



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:57 PM UTC

PDB ID : 2DQN / pdb_00002dqn
Title : Structure of tRNA-Dependent Amidotransferase GatCAB complexed with Asn
Authors : Nakamura, A.; Yao, M.; Tanaka, I.
Deposited on : 2006-05-29
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

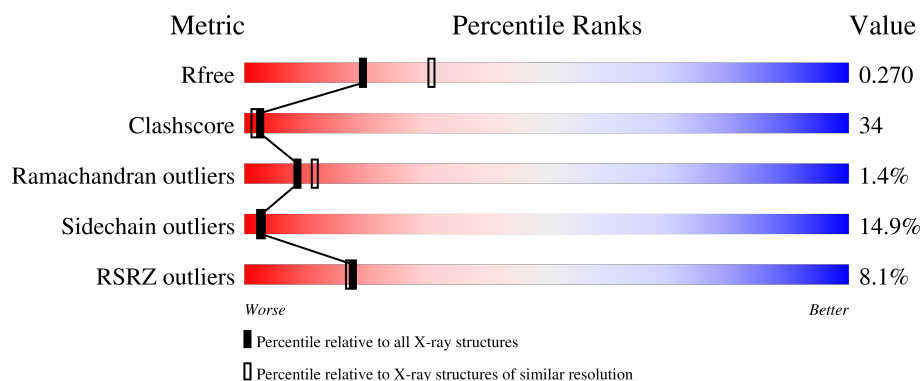
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	485	13% 53% 37% 9% .
2	B	483	13% 33% 37% 13% . 16%
3	C	100	11% 49% 31% 16% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7925 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 Glutamyl-tRNA(Gln) amidotransferase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3716	2359	605	739	13			

- Molecule 2 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	0	0
			3228	2034	542	639	13			

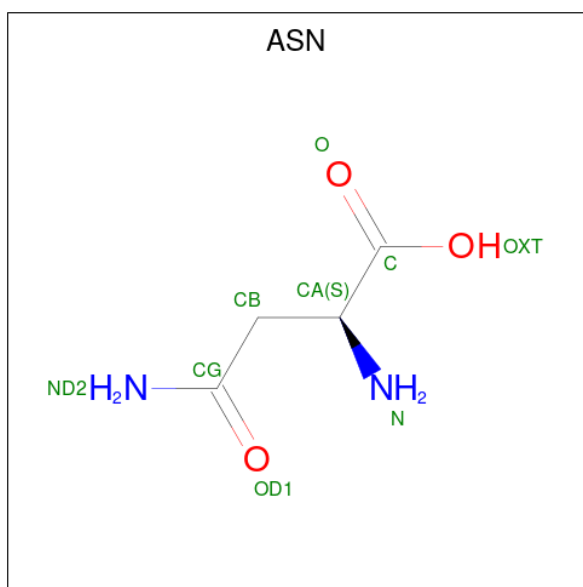
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	476	LEU	-	expression tag	UNP P64201
B	477	GLU	-	expression tag	UNP P64201
B	478	HIS	-	expression tag	UNP P64201
B	479	HIS	-	expression tag	UNP P64201
B	480	HIS	-	expression tag	UNP P64201
B	481	HIS	-	expression tag	UNP P64201
B	482	HIS	-	expression tag	UNP P64201
B	483	HIS	-	expression tag	UNP P64201

- Molecule 3 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	98	Total	C	N	O	S	0	0	0
			774	476	129	167	2			

- Molecule 4 is ASPARAGINE (CCD ID: ASN) (formula: C₄H₈N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	4	2	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

