A	367	GLU
1	A	388	HIS
1	B	12	LYS
1	B	13	GLN
1	B	16	ARG

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Mol	Chain	Res	Type
1	B	28	LEU
1	B	33	LYS
1	B	52	LYS
1	B	73	ARG
1	B	89	TRP
1	B	93	LYS
1	B	145	ASP
1	B	167	LYS
1	B	220	TYR
1	B	235	LEU
1	B	282	GLU
1	B	299	GLU
1	B	388	HIS
1	C	4	ILE
1	C	28	LEU
1	C	33	LYS
1	C	82	THR
1	C	206	LEU
1	C	220	TYR
1	C	230	LEU
1	C	266	GLU
1	C	277	THR
1	C	312	LYS
1	C	367	GLU
1	C	370	ARG
1	C	372	LYS
1	C	379	LYS
1	C	388	HIS
1	C	419	LYS
1	D	8	GLU
1	D	12	LYS
1	D	28	LEU
1	D	97	VAL
1	D	145	ASP
1	D	206	LEU
1	D	220	TYR
1	D	246	ARG
1	D	265	ARG
1	D	292	LEU
1	D	388	HIS
1	E	16	ARG
1	E	23	ILE

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Mol	Chain	Res	Type
1	E	28	LEU
1	E	60	GLN
1	E	96	VAL
1	E	97	VAL
1	E	118	ARG
1	E	211	LYS
1	E	220	TYR
1	E	230	LEU
1	E	234	GLN
1	E	310	LYS
1	E	336	LEU
1	E	370	ARG
1	E	372	LYS
1	E	376	LYS
1	E	388	HIS
1	F	3	GLU
1	F	22	ASP
1	F	28	LEU
1	F	73	ARG
1	F	96	VAL
1	F	97	VAL
1	F	113	LYS
1	F	206	LEU
1	F	210	LEU
1	F	220	TYR
1	F	262	LYS
1	F	266	GLU
1	F	277	THR
1	F	287	LEU
1	F	288	GLU
1	F	304	LYS
1	F	312	LYS
1	F	323	THR
1	F	332	GLU
1	F	333	LYS
1	F	372	LYS
1	F	388	HIS
1	F	389	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	281	ASN
1	A	358	ASN
1	A	360	ASN
1	A	386	ASN
1	B	120	GLN
1	B	234	GLN
1	B	360	ASN
1	B	386	ASN
1	B	392	ASN
1	C	62	ASN
1	C	75	HIS
1	C	222	ASN
1	C	278	ASN
1	C	386	ASN
1	C	388	HIS
1	D	75	HIS
1	D	218	GLN
1	D	234	GLN
1	D	281	ASN
1	D	358	ASN
1	E	120	GLN
1	E	234	GLN
1	E	360	ASN
1	F	13	GLN
1	F	75	HIS
1	F	120	GLN
1	F	222	ASN
1	F	360	ASN
1	F	388	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

17 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	600	-	4,4,4	1.18	1 (25%)	6,6,6	0.67	0
2	SO4	A	601	-	4,4,4	0.53	0	6,6,6	0.92	0
2	SO4	A	602	-	4,4,4	0.52	0	6,6,6	0.60	0
2	SO4	A	603	-	4,4,4	0.14	0	6,6,6	0.32	0
2	SO4	A	605	-	4,4,4	0.51	0	6,6,6	0.28	0
2	SO4	B	606	-	4,4,4	0.36	0	6,6,6	0.45	0
2	SO4	B	607	-	4,4,4	0.47	0	6,6,6	0.25	0
2	SO4	B	608	-	4,4,4	0.77	0	6,6,6	0.65	0
2	SO4	C	604	-	4,4,4	0.73	0	6,6,6	1.09	0
2	SO4	C	609	-	4,4,4	0.67	0	6,6,6	0.77	0
2	SO4	D	610	-	4,4,4	0.62	0	6,6,6	0.46	0
2	SO4	E	611	-	4,4,4	0.60	0	6,6,6	0.55	0
2	SO4	E	612	-	4,4,4	0.99	0	6,6,6	1.27	1 (16%)
2	SO4	E	613	-	4,4,4	0.74	0	6,6,6	0.71	0
2	SO4	E	614	-	4,4,4	1.01	0	6,6,6	0.52	0
2	SO4	F	615	-	4,4,4	0.98	0	6,6,6	0.42	0
2	SO4	F	616	-	4,4,4	0.25	0	6,6,6	0.47	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	600	-	-	0/0/0/0	0/0/0/0
2	SO4	A	601	-	-	0/0/0/0	0/0/0/0
2	SO4	A	602	-	-	0/0/0/0	0/0/0/0
2	SO4	A	603	-	-	0/0/0/0	0/0/0/0
2	SO4	A	605	-	-	0/0/0/0	0/0/0/0
2	SO4	B	606	-	-	0/0/0/0	0/0/0/0
2	SO4	B	607	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	B	608	-	-	0/0/0/0	0/0/0/0
2	SO4	C	604	-	-	0/0/0/0	0/0/0/0
2	SO4	C	609	-	-	0/0/0/0	0/0/0/0
2	SO4	D	610	-	-	0/0/0/0	0/0/0/0
2	SO4	E	611	-	-	0/0/0/0	0/0/0/0
2	SO4	E	612	-	-	0/0/0/0	0/0/0/0
2	SO4	E	613	-	-	0/0/0/0	0/0/0/0
2	SO4	E	614	-	-	0/0/0/0	0/0/0/0
2	SO4	F	615	-	-	0/0/0/0	0/0/0/0
2	SO4	F	616	-	-	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	600	SO4	O2-S	-2.06	1.40	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	612	SO4	O2-S-O1	-2.65	101.11	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	605	SO4	1	0
2	B	606	SO4	1	0
2	E	612	SO4	1	0
2	E	613	SO4	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 will therefore be empty.

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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