



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2024 – 01:44 PM EST

PDB ID : 1HRD
Title : GLUTAMATE DEHYDROGENASE
Authors : Britton, K.L.; Baker, P.J.; Stillman, T.J.; Rice, D.W.
Deposited on : 1996-04-03
Resolution : 1.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

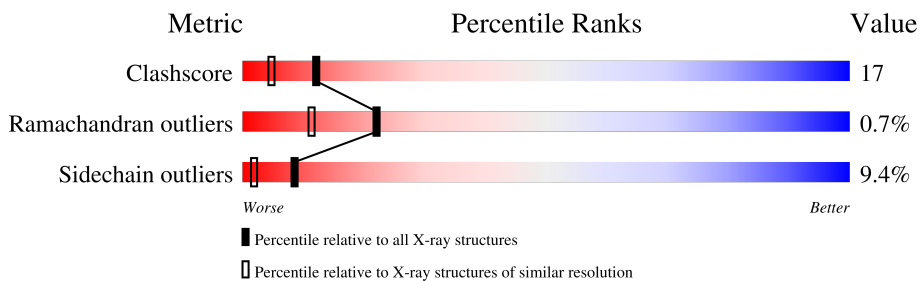
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	449	
1	B	449	
1	C	449	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10901 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
			Total	C	N	O	S			
1	A	449	3460	2198	583	660	19	0	0	0
1	B	449	3460	2198	583	660	19	0	0	0
1	C	449	3460	2198	583	660	19	0	0	0

- Molecule 2 is water.

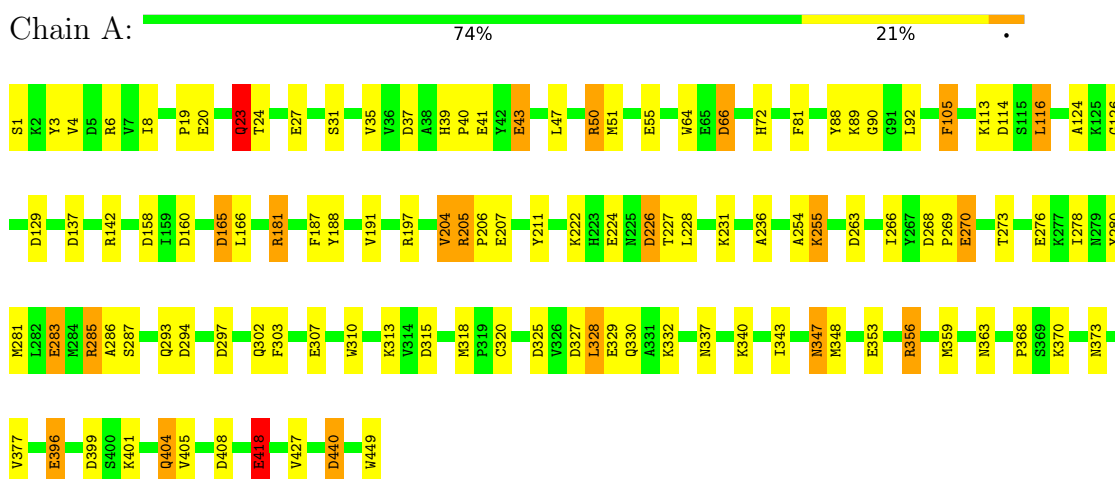
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	191	Total 191	O 191	0	0
2	B	152	Total 152	O 152	0	0
2	C	178	Total 178	O 178	0	0

3 Residue-property plots [i](#)

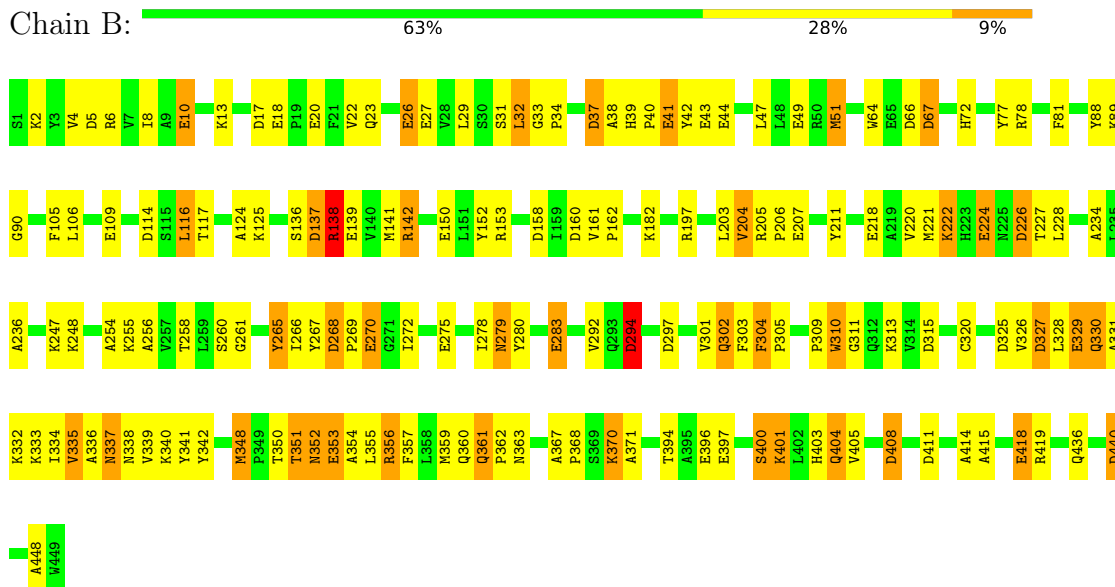
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: GLUTAMATE DEHYDROGENASE