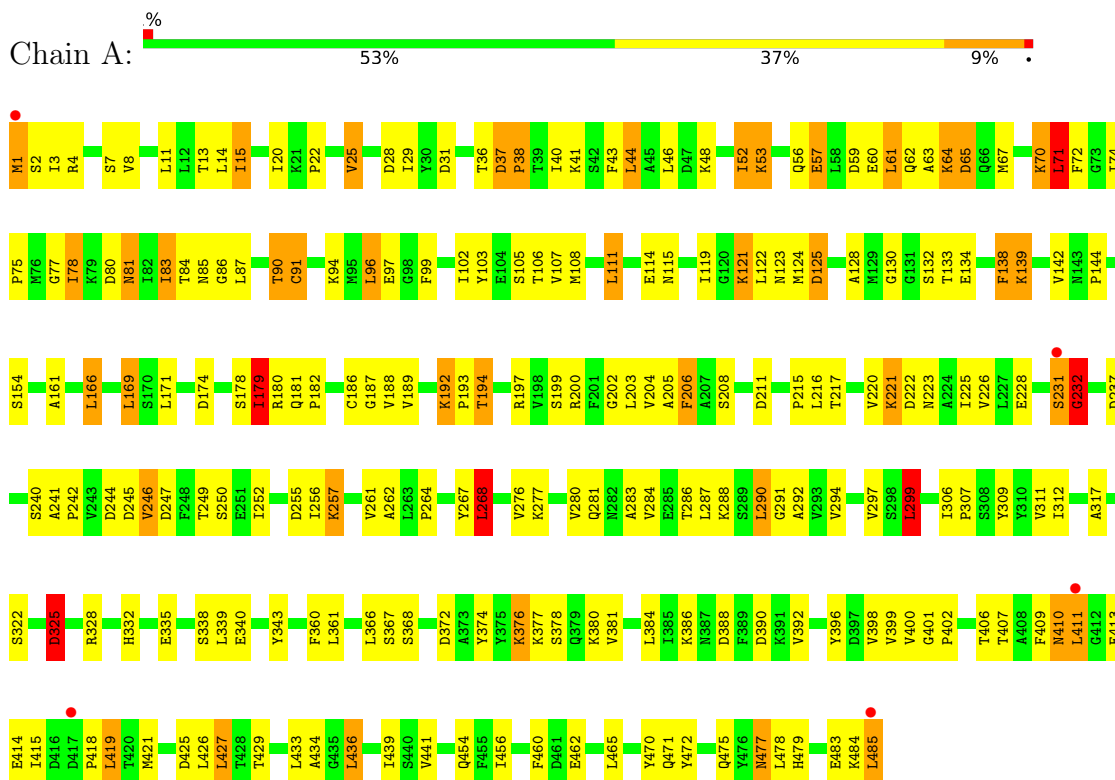
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	121	Total	O	0	0
			121	121		
6	B	61	Total	O	0	0
			61	61		
6	C	15	Total	O	0	0
			15	15		

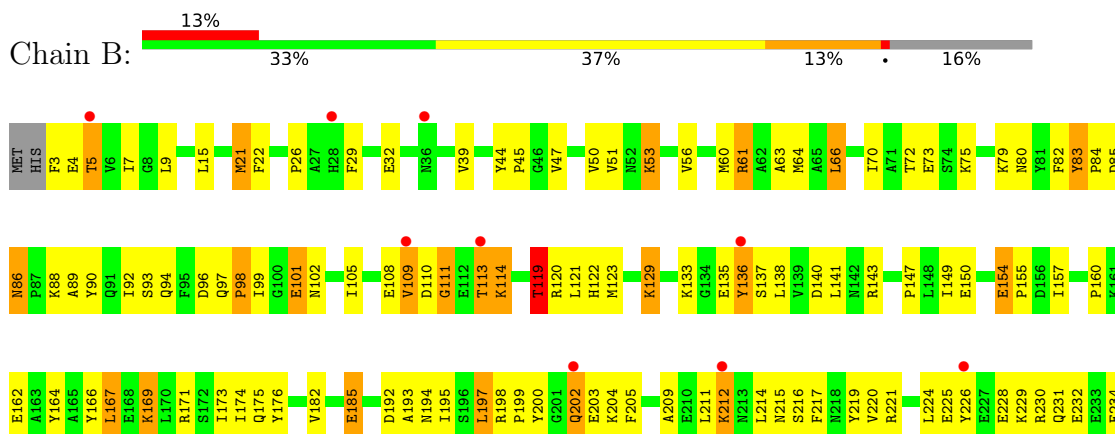
3 Residue-property plots

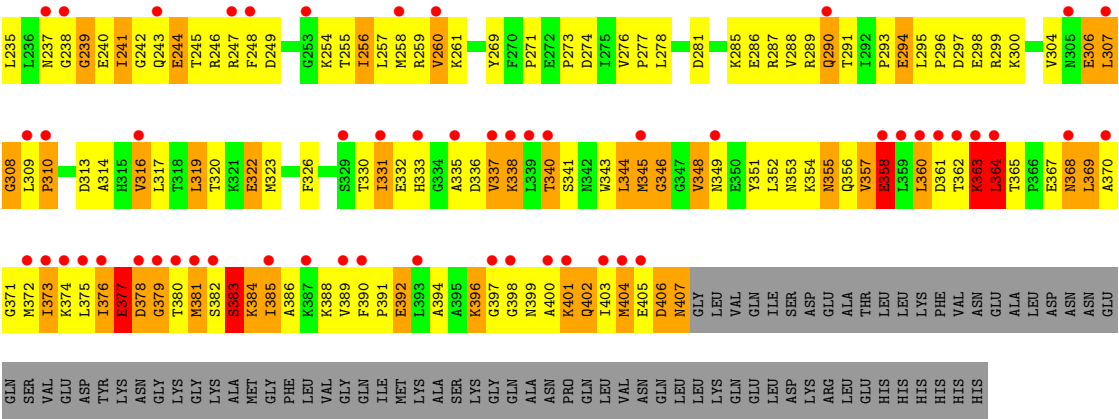
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

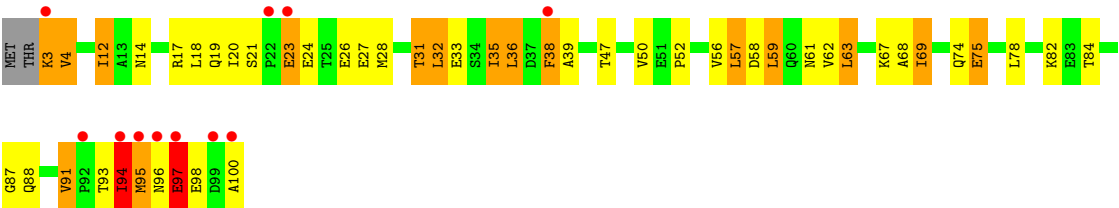


• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B





● Molecule 3: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.81Å 92.36Å 182.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.55 20.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.55) 98.6 (20.00-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.271 0.233 , 0.270	Depositor DCC
R_{free} test set	3915 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7925	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.58	0/3784	1.13	28/5116 (0.5%)
2	B	0.57	2/3290 (0.1%)	1.20	43/4442 (1.0%)
3	C	0.49	0/782	1.31	8/1056 (0.8%)
All	All	0.56	2/7856 (0.0%)	1.18	79/10614 (0.7%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	383	SER	CA-C	5.98	1.60	1.52
2	B	383	SER	N-CA	5.57	1.53	1.46