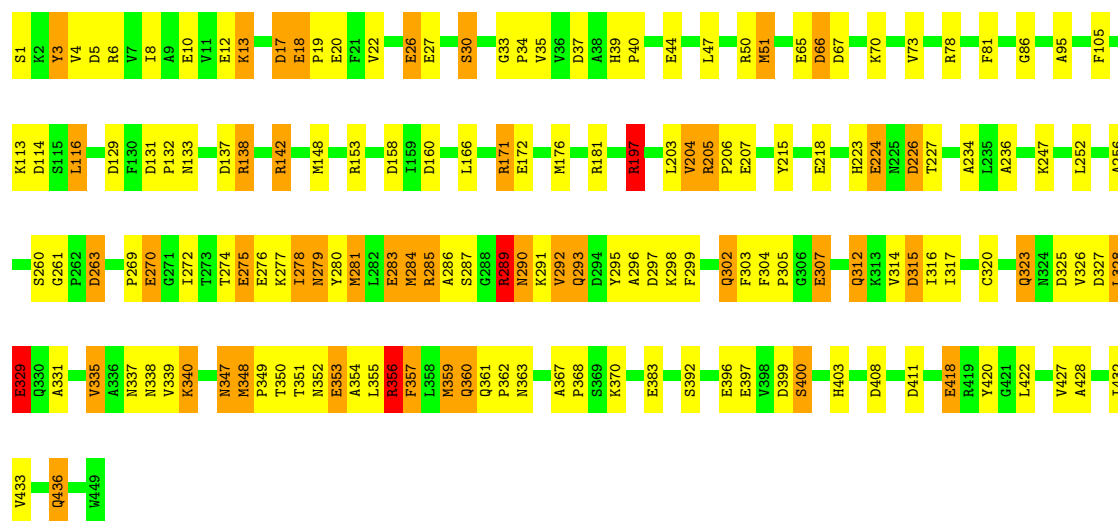


- Molecule 1: GLUTAMATE DEHYDROGENASE



- Molecule 1: GLUTAMATE DEHYDROGENASE

Chain C:  64% 25% 10%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.10Å 151.30Å 94.60Å 90.00° 132.75° 90.00°	Depositor
Resolution (Å)	37.80 – 1.96	Depositor
% Data completeness (in resolution range)	88.0 (37.80-1.96)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	10901	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	0.79	13/3535 (0.4%)	1.28	38/4781 (0.8%)
1	B	0.79	12/3535 (0.3%)	1.31	41/4781 (0.9%)
1	C	0.79	17/3535 (0.5%)	1.28	37/4781 (0.8%)
All	All	0.79	42/10605 (0.4%)	1.29	116/14343 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	2	0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	GLU	CD-OE2	6.64	1.32	1.25
1	B	329	GLU	CD-OE1	6.60	1.32	1.25
1	C	27	GLU	CD-OE2	6.50	1.32	1.25
1	C	270	GLU	CD-OE2	6.41	1.32	1.25
1	A	27	GLU	CD-OE2	6.03	1.32	1.25
1	C	418	GLU	CD-OE2	6.01	1.32	1.25
1	B	353	GLU	CD-OE2	5.94	1.32	1.25
1	A	43	GLU	CD-OE1	5.94	1.32	1.25
1	B	283	GLU	CD-OE1	5.89	1.32	1.25
1	C	218	GLU	CD-OE1	5.83	1.32	1.25
1	B	41	GLU	CD-OE1	5.74	1.31	1.25
1	C	26	GLU	CD-OE2	5.73	1.31	1.25
1	A	329	GLU	CD-OE1	5.72	1.31	1.25
1	A	418	GLU	CD-OE1	5.70	1.31	1.25
1	B	10	GLU	CD-OE1	5.68	1.31	1.25
1	B	218	GLU	CD-OE2	5.65	1.31	1.25
1	B	44	GLU	CD-OE1	5.63	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	109	GLU	CD-OE1	5.63	1.31	1.25
1	C	307	GLU	CD-OE1	5.53	1.31	1.25
1	A	270	GLU	CD-OE1	5.53	1.31	1.25
1	A	20	GLU	CD-OE1	5.52	1.31	1.25
1	A	224	GLU	CD-OE2	5.52	1.31	1.25
1	A	307	GLU	CD-OE2	5.51	1.31	1.25
1	A	276	GLU	CD-OE2	5.49	1.31	1.25
1	C	275	GLU	CD-OE2	5.49	1.31	1.25
1	C	224	GLU	CD-OE2	5.44	1.31	1.25
1	C	18	GLU	CD-OE1	5.41	1.31	1.25
1	A	55	GLU	CD-OE1	5.40	1.31	1.25
1	C	12	GLU	CD-OE1	5.32	1.31	1.25
1	B	20	GLU	CD-OE1	5.30	1.31	1.25
1	A	207	GLU	CD-OE2	5.21	1.31	1.25
1	C	20	GLU	CD-OE1	5.21	1.31	1.25
1	A	396	GLU	CD-OE2	5.20	1.31	1.25
1	B	43	GLU	CD-OE1	5.20	1.31	1.25
1	C	283	GLU	CD-OE1	5.18	1.31	1.25
1	C	329	GLU	CD-OE1	5.15	1.31	1.25
1	C	383	GLU	CD-OE1	5.15	1.31	1.25
1	C	207	GLU	CD-OE2	5.08	1.31	1.25
1	C	397	GLU	CD-OE1	5.07	1.31	1.25
1	C	65	GLU	CD-OE1	5.05	1.31	1.25
1	B	49	GLU	CD-OE1	5.05	1.31	1.25
1	B	150	GLU	CD-OE1	5.03	1.31	1.25

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	ARG	NE-CZ-NH1	9.39	124.99	120.30
1	C	142	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	A	50	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	A	285	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	66	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	A	142	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	A	165	ASP	CB-CG-OD1	-7.21	111.81	118.30
1	C	142	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	C	50	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	A	211	TYR	CB-CG-CD2	-7.12	116.73	121.00
1	B	325	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	A	325	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	C	285	ARG	NE-CZ-NH1	6.78	123.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	ASP	CB-CG-OD1	-6.75	112.22	118.30
1	A	142	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	66	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	C	153	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	297	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	A	197	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	B	294	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	A	37	ASP	CB-CG-OD1	6.41	124.06	118.30
1	B	37	ASP	CB-CG-OD1	6.41	124.07	118.30
1	B	408	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	A	285	ARG	N-CA-CB	6.39	122.11	110.60
1	B	297	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	B	37	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	C	153	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	C	408	ASP	CB-CG-OD1	-6.33	112.61	118.30
1	B	29	LEU	CB-CA-C	-6.29	98.24	110.20
1	A	315	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	A	268	ASP	CB-CG-OD2	6.26	123.94	118.30
1	A	37	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	C	315	ASP	CB-CG-OD1	-6.24	112.69	118.30
1	A	268	ASP	CB-CG-OD1	-6.18	112.73	118.30
1	C	160	ASP	CB-CG-OD1	-6.17	112.75	118.30
1	C	297	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	B	114	ASP	CB-CG-OD2	6.10	123.79	118.30
1	C	66	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	C	158	ASP	CB-CG-OD1	-6.06	112.85	118.30
1	B	211	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	C	17	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	160	ASP	CB-CG-OD1	-5.96	112.94	118.30
1	C	137	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	A	137	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	A	294	ASP	CB-CG-OD1	-5.83	113.05	118.30
1	B	114	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	C	3	TYR	CB-CG-CD2	-5.81	117.51	121.00
1	A	158	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	A	226	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	C	37	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	B	77	TYR	CB-CA-C	-5.79	98.83	110.40
1	C	114	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	325	ASP	CB-CG-OD1	5.76	123.48	118.30
1	C	226	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	B	297	ASP	CB-CG-OD1	5.74	123.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	B	411	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	C	289	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	B	17	ASP	CB-CG-OD1	-5.66	113.20	118.30
1	C	347	ASN	N-CA-CB	5.66	120.79	110.60
1	B	315	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	B	142	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	138	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	C	359	MET	CA-CB-CG	-5.64	103.71	113.30
1	B	448	ALA	N-CA-C	-5.58	95.94	111.00
1	C	356	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	285	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	165	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	329	GLU	CB-CA-C	5.53	121.45	110.40
1	A	160	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	78	ARG	N-CA-CB	5.48	120.47	110.60
1	B	160	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	C	197	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	226	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	B	5	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	A	399	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	A	114	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	A	408	ASP	CB-CG-OD2	5.42	123.17	118.30
1	B	27	GLU	N-CA-CB	-5.39	100.89	110.60
1	B	268	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	138	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	205	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	263	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	C	276	GLU	N-CA-CB	-5.36	100.95	110.60
1	C	226	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	182	LYS	CA-CB-CG	-5.35	101.63	113.40
1	B	411	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	181	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	330	GLN	CB-CA-C	5.28	120.95	110.40
1	B	137	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	B	67	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	129	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	B	158	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	C	411	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	A	6	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	17	ASP	CB-CG-OD1	5.21	122.98	118.30
1	A	23	GLN	N-CA-CB	-5.20	101.25	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	325	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	B	78	ARG	N-CA-CB	5.19	119.94	110.60
1	A	66	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	280	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	B	265	TYR	CB-CG-CD2	-5.16	117.91	121.00
1	A	285	ARG	CD-NE-CZ	5.15	130.81	123.60
1	B	327	ASP	CB-CG-OD2	5.14	122.93	118.30
1	C	399	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	A	129	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	181	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	408	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	B	327	ASP	CB-CG-OD1	-5.07	113.73	118.30
1	B	440	ASP	CB-CG-OD1	-5.06	113.74	118.30
1	A	440	ASP	CB-CG-OD1	-5.05	113.75	118.30
1	B	226	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	67	ASP	CB-CG-OD1	-5.05	113.76	118.30
1	C	137	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	211	TYR	CB-CG-CD1	5.02	124.01	121.00
1	C	263	ASP	CB-CG-OD1	-5.00	113.80	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	278	ILE	CA
1	C	329	GLU	CA

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3460	0	3390	71	0
1	B	3460	0	3390	144	0
1	C	3460	0	3390	137	0
2	A	191	0	0	2	0
2	B	152	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	178	0	0	4	0
All	All	10901	0	10170	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 17.