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	97	GLU	N-CA-C	22.70	136.02	111.28
1	A	231	SER	N-CA-C	15.22	127.92	111.03
2	B	111	GLY	N-CA-C	-11.87	85.04	113.18
2	B	397	GLY	N-CA-C	10.56	126.28	112.13
3	C	38	PHE	N-CA-C	-9.73	101.54	113.41
1	A	71	LEU	N-CA-C	-9.65	94.60	109.85
2	B	383	SER	N-CA-C	9.64	131.33	110.80
2	B	382	SER	N-CA-C	9.55	124.99	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	380	THR	N-CA-C	-9.43	98.08	110.53
2	B	363	LYS	N-CA-C	9.09	122.87	111.69
2	B	86	ASN	CA-C-N	8.82	128.15	118.97
2	B	86	ASN	C-N-CA	8.82	128.15	118.97
1	A	205	ALA	N-CA-C	8.71	122.19	110.35
2	B	377	GLU	N-CA-C	7.65	119.26	111.07
2	B	364	LEU	N-CA-C	-7.46	98.07	109.41
2	B	404	MET	N-CA-C	-7.43	103.17	111.71
2	B	237	ASN	N-CA-C	7.41	119.35	111.28
2	B	154	GLU	N-CA-C	-7.37	99.59	110.20
2	B	401	LYS	N-CA-C	-6.76	103.06	112.25
2	B	307	LEU	N-CA-C	-6.72	102.11	111.52
2	B	51	VAL	N-CA-C	6.67	117.93	108.93
1	A	268	LEU	N-CA-C	-6.65	104.48	112.59
1	A	91	CYS	N-CA-C	-6.43	105.02	112.86
1	A	36	THR	N-CA-C	6.43	121.15	113.12
2	B	120	ARG	N-CA-C	6.36	117.89	108.60
1	A	441	VAL	N-CA-C	-6.32	104.01	109.19
2	B	113	THR	N-CA-C	6.25	119.06	110.24
1	A	367	SER	N-CA-C	6.25	118.78	110.53
2	B	96	ASP	N-CA-C	-6.16	101.40	110.52
2	B	232	GLU	N-CA-C	-6.14	104.14	111.69
2	B	5	THR	N-CA-C	-6.12	98.56	108.41
2	B	358	GLU	N-CA-C	-6.08	105.89	113.38
1	A	83	ILE	N-CA-C	6.08	117.58	109.37
2	B	381	MET	N-CA-C	6.07	123.73	110.80
2	B	21	MET	N-CA-C	6.05	117.55	111.07
3	C	94	ILE	N-CA-C	-6.04	96.78	109.34
2	B	72	THR	N-CA-C	-6.03	105.59	113.12
2	B	244	GLU	N-CA-C	6.03	118.23	109.07
1	A	410	ASN	N-CA-C	5.99	118.63	110.55
1	A	70	LYS	N-CA-C	-5.98	104.69	112.23
2	B	80	ASN	N-CA-C	5.95	118.42	108.96
2	B	61	ARG	N-CA-C	-5.92	104.18	111.40
2	B	346	GLY	N-CA-C	-5.89	102.54	111.14
2	B	154	GLU	CA-C-N	-5.89	113.96	121.91
2	B	154	GLU	C-N-CA	-5.89	113.96	121.91
1	A	81	ASN	N-CA-C	-5.88	104.65	112.94
2	B	119	THR	N-CA-C	5.84	118.59	111.82
1	A	125	ASP	N-CA-C	-5.82	102.70	110.55
1	A	325	ASP	N-CA-C	-5.77	106.22	113.72
1	A	99	PHE	N-CA-C	5.73	118.49	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ILE	N-CA-C	-5.67	107.14	111.62
2	B	361	ASP	N-CA-C	5.64	120.28	113.17
2	B	396	LYS	N-CA-C	5.58	119.66	111.34
3	C	91	VAL	N-CA-C	5.57	113.76	109.19
2	B	83	TYR	CA-C-N	-5.56	113.95	119.56
2	B	83	TYR	C-N-CA	-5.56	113.95	119.56
1	A	138	PHE	N-CA-C	5.52	120.02	112.68
1	A	407	THR	N-CA-C	-5.47	103.48	110.53
3	C	97	GLU	CA-C-N	-5.46	111.58	121.14
3	C	97	GLU	C-N-CA	-5.46	111.58	121.14
1	A	31	ASP	N-CA-C	-5.45	105.42	111.36
1	A	57	GLU	N-CA-C	-5.43	105.26	111.07
2	B	53	LYS	N-CA-C	5.41	117.18	111.28
2	B	98	PRO	N-CA-C	-5.39	102.81	111.38
1	A	94	LYS	N-CA-C	-5.39	105.57	111.82
2	B	215	ASN	N-CA-C	5.37	119.93	113.17
2	B	376	ILE	N-CA-C	-5.31	105.21	111.00
2	B	306	GLU	N-CA-C	-5.24	100.76	109.46
1	A	90	THR	N-CA-C	5.22	119.92	113.50
3	C	91	VAL	CA-C-N	5.20	125.14	119.78
3	C	91	VAL	C-N-CA	5.20	125.14	119.78
1	A	25	VAL	N-CA-C	-5.20	104.90	110.36
1	A	232	GLY	N-CA-C	5.17	125.42	113.18
1	A	299	LEU	CA-C-N	5.09	126.20	119.84
1	A	299	LEU	C-N-CA	5.09	126.20	119.84
2	B	294	GLU	N-CA-C	-5.07	100.91	108.96
1	A	220	VAL	N-CA-C	5.03	115.25	110.42
2	B	101	GLU	N-CA-C	5.01	116.81	109.24
1	A	78	ILE	N-CA-C	5.00	115.33	108.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	472	TYR	Sidechain

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	3716	0	3709	192	0
2	B	3228	0	3176	303	0
3	C	774	0	753	73	0
4	A	9	0	5	3	0
5	B	1	0	0	0	0
6	A	121	0	0	5	0
6	B	61	0	0	6	0
6	C	15	0	0	1	0
All	All	7925	0	7643	526	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 34.