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:A:347:ASN:HD22	1:A:348:MET:N	1.27	1.32
1:B:360:GLN:O	1:B:362:PRO:HD3	1.33	1.24
1:C:280:TYR:O	1:C:283:GLU:HB2	1.44	1.17
1:C:302:GLN:HA	1:C:302:GLN:OE1	1.46	1.10
1:C:323:GLN:OE1	1:C:348:MET:HG2	1.50	1.08
1:B:313:LYS:HG3	1:B:337:ASN:HB3	1.34	1.06
1:C:289:ARG:NH2	1:C:291:LYS:HD2	1.70	1.05
1:A:347:ASN:ND2	1:A:348:MET:N	2.05	1.03
1:B:267:TYR:CE2	1:B:269:PRO:HG3	1.95	1.01
1:C:280:TYR:HA	1:C:283:GLU:HG3	1.47	0.94
1:A:347:ASN:HD22	1:A:348:MET:H	1.09	0.94
1:C:280:TYR:CE2	1:C:284:MET:CE	2.51	0.94
1:C:280:TYR:CE2	1:C:284:MET:HE2	2.02	0.93
1:B:394:THR:OG1	1:B:397:GLU:HG3	1.68	0.92
1:A:35:VAL:O	1:A:39:HIS:HD2	1.53	0.90
1:B:360:GLN:O	1:B:362:PRO:CD	2.21	0.89
1:C:347:ASN:OD1	1:C:348:MET:N	2.05	0.88
1:C:1:SER:O	1:C:5:ASP:OD2	1.91	0.87
1:C:352:ASN:O	1:C:356:ARG:HG2	1.75	0.85
1:B:331:ALA:O	1:B:335:VAL:HG22	1.77	0.84
1:C:323:GLN:HG2	1:C:348:MET:O	1.77	0.84
1:B:236:ALA:HB2	1:B:310:TRP:CZ2	2.13	0.83
1:B:302:GLN:HB3	1:B:304:PHE:CE1	2.14	0.83
1:B:331:ALA:O	1:B:335:VAL:CG2	2.26	0.83
1:C:26:GLU:O	1:C:30:SER:OG	1.97	0.82
1:C:323:GLN:CD	1:C:348:MET:HG2	1.99	0.82
1:A:89:LYS:HE3	2:A:573:HOH:O	1.76	0.82
1:B:313:LYS:HE2	1:B:337:ASN:HB3	1.60	0.82
1:C:35:VAL:O	1:C:39:HIS:HD2	1.62	0.82
1:B:221:MET:HA	1:B:221:MET:CE	2.10	0.82
1:C:323:GLN:CG	1:C:348:MET:HG2	2.11	0.80
1:B:313:LYS:HE2	1:B:337:ASN:CA	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LYS:CE	1:B:337:ASN:HB3	2.12	0.80
1:B:116:LEU:C	1:B:116:LEU:HD23	2.02	0.80
1:B:313:LYS:HE2	1:B:337:ASN:CB	2.12	0.79
1:B:4:VAL:O	1:B:8:ILE:HG13	1.82	0.79
1:A:348:MET:CG	1:A:348:MET:O	2.26	0.79
1:B:226:ASP:OD1	1:B:227:THR:N	2.16	0.79
1:A:227:THR:O	1:A:231:LYS:HE3	1.83	0.78
1:B:310:TRP:HB2	1:B:330:GLN:HB3	1.64	0.78
1:C:340:LYS:O	1:C:340:LYS:HG3	1.81	0.78
1:C:323:GLN:HG2	1:C:348:MET:HG2	1.66	0.78
1:C:331:ALA:O	1:C:335:VAL:HG23	1.83	0.77
1:B:340:LYS:HG2	1:B:340:LYS:O	1.83	0.77
1:C:323:GLN:OE1	1:C:348:MET:CG	2.31	0.77
1:B:330:GLN:OE1	1:B:333:LYS:HE3	1.84	0.76
1:C:355:LEU:O	1:C:359:MET:HB2	1.86	0.76
1:B:23:GLN:O	1:B:26:GLU:HB3	1.85	0.75
1:B:313:LYS:HG3	1:B:337:ASN:CB	2.14	0.74
1:B:236:ALA:HB2	1:B:310:TRP:HZ2	1.53	0.74
1:B:313:LYS:HE2	1:B:337:ASN:HA	1.70	0.74
1:C:280:TYR:CE2	1:C:284:MET:HE3	2.21	0.74
1:A:116:LEU:C	1:A:116:LEU:HD23	2.08	0.73
1:B:313:LYS:CG	1:B:337:ASN:HB3	2.14	0.73
1:C:280:TYR:HD1	1:C:283:GLU:HG3	1.52	0.73
1:C:304:PHE:O	1:C:307:GLU:HB2	1.87	0.73
1:C:328:LEU:HB2	1:C:353:GLU:OE1	1.89	0.72
1:B:138:ARG:HD2	1:B:141:MET:HE1	1.71	0.72
1:B:224:GLU:OE1	1:B:224:GLU:HA	1.90	0.71
1:B:302:GLN:HB3	1:B:304:PHE:HE1	1.55	0.71
1:A:418:GLU:HB2	2:A:602:HOH:O	1.91	0.71
1:A:340:LYS:HG3	1:A:363:ASN:O	1.91	0.70
1:B:267:TYR:CZ	1:B:269:PRO:HG3	2.25	0.70
1:C:263:ASP:O	1:C:305:PRO:HA	1.91	0.69
1:B:313:LYS:CE	1:B:337:ASN:CB	2.70	0.69
1:B:138:ARG:HD3	1:B:141:MET:HE2	1.74	0.69
1:B:221:MET:HA	1:B:221:MET:HE2	1.74	0.69
1:A:4:VAL:O	1:A:8:ILE:HD12	1.92	0.69
1:A:204:VAL:HG12	1:A:204:VAL:O	1.91	0.69
1:B:404:GLN:O	1:B:408:ASP:OD2	2.10	0.68
1:B:138:ARG:HD2	1:B:141:MET:CE	2.23	0.68
1:A:35:VAL:O	1:A:39:HIS:CD2	2.42	0.68
1:A:327:ASP:OD1	1:A:330:GLN:HG2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:LYS:HD2	1:C:13:LYS:N	2.07	0.67
1:B:337:ASN:N	1:B:337:ASN:HD22	1.91	0.67
1:C:284:MET:HE1	1:C:295:TYR:N	2.10	0.67
1:B:138:ARG:CD	1:B:141:MET:HE2	2.24	0.66
1:B:265:TYR:CE2	1:B:309:PRO:HA	2.30	0.66
1:B:335:VAL:HG21	1:B:357:PHE:CZ	2.31	0.66
1:C:275:GLU:O	1:C:279:ASN:ND2	2.29	0.66
1:C:289:ARG:O	1:C:291:LYS:N	2.28	0.66
1:C:280:TYR:CD1	1:C:283:GLU:HG3	2.31	0.66
1:B:267:TYR:O	1:B:301:VAL:HB	1.96	0.65
1:C:420:TYR:C	1:C:422:LEU:HD12	2.17	0.65
1:C:289:ARG:HH21	1:C:291:LYS:HD2	1.58	0.64
1:C:1:SER:HB3	1:C:4:VAL:HB	1.79	0.64
1:C:223:HIS:ND1	1:C:224:GLU:OE2	2.30	0.64
1:A:348:MET:O	1:A:348:MET:HG3	1.97	0.64
1:C:17:ASP:C	1:C:19:PRO:HD3	2.18	0.64
1:B:304:PHE:CD1	1:B:304:PHE:N	2.66	0.64
1:A:328:LEU:HD13	1:A:332:LYS:HE3	1.79	0.64
1:C:226:ASP:OD1	1:C:227:THR:N	2.30	0.63
1:B:348:MET:O	1:B:348:MET:CG	2.46	0.63
1:C:3:TYR:CD1	1:C:6:ARG:NH2	2.66	0.63
1:C:256:ALA:O	1:C:272:ILE:HD12	1.98	0.63
1:C:420:TYR:O	1:C:422:LEU:HD12	1.99	0.63
1:B:224:GLU:OE1	1:B:224:GLU:CA	2.44	0.63
1:B:228:LEU:O	1:B:254:ALA:HB2	1.99	0.63
1:C:354:ALA:O	1:C:357:PHE:HB3	1.98	0.62
1:A:347:ASN:ND2	1:A:347:ASN:C	2.46	0.62
1:C:323:GLN:HG2	1:C:348:MET:CG	2.30	0.62
1:B:205:ARG:HB3	1:B:206:PRO:HD3	1.82	0.62
1:B:221:MET:HE1	1:B:341:TYR:CZ	2.35	0.62
1:C:35:VAL:O	1:C:39:HIS:CD2	2.50	0.61
1:C:348:MET:O	1:C:348:MET:HG3	2.00	0.61
1:B:275:GLU:O	1:B:279:ASN:OD1	2.18	0.61
1:A:3:TYR:CD2	1:A:43:GLU:HB2	2.36	0.61
1:C:33:GLY:N	1:C:34:PRO:HD2	2.15	0.61
1:C:348:MET:O	1:C:348:MET:CG	2.45	0.61
1:C:420:TYR:O	1:C:422:LEU:CD1	2.50	0.60
1:C:204:VAL:HG12	1:C:204:VAL:O	2.01	0.60
1:B:138:ARG:CD	1:B:141:MET:CE	2.79	0.60
1:A:404:GLN:HG2	1:A:405:VAL:N	2.15	0.60
1:C:348:MET:HA	2:C:576:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:TYR:HH	1:B:350:THR:HG1	1.51	0.59
1:C:302:GLN:HB3	1:C:304:PHE:CE1	2.37	0.59
1:C:337:ASN:O	1:C:338:ASN:HB2	2.02	0.59
1:A:3:TYR:CE2	1:A:43:GLU:HB2	2.38	0.59
1:A:368:PRO:HG3	1:A:427:VAL:HA	1.85	0.59
1:C:338:ASN:HD22	1:C:338:ASN:N	2.01	0.59
1:C:261:GLY:HA3	1:C:292:VAL:HB	1.86	0.58
1:B:268:ASP:OD1	1:B:268:ASP:C	2.42	0.58
1:B:348:MET:O	1:B:348:MET:HG3	2.05	0.57
1:B:414:ALA:O	1:B:418:GLU:HB2	2.05	0.57
1:C:327:ASP:OD1	1:C:329:GLU:N	2.37	0.57
1:A:266:ILE:C	1:A:266:ILE:HD12	2.24	0.57
1:C:280:TYR:HE2	1:C:284:MET:CE	2.16	0.57
1:B:221:MET:CE	1:B:221:MET:CA	2.81	0.57
1:B:40:PRO:HD2	1:B:41:GLU:OE1	2.05	0.56
1:C:280:TYR:HA	1:C:283:GLU:CG	2.28	0.56
1:C:328:LEU:HD22	1:C:328:LEU:O	2.06	0.56
1:C:352:ASN:H	1:C:352:ASN:ND2	2.03	0.56
1:C:280:TYR:CE1	1:C:298:LYS:HD3	2.41	0.55
1:C:302:GLN:OE1	1:C:302:GLN:CA	2.31	0.55
1:B:313:LYS:CE	1:B:337:ASN:HA	2.36	0.55
1:C:317:ILE:HG12	1:C:339:VAL:HG11	1.88	0.55
1:C:422:LEU:HD12	1:C:422:LEU:N	2.22	0.55
1:B:331:ALA:HB1	1:B:357:PHE:CD2	2.41	0.55
1:A:19:PRO:O	1:A:23:GLN:HB2	2.05	0.55
1:C:327:ASP:HA	1:C:351:THR:CG2	2.37	0.55
1:B:236:ALA:O	1:B:320:CYS:HB2	2.07	0.54
1:B:415:ALA:HA	1:B:418:GLU:HB2	1.89	0.54
1:B:348:MET:HA	2:B:528:HOH:O	2.06	0.54
1:A:236:ALA:HB2	1:A:310:TRP:CZ2	2.42	0.54
1:B:335:VAL:HG21	1:B:357:PHE:CE2	2.43	0.54
1:B:335:VAL:O	1:B:338:ASN:N	2.39	0.54
1:B:400:SER:O	1:B:404:GLN:HG3	2.08	0.54
1:B:327:ASP:O	1:B:331:ALA:N	2.34	0.53
1:A:348:MET:O	1:A:348:MET:HG2	2.06	0.53
1:B:272:ILE:O	1:B:278:ILE:HD11	2.08	0.53
1:A:280:TYR:HA	1:A:283:GLU:HG3	1.89	0.53
1:A:440:ASP:HB3	2:B:505:HOH:O	2.09	0.53
1:A:280:TYR:CD1	1:A:283:GLU:HG3	2.44	0.53
1:C:236:ALA:O	1:C:320:CYS:HB2	2.09	0.53
1:B:32:LEU:C	1:B:34:PRO:HD2	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:GLN:HB2	1:C:303:PHE:CD1	2.43	0.53
1:C:347:ASN:OD1	1:C:347:ASN:C	2.39	0.53
1:C:280:TYR:CZ	1:C:298:LYS:HD3	2.44	0.53
1:C:327:ASP:OD1	1:C:327:ASP:C	2.48	0.52
1:A:88:TYR:HB3	1:A:124:ALA:HB2	1.91	0.52
1:A:50:ARG:HD2	1:A:449:TRP:OXT	2.10	0.52
1:A:347:ASN:ND2	1:A:348:MET:CB	2.73	0.52
1:B:67:ASP:OD1	1:B:142:ARG:NH2	2.35	0.52
1:A:328:LEU:O	1:A:332:LYS:HG3	2.10	0.51
1:A:269:PRO:HD2	1:A:270:GLU:H	1.75	0.51
1:B:403:HIS:HD2	1:B:403:HIS:O	1.93	0.51
1:C:113:LYS:HE3	1:C:370:LYS:O	2.10	0.51
1:C:327:ASP:HA	1:C:351:THR:HG23	1.92	0.51
1:A:165:ASP:CG	1:A:166:LEU:H	2.13	0.51
1:B:261:GLY:HA3	1:B:292:VAL:HB	1.92	0.51
1:B:330:GLN:NE2	2:B:564:HOH:O	2.43	0.51
1:B:90:GLY:HA3	1:B:124:ALA:O	2.10	0.51
1:B:340:LYS:O	1:B:340:LYS:CG	2.55	0.51
1:B:6:ARG:O	1:B:10:GLU:HG3	2.11	0.51
1:C:47:LEU:O	1:C:51:MET:HG3	2.11	0.51
1:C:171:ARG:HD2	1:C:172:GLU:OE2	2.10	0.51
1:C:280:TYR:CZ	1:C:284:MET:HE2	2.45	0.51
1:B:116:LEU:C	1:B:116:LEU:CD2	2.79	0.51
1:B:332:LYS:O	1:B:335:VAL:HG23	2.11	0.51
1:C:283:GLU:O	1:C:286:ALA:HB3	2.10	0.51