All (526) 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)
2:B:199:PRO:HG2	2:B:202:GLN:HE22	1.12	1.12
2:B:357:VAL:HG11	2:B:363:LYS:HE2	1.32	1.09
2:B:192:ASP:OD2	2:B:212:LYS:HD3	1.63	0.98
3:C:23:GLU:OE1	3:C:24:GLU:HG3	1.63	0.96
2:B:247:ARG:HB3	2:B:258:MET:HE2	1.50	0.93
2:B:56:VAL:HG22	2:B:123:MET:HE1	1.50	0.93
1:A:194:THR:HG22	1:A:462:GLU:OE2	1.68	0.92
2:B:355:ASN:HB3	2:B:357:VAL:HG22	1.53	0.90
2:B:344:LEU:HD12	2:B:348:VAL:HG21	1.52	0.89
2:B:368:ASN:HD22	2:B:369:LEU:N	1.71	0.88
2:B:383:SER:O	2:B:384:LYS:C	2.14	0.88
2:B:368:ASN:HD22	2:B:368:ASN:C	1.82	0.88
2:B:357:VAL:HG11	2:B:363:LYS:CE	2.05	0.87
1:A:286:THR:O	1:A:290:LEU:HD12	1.74	0.86
2:B:371:GLY:O	2:B:374:LYS:HG2	1.76	0.85
3:C:47:THR:O	3:C:50:VAL:HG12	1.77	0.85
2:B:331:ILE:HD11	2:B:337:VAL:HG13	1.58	0.85
1:A:477:ASN:C	1:A:477:ASN:HD22	1.83	0.85
2:B:309:LEU:HD11	2:B:338:LYS:HD2	1.57	0.84
1:A:255:ASP:OD1	1:A:257:LYS:HE2	1.78	0.84
2:B:199:PRO:HG2	2:B:202:GLN:NE2	1.92	0.84
2:B:26:PRO:HG3	3:C:68:ALA:HB1	1.60	0.83
1:A:180:ARG:HD2	1:A:192:LYS:HB3	1.60	0.83
2:B:343:TRP:O	2:B:348:VAL:HG13	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HG2	1:A:4:ARG:HD2	1.60	0.82
1:A:372:ASP:HA	1:A:376:LYS:HB2	1.59	0.82
2:B:368:ASN:ND2	2:B:369:LEU:N	2.28	0.82
2:B:304:VAL:O	2:B:308:GLY:HA2	1.81	0.81
2:B:309:LEU:CD1	2:B:338:LYS:HD2	2.10	0.81
2:B:364:LEU:HD12	2:B:365:THR:H	1.45	0.81
1:A:194:THR:HG21	1:A:460:PHE:HA	1.63	0.81
1:A:247:ASP:OD2	1:A:250:SER:HB3	1.80	0.81
1:A:84:THR:OG1	1:A:121:LYS:HE3	1.81	0.81
2:B:364:LEU:HD12	2:B:365:THR:N	1.96	0.80
2:B:403:ILE:O	2:B:407:ASN:HB2	1.81	0.79
2:B:390:PHE:HB3	2:B:391:PRO:HD3	1.64	0.79
2:B:388:LYS:O	2:B:388:LYS:HD3	1.82	0.79
2:B:140:ASP:HB2	3:C:88:GLN:NE2	1.97	0.79
2:B:348:VAL:HG12	2:B:390:PHE:CZ	2.18	0.78
1:A:339:LEU:CB	3:C:95:MET:HE1	2.14	0.77
2:B:356:GLN:HA	2:B:356:GLN:NE2	1.99	0.77
2:B:82:PHE:HB2	3:C:17:ARG:HE	1.48	0.77
1:A:306:ILE:HG22	3:C:38:PHE:HZ	1.50	0.76
2:B:400:ALA:O	2:B:404:MET:HG3	1.85	0.76
2:B:198:ARG:O	2:B:198:ARG:HG3	1.86	0.75
2:B:217:PHE:O	2:B:220:VAL:HG22	1.87	0.74
1:A:204:VAL:HG22	2:B:45:PRO:HB2	1.70	0.74
2:B:375:LEU:HD21	2:B:404:MET:SD	2.26	0.74
2:B:313:ASP:HA	2:B:345:MET:SD	2.28	0.74
3:C:75:GLU:OE1	3:C:75:GLU:HA	1.88	0.74
3:C:93:THR:C	3:C:95:MET:H	1.96	0.74
3:C:94:ILE:HG12	3:C:94:ILE:O	1.87	0.74
1:A:340:GLU:HB2	3:C:100:ALA:O	1.88	0.73