1:B:221:MET:HE3	1:B:221:MET:N	2.26	0.50
1:C:274:THR:OG1	1:C:277:LYS:HB2	2.11	0.50
1:B:38:ALA:C	1:B:40:PRO:HD3	2.31	0.50
1:B:234:ALA:HA	1:B:258:THR:OG1	2.12	0.50
1:B:396:GLU:HB2	2:B:576:HOH:O	2.10	0.50
1:A:313:LYS:HB2	1:A:337:ASN:OD1	2.12	0.50
1:B:221:MET:CA	1:B:221:MET:HE3	2.41	0.50
1:B:440:ASP:HB3	2:C:532:HOH:O	2.11	0.50
1:C:348:MET:HA	2:C:578:HOH:O	2.12	0.50
1:C:312:GLN:OE1	1:C:312:GLN:HA	2.11	0.49
1:B:335:VAL:HG21	1:B:357:PHE:HZ	1.74	0.49
1:A:255:LYS:HB2	1:A:273:THR:CG2	2.42	0.49
1:C:8:ILE:HD13	1:C:26:GLU:HA	1.95	0.49
1:B:203:LEU:C	1:B:204:VAL:HG23	2.31	0.49
1:B:33:GLY:O	1:B:37:ASP:N	2.30	0.49
1:B:302:GLN:HA	1:B:302:GLN:HE21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LYS:HD2	1:B:161:VAL:O	2.12	0.49
1:B:304:PHE:N	1:B:304:PHE:HD1	2.11	0.49
1:A:47:LEU:O	1:A:51:MET:HG3	2.13	0.48
1:B:302:GLN:HE21	1:B:302:GLN:CA	2.26	0.48
1:B:335:VAL:O	1:B:338:ASN:HA	2.13	0.48
1:A:1:SER:HB3	1:A:4:VAL:HB	1.96	0.48
1:C:116:LEU:HD23	1:C:433:VAL:HG13	1.94	0.48
1:A:90:GLY:HA3	1:A:124:ALA:O	2.13	0.48
1:A:236:ALA:O	1:A:320:CYS:HB2	2.14	0.48
1:B:333:LYS:NZ	2:B:597:HOH:O	2.47	0.48
1:B:355:LEU:HG	1:B:359:MET:CE	2.44	0.48
1:C:280:TYR:CD2	1:C:299:PHE:HE2	2.31	0.48
1:A:205:ARG:N	1:A:206:PRO:CD	2.77	0.48
1:A:204:VAL:O	1:A:204:VAL:CG1	2.61	0.47
1:B:39:HIS:N	1:B:40:PRO:HD3	2.29	0.47
1:B:64:TRP:CE2	1:B:72:HIS:HB2	2.49	0.47
1:B:303:PHE:CD2	1:B:305:PRO:HD3	2.49	0.47
1:B:396:GLU:CD	1:B:396:GLU:H	2.17	0.47
1:A:278:ILE:O	1:A:281:MET:HB2	2.13	0.47
1:B:47:LEU:O	1:B:51:MET:HG3	2.14	0.47
1:B:401:LYS:O	1:B:405:VAL:HG23	2.14	0.47
1:C:116:LEU:HD23	1:C:433:VAL:CG1	2.42	0.47
1:B:330:GLN:OE1	1:B:333:LYS:CE	2.59	0.47
1:C:289:ARG:C	1:C:291:LYS:N	2.68	0.47
1:B:331:ALA:O	1:B:335:VAL:HG23	2.11	0.47
1:C:289:ARG:O	1:C:290:ASN:C	2.50	0.47
1:B:224:GLU:HG3	1:B:340:LYS:NZ	2.30	0.47
1:C:347:ASN:O	1:C:348:MET:HB3	2.14	0.47
1:C:260:SER:HA	1:C:292:VAL:HG21	1.97	0.47
1:B:335:VAL:CG1	1:B:361:GLN:HG3	2.45	0.47
1:C:350:THR:HG22	1:C:354:ALA:HB3	1.97	0.47
1:A:187:PHE:CZ	1:C:86:GLY:HA2	2.49	0.47
1:C:263:ASP:HB2	1:C:303:PHE:HZ	1.80	0.46
1:C:368:PRO:HG3	1:C:427:VAL:HA	1.96	0.46
1:B:294:ASP:N	1:B:294:ASP:OD1	2.47	0.46
1:C:296:ALA:CB	1:C:303:PHE:HB2	2.46	0.46
1:B:403:HIS:C	1:B:403:HIS:CD2	2.89	0.46
1:A:347:ASN:ND2	1:A:348:MET:H	1.91	0.46
1:A:283:GLU:H	1:A:283:GLU:HG2	1.42	0.46
1:B:332:LYS:C	1:B:335:VAL:HG23	2.36	0.46
1:C:323:GLN:HG3	1:C:348:MET:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:HIS:HA	1:A:40:PRO:HD2	1.82	0.46
1:A:226:ASP:OD1	1:A:231:LYS:NZ	2.37	0.46
1:C:428:ALA:O	1:C:432:ILE:HG13	2.16	0.46
1:B:332:LYS:HA	1:B:335:VAL:CG2	2.46	0.46
1:C:348:MET:N	1:C:349:PRO:HD3	2.31	0.46
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.71	0.46
1:A:280:TYR:HA	1:A:283:GLU:CG	2.46	0.46
1:C:247:LYS:HD2	1:C:278:ILE:HD11	1.98	0.45
1:C:261:GLY:CA	1:C:292:VAL:HB	2.46	0.45
1:B:4:VAL:O	1:B:8:ILE:CG1	2.59	0.45
1:C:354:ALA:O	1:C:357:PHE:CB	2.65	0.45
1:C:315:ASP:C	1:C:316:ILE:HG13	2.36	0.45
1:C:396:GLU:O	1:C:400:SER:HB2	2.17	0.45
1:C:355:LEU:HG	1:C:359:MET:CE	2.47	0.45
1:B:256:ALA:O	1:B:272:ILE:HD12	2.16	0.45
1:A:330:GLN:HA	1:A:330:GLN:NE2	2.32	0.45
1:C:263:ASP:OD1	1:C:263:ASP:N	2.42	0.45
1:C:280:TYR:C	1:C:283:GLU:HB2	2.30	0.45
1:B:39:HIS:HA	1:B:40:PRO:HD2	1.78	0.45
1:B:106:LEU:HB2	1:B:125:LYS:HG2	1.99	0.45
1:B:351:THR:O	1:B:354:ALA:N	2.50	0.45
1:C:18:GLU:N	1:C:19:PRO:HD3	2.32	0.45
1:C:280:TYR:CD2	1:C:299:PHE:CE2	3.05	0.45
1:C:292:VAL:HG12	1:C:303:PHE:HE1	1.81	0.45
1:A:43:GLU:O	1:A:43:GLU:HG2	2.16	0.45
1:A:113:LYS:HE2	1:A:377:VAL:HG21	1.98	0.45
1:B:327:ASP:OD1	1:B:330:GLN:N	2.41	0.45
1:C:148:MET:CE	1:C:176:MET:HB3	2.47	0.45
1:B:367:ALA:HA	1:B:368:PRO:HD3	1.84	0.44
1:B:436:GLN:OE1	1:B:436:GLN:HA	2.17	0.44
1:C:171:ARG:NH1	1:C:172:GLU:OE2	2.45	0.44
1:C:215:TYR:CD2	1:C:403:HIS:HA	2.52	0.44
1:C:280:TYR:CD1	1:C:283:GLU:CG	2.99	0.44
1:C:338:ASN:N	1:C:338:ASN:ND2	2.66	0.44
1:B:266:ILE:C	1:B:266:ILE:HD12	2.38	0.44
1:C:280:TYR:CD2	1:C:284:MET:HE3	2.52	0.44
1:A:269:PRO:CD	1:A:270:GLU:H	2.31	0.44
1:B:352:ASN:O	1:B:356:ARG:HG2	2.17	0.44
1:A:66:ASP:OD1	1:A:66:ASP:C	2.55	0.44
1:A:293:GLN:HG3	1:A:303:PHE:CG	2.52	0.44
1:A:64:TRP:CE2	1:A:72:HIS:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ARG:N	1:C:206:PRO:CD	2.81	0.44
1:B:33:GLY:N	1:B:34:PRO:HD2	2.33	0.43
1:B:116:LEU:HD23	1:B:117:THR:N	2.33	0.43
1:C:39:HIS:HA	1:C:40:PRO:HD2	1.74	0.43
1:C:66:ASP:OD1	1:C:66:ASP:C	2.57	0.43
1:C:293:GLN:HB2	1:C:303:PHE:CG	2.52	0.43
1:B:88:TYR:HB3	1:B:124:ALA:HB2	1.99	0.43
1:B:309:PRO:C	1:B:311:GLY:H	2.21	0.43
1:C:131:ASP:HA	1:C:132:PRO:HD3	1.78	0.43
1:B:337:ASN:N	1:B:337:ASN:ND2	2.64	0.43
1:C:278:ILE:HD13	1:C:278:ILE:C	2.39	0.43
1:A:228:LEU:O	1:A:254:ALA:HB2	2.18	0.43
1:C:18:GLU:N	1:C:19:PRO:CD	2.79	0.43
1:C:95:ALA:O	1:C:129:ASP:HA	2.18	0.43
1:C:436:GLN:O	1:C:436:GLN:HG3	2.17	0.43
1:B:33:GLY:N	1:B:34:PRO:CD	2.82	0.43
1:C:138:ARG:HG3	1:C:142:ARG:NH1	2.34	0.43
1:C:197:ARG:HD3	1:C:203:LEU:HD23	2.00	0.43
1:C:323:GLN:CG	1:C:348:MET:CG	2.89	0.43
1:C:326:VAL:O	1:C:351:THR:HG23	2.18	0.43
1:B:203:LEU:O	1:B:204:VAL:HB	2.18	0.43
1:B:270:GLU:H	1:B:270:GLU:HG2	1.68	0.43
1:C:367:ALA:HA	1:C:368:PRO:HD3	1.80	0.43
1:C:357:PHE:C	1:C:359:MET:N	2.71	0.43
1:A:266:ILE:HD12	1:A:266:ILE:O	2.19	0.42
1:B:310:TRP:CD1	1:B:326:VAL:HG22	2.53	0.42
1:B:370:LYS:HG3	1:B:371:ALA:N	2.34	0.42
1:B:18:GLU:O	1:B:22:VAL:HG23	2.19	0.42
1:B:265:TYR:CD2	1:B:309:PRO:HA	2.54	0.42
1:C:289:ARG:NH2	1:C:291:LYS:CD	2.61	0.42
1:B:313:LYS:HE3	1:B:337:ASN:CG	2.40	0.42
1:B:332:LYS:CA	1:B:335:VAL:HG23	2.50	0.42
1:B:400:SER:O	1:B:404:GLN:CG	2.66	0.42
1:C:67:ASP:OD1	1:C:142:ARG:NH2	2.41	0.42
1:B:332:LYS:HA	1:B:335:VAL:HG23	2.02	0.42
1:B:334:ILE:HG22	1:B:335:VAL:N	2.34	0.42
1:C:18:GLU:O	1:C:22:VAL:HG23	2.19	0.42
1:A:92:LEU:O	1:A:165:ASP:HB3	2.20	0.42
1:C:350:THR:HG22	1:C:351:THR:O	2.20	0.42
1:B:41:GLU:HG2	1:B:42:TYR:N	2.34	0.42
1:B:203:LEU:HA	1:B:203:LEU:HD23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:LEU:HD23	1:C:203:LEU:HA	1.83	0.42
1:C:323:GLN:CG	1:C:348:MET:HB3	2.50	0.42
1:C:360:GLN:HG3	2:C:609:HOH:O	2.19	0.42
1:A:24:THR:HG1	1:A:105:PHE:HD1	1.68	0.42
1:B:136:SER:OG	1:B:139:GLU:HG3	2.20	0.42
1:A:41:GLU:OE1	1:A:41:GLU:N	2.35	0.41
1:C:361:GLN:HA	1:C:362:PRO:HD3	1.64	0.41
1:A:116:LEU:C	1:A:116:LEU:CD2	2.85	0.41
1:B:221:MET:O	1:B:222:LYS:C	2.59	0.41
1:C:278:ILE:O	1:C:281:MET:HB2	2.20	0.41
1:A:236:ALA:HB2	1:A:310:TRP:CH2	2.56	0.41
1:B:331:ALA:O	1:B:334:ILE:HB	2.21	0.41
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.89	0.41
1:B:350:THR:CG2	1:B:354:ALA:HB3	2.51	0.41
1:C:323:GLN:OE1	1:C:348:MET:SD	2.78	0.41
1:A:356:ARG:HA	1:A:356:ARG:HD3	1.31	0.41
1:B:152:TYR:CD1	1:B:152:TYR:C	2.93	0.41
1:C:113:LYS:HZ2	1:C:370:LYS:HA	1.86	0.41
1:A:188:TYR:O	1:A:191:VAL:HG12	2.21	0.41
1:B:313:LYS:CD	1:B:337:ASN:HB3	2.51	0.41
1:A:318:MET:HG2	1:A:343:ILE:HB	2.02	0.41
1:A:113:LYS:NZ	1:A:373:ASN:OD1	2.51	0.41
1:B:152:TYR:CG	1:B:153:ARG:N	2.88	0.41
1:B:336:ALA:C	1:B:338:ASN:H	2.25	0.41
1:B:220:VAL:O	1:B:221:MET:C	2.60	0.40
1:B:228:LEU:HA	1:B:228:LEU:HD23	1.78	0.40
1:A:92:LEU:HA	1:A:126:GLY:O	2.22	0.40
1:A:286:ALA:O	1:A:287:SER:C	2.60	0.40
1:A:340:LYS:O	1:A:340:LYS:HG2	2.21	0.40
1:C:234:ALA:HB2	1:C:314:VAL:HG11	2.03	0.40
1:B:207:GLU:OE1	1:B:207:GLU:N	2.47	0.40
1:B:267:TYR:HB3	1:B:302:GLN:HB2	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	447/449 (100%)	432 (97%)	14 (3%)	1 (0%)	47	38
1	B	447/449 (100%)	424 (95%)	18 (4%)	5 (1%)	14	5
1	C	447/449 (100%)	420 (94%)	23 (5%)	4 (1%)	17	8
All	All	1341/1347 (100%)	1276 (95%)	55 (4%)	10 (1%)	22	11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	290	ASN
1	B	204	VAL
1	B	310	TRP
1	B	361	GLN
1	C	289	ARG
1	A	204	VAL
1	B	329	GLU
1	B	352	ASN
1	C	204	VAL
1	C	357	PHE