2:B:221:ARG:O	2:B:225:GLU:HG2	1.89	0.73
2:B:247:ARG:CB	2:B:258:MET:HE2	2.19	0.73
2:B:399:ASN:HD21	2:B:401:LYS:HB3	1.53	0.73
2:B:281:ASP:O	2:B:285:LYS:HG3	1.87	0.73
2:B:316:VAL:HG13	2:B:345:MET:HE2	1.69	0.72
1:A:1:MET:H2	1:A:28:ASP:CG	1.97	0.72
2:B:288:VAL:O	2:B:291:THR:HG22	1.88	0.72
3:C:35:ILE:O	3:C:38:PHE:HB3	1.88	0.72
2:B:352:LEU:HA	2:B:357:VAL:HG23	1.72	0.72
1:A:249:THR:HA	1:A:252:ILE:HD12	1.72	0.72
2:B:386:ALA:HA	2:B:389:VAL:HG22	1.69	0.72
2:B:94:GLN:HB2	2:B:122:HIS:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LYS:O	1:A:225:ILE:HD12	1.89	0.71
2:B:388:LYS:HE2	2:B:392:GLU:CG	2.20	0.71
2:B:5:THR:HG21	2:B:228:GLU:HG3	1.72	0.71
2:B:75:LYS:HG3	2:B:97:GLN:OE1	1.90	0.71
3:C:27:GLU:O	3:C:31:THR:HG22	1.90	0.71
2:B:348:VAL:O	2:B:352:LEU:HD13	1.90	0.71
1:A:264:PRO:HB3	1:A:299:LEU:HD22	1.73	0.70
2:B:243:GLN:HG3	2:B:261:LYS:HG3	1.74	0.70
2:B:364:LEU:HD13	2:B:368:ASN:HD21	1.56	0.70
2:B:375:LEU:CD2	2:B:404:MET:SD	2.80	0.70
2:B:202:GLN:HG2	2:B:203:GLU:N	2.05	0.70
1:A:339:LEU:HB2	3:C:95:MET:HE1	1.74	0.69
2:B:364:LEU:HD11	2:B:369:LEU:HB2	1.74	0.69
1:A:81:ASN:HB3	1:A:124:MET:HE1	1.73	0.69
1:A:178:SER:OG	4:A:511:ASN:ND2	2.25	0.69
2:B:256:ILE:HD12	2:B:256:ILE:N	2.07	0.69
1:A:360:PHE:CD2	3:C:28:MET:HE3	2.28	0.69
2:B:404:MET:HB2	6:B:547:HOH:O	1.91	0.68
2:B:300:LYS:HG3	6:B:553:HOH:O	1.92	0.68
1:A:306:ILE:HG22	3:C:38:PHE:CZ	2.29	0.67
1:A:78:ILE:HD12	1:A:108:MET:HE1	1.77	0.67
2:B:307:LEU:HD23	2:B:307:LEU:O	1.95	0.67
2:B:61:ARG:CD	2:B:291:THR:HG23	2.24	0.67
1:A:192:LYS:O	1:A:192:LYS:HG3	1.94	0.66
3:C:96:ASN:OD1	3:C:97:GLU:N	2.29	0.66
2:B:386:ALA:HA	2:B:389:VAL:CG2	2.25	0.66
1:A:57:GLU:O	1:A:61:LEU:HD23	1.96	0.66
2:B:160:PRO:HB3	2:B:224:LEU:HB3	1.78	0.65
1:A:280:VAL:HG21	1:A:402:PRO:HB3	1.77	0.65
2:B:388:LYS:HE2	2:B:392:GLU:HG3	1.78	0.65
1:A:72:PHE:H	1:A:74:ILE:HG12	1.62	0.65
1:A:434:ALA:HB3	1:A:436:LEU:HD22	1.78	0.64
2:B:171:ARG:NH1	2:B:175:GLN:HG3	2.13	0.64
2:B:241:ILE:HD13	2:B:241:ILE:C	2.23	0.64
1:A:139:LYS:NZ	1:A:139:LYS:HB3	2.13	0.64
2:B:259:ARG:HG3	2:B:259:ARG:HH11	1.62	0.64
1:A:194:THR:HG21	1:A:460:PHE:CA	2.28	0.63
3:C:97:GLU:OE2	3:C:97:GLU:HA	1.98	0.63
2:B:7:ILE:HG22	2:B:195:ILE:HG13	1.81	0.63
3:C:57:LEU:HD23	3:C:58:ASP:H	1.62	0.63
1:A:70:LYS:HZ3	1:A:70:LYS:HB3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LYS:O	1:A:281:GLN:HG3	1.99	0.63