5.3.2 Protein sidechains [i](#)

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	358/358 (100%)	338 (94%)	20 (6%)	21	9
1	B	358/358 (100%)	318 (89%)	40 (11%)	6	1
1	C	358/358 (100%)	317 (88%)	41 (12%)	5	1
All	All	1074/1074 (100%)	973 (91%)	101 (9%)	8	2

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	31	SER
1	A	81	PHE
1	A	105	PHE
1	A	116	LEU
1	A	181	ARG
1	A	222	LYS
1	A	255	LYS
1	A	283	GLU
1	A	285	ARG
1	A	302	GLN
1	A	328	LEU
1	A	347	ASN
1	A	356	ARG
1	A	359	MET
1	A	370	LYS
1	A	396	GLU
1	A	401	LYS
1	A	404	GLN
1	A	418	GLU
1	B	2	LYS
1	B	13	LYS
1	B	26	GLU
1	B	31	SER
1	B	32	LEU
1	B	51	MET
1	B	81	PHE
1	B	105	PHE
1	B	116	LEU
1	B	137	ASP
1	B	138	ARG
1	B	162	PRO
1	B	197	ARG
1	B	222	LYS
1	B	224	GLU
1	B	247	LYS
1	B	248	LYS
1	B	255	LYS
1	B	260	SER
1	B	270	GLU
1	B	279	ASN
1	B	283	GLU
1	B	294	ASP

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Mol	Chain	Res	Type
1	B	302	GLN
1	B	304	PHE
1	B	328	LEU
1	B	335	VAL
1	B	337	ASN
1	B	339	VAL
1	B	348	MET
1	B	351	THR
1	B	353	GLU
1	B	356	ARG
1	B	363	ASN
1	B	370	LYS
1	B	400	SER
1	B	401	LYS
1	B	404	GLN
1	B	418	GLU
1	B	419	ARG
1	C	10	GLU
1	C	13	LYS
1	C	30	SER
1	C	44	GLU
1	C	51	MET
1	C	70	LYS
1	C	73	VAL
1	C	81	PHE
1	C	105	PHE
1	C	116	LEU
1	C	133	ASN
1	C	166	LEU
1	C	171	ARG
1	C	197	ARG
1	C	205	ARG
1	C	269	PRO
1	C	270	GLU
1	C	278	ILE
1	C	279	ASN
1	C	281	MET
1	C	284	MET
1	C	285	ARG
1	C	287	SER
1	C	292	VAL
1	C	293	GLN

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Mol	Chain	Res	Type
1	C	302	GLN
1	C	312	GLN
1	C	323	GLN
1	C	328	LEU
1	C	329	GLU
1	C	335	VAL
1	C	340	LYS
1	C	348	MET
1	C	353	GLU
1	C	356	ARG
1	C	360	GLN
1	C	363	ASN
1	C	392	SER
1	C	400	SER
1	C	418	GLU
1	C	436	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	68	ASN
1	A	312	GLN
1	A	330	GLN
1	A	347	ASN
1	A	360	GLN
1	B	23	GLN
1	B	302	GLN
1	B	337	ASN
1	B	363	ASN
1	B	403	HIS
1	B	404	GLN
1	C	23	GLN
1	C	39	HIS
1	C	133	ASN
1	C	279	ASN
1	C	330	GLN
1	C	338	ASN
1	C	352	ASN
1	C	360	GLN
1	C	361	GLN
1	C	436	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.