3:C:28:MET:HA	3:C:31:THR:HG23	1.80	0.63
3:C:59:LEU:HD23	3:C:59:LEU:N	2.13	0.62
2:B:320:THR:OG1	2:B:323:MET:HB3	2.00	0.62
1:A:132:SER:O	1:A:133:THR:HB	2.00	0.62
2:B:288:VAL:HA	2:B:291:THR:HG22	1.81	0.62
1:A:484:LYS:C	1:A:485:LEU:HD23	2.25	0.62
2:B:82:PHE:CD1	3:C:17:ARG:HG3	2.34	0.62
2:B:344:LEU:HA	2:B:348:VAL:HG22	1.81	0.62
2:B:3:PHE:HE1	2:B:197:LEU:HD23	1.65	0.62
1:A:377:LYS:O	1:A:381:VAL:HG23	1.99	0.62
1:A:284:VAL:HG12	1:A:288:LYS:HE3	1.82	0.61
3:C:3:LYS:HA	6:C:109:HOH:O	2.00	0.61
1:A:221:LYS:HZ2	1:A:252:ILE:HG21	1.65	0.61
1:A:409:PHE:CD1	1:A:414:GLU:HG3	2.35	0.61
2:B:309:LEU:HG	2:B:310:PRO:HD2	1.82	0.61
2:B:388:LYS:HE2	2:B:392:GLU:HG2	1.82	0.61
1:A:29:ILE:HG21	1:A:119:ILE:HG12	1.82	0.61
2:B:133:LYS:HB2	2:B:138:LEU:HD23	1.81	0.61
2:B:5:THR:HG22	2:B:197:LEU:HG	1.82	0.61
2:B:88:LYS:O	2:B:89:ALA:HB3	1.99	0.61
2:B:364:LEU:CD1	2:B:369:LEU:HB2	2.30	0.61
2:B:368:ASN:HB2	2:B:398:GLY:O	2.00	0.61
2:B:197:LEU:HD13	2:B:231:GLN:OE1	2.01	0.61
2:B:105:ILE:HD11	2:B:166:TYR:CD1	2.36	0.61
2:B:140:ASP:HB2	3:C:88:GLN:HE21	1.64	0.60
1:A:252:ILE:HG23	1:A:470:TYR:CG	2.37	0.60
2:B:300:LYS:HG2	2:B:314:ALA:HB1	1.82	0.60
1:A:139:LYS:HB3	1:A:139:LYS:HZ3	1.67	0.60
2:B:378:ASP:OD1	2:B:379:GLY:N	2.35	0.60
3:C:93:THR:C	3:C:95:MET:N	2.57	0.60
1:A:374:TYR:HE2	3:C:36:LEU:HG	1.66	0.60
2:B:44:TYR:O	2:B:47:VAL:HG22	2.01	0.60
2:B:333:HIS:CE1	2:B:367:GLU:HA	2.37	0.59
2:B:61:ARG:HD3	2:B:291:THR:HG23	1.84	0.59
2:B:331:ILE:CG2	2:B:332:GLU:N	2.65	0.59
1:A:84:THR:HG23	1:A:121:LYS:HE2	1.85	0.59
1:A:256:ILE:HG23	1:A:471:GLN:HG3	1.84	0.59
1:A:332:HIS:HB3	3:C:82:LYS:HD2	1.84	0.59
1:A:276:VAL:HG21	1:A:406:THR:HA	1.85	0.58
2:B:307:LEU:CD2	2:B:337:VAL:HG11	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:HIS:HE1	2:B:367:GLU:HA	1.67	0.58
1:A:244:ASP:O	1:A:246:VAL:HG22	2.04	0.58
2:B:61:ARG:HD2	2:B:291:THR:HG23	1.85	0.58
2:B:202:GLN:HG2	2:B:204:LYS:H	1.68	0.58
1:A:197:ARG:O	1:A:231:SER:O	2.22	0.58
2:B:249:ASP:HB2	2:B:256:ILE:HD11	1.86	0.58
3:C:20:ILE:HD11	3:C:24:GLU:HB3	1.86	0.58
1:A:194:THR:HG21	1:A:460:PHE:H	1.69	0.57
1:A:67:MET:HE2	1:A:72:PHE:CE2	2.40	0.57
1:A:84:THR:CG2	1:A:121:LYS:HE2	2.34	0.57
2:B:121:LEU:C	2:B:121:LEU:HD23	2.30	0.57
2:B:383:SER:O	2:B:386:ALA:N	2.35	0.57
2:B:295:LEU:O	2:B:299:ARG:HB2	2.05	0.57
1:A:284:VAL:HG13	1:A:294:VAL:HG11	1.87	0.57
2:B:109:VAL:O	2:B:111:GLY:N	2.38	0.57
2:B:226:TYR:HB2	6:B:522:HOH:O	2.03	0.57
1:A:290:LEU:HD11	1:A:475:GLN:HG3	1.87	0.57
1:A:41:LYS:HB3	1:A:139:LYS:HD3	1.85	0.57
1:A:264:PRO:HA	1:A:297:VAL:O	2.05	0.57
1:A:339:LEU:HB3	3:C:95:MET:HE1	1.85	0.57
1:A:60:GLU:O	1:A:64:LYS:HG3	2.05	0.56
1:A:71:LEU:O	1:A:114:GLU:O	2.22	0.56
2:B:219:TYR:CD1	2:B:248:PHE:HE2	2.23	0.56
2:B:230:ARG:NH1	2:B:246:ARG:HE	2.04	0.56
2:B:176:TYR:CE1	2:B:296:PRO:HG3	2.40	0.56
2:B:383:SER:O	2:B:385:ILE:N	2.37	0.56
2:B:344:LEU:HA	2:B:348:VAL:CG2	2.36	0.56
1:A:188:VAL:CG1	1:A:217:THR:O	2.54	0.56
2:B:193:ALA:CB	2:B:224:LEU:HD11	2.36	0.56
2:B:169:LYS:HZ1	2:B:297:ASP:CG	2.14	0.56
3:C:97:GLU:OE2	3:C:97:GLU:CA	2.53	0.56
2:B:288:VAL:C	2:B:291:THR:HG22	2.31	0.56
2:B:211:LEU:HD12	2:B:224:LEU:HD12	1.88	0.56
2:B:133:LYS:HB2	2:B:138:LEU:CD2	2.36	0.56
2:B:290:GLN:C	2:B:290:GLN:CD	2.74	0.56
2:B:295:LEU:HD22	2:B:295:LEU:N	2.21	0.56
2:B:340:THR:O	2:B:344:LEU:HD22	2.05	0.56
1:A:299:LEU:HD12	1:A:388:ASP:HB3	1.88	0.55
2:B:247:ARG:HB3	2:B:258:MET:CE	2.32	0.55
2:B:83:TYR:HD2	2:B:85:ASP:CG	2.14	0.55
1:A:411:LEU:HB2	6:A:624:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:VAL:CG2	3:C:59:LEU:O	2.55	0.55
2:B:352:LEU:HD21	2:B:360:LEU:CD1	2.37	0.55
2:B:22:PHE:CE2	2:B:92:ILE:HB	2.42	0.55
1:A:485:LEU:HD23	1:A:485:LEU:N	2.22	0.55
2:B:316:VAL:HG13	2:B:345:MET:CE	2.36	0.55
1:A:242:PRO:HD2	3:C:59:LEU:HD11	1.87	0.55
1:A:134:GLU:HB2	1:A:415:ILE:HD13	1.88	0.55
2:B:60:MET:HE2	2:B:288:VAL:HG21	1.89	0.55
1:A:206:PHE:CE1	1:A:317:ALA:HB2	2.42	0.54
2:B:276:VAL:HG21	3:C:59:LEU:O	2.06	0.54
2:B:294:GLU:HB2	2:B:299:ARG:HH11	1.72	0.54
3:C:78:LEU:HD22	3:C:84:THR:HG21	1.88	0.54
2:B:26:PRO:HD3	3:C:69:ILE:O	2.08	0.54
1:A:228:GLU:HG2	1:A:246:VAL:O	2.08	0.54
2:B:276:VAL:HG21	3:C:59:LEU:C	2.33	0.54
2:B:343:TRP:O	2:B:346:GLY:O	2.26	0.54
2:B:364:LEU:CD1	2:B:368:ASN:HD21	2.20	0.54
2:B:369:LEU:HD22	2:B:369:LEU:O	2.06	0.54
2:B:199:PRO:HD3	2:B:235:LEU:HD21	1.90	0.54
2:B:330:THR:HG21	2:B:369:LEU:HD13	1.88	0.54
1:A:325:ASP:HB3	1:A:343:TYR:CE1	2.43	0.54
2:B:278:LEU:HD21	3:C:63:LEU:HD11	1.89	0.54
2:B:352:LEU:HD21	2:B:360:LEU:HD12	1.89	0.54
2:B:15:LEU:HD11	2:B:149:ILE:HG23	1.90	0.53
1:A:206:PHE:CD1	1:A:206:PHE:C	2.84	0.53
1:A:328:ARG:HG3	1:A:328:ARG:HH11	1.74	0.53
1:A:306:ILE:CG2	3:C:38:PHE:HZ	2.21	0.53
1:A:84:THR:OG1	1:A:87:LEU:HB3	2.09	0.53
1:A:188:VAL:HG12	1:A:189:VAL:N	2.24	0.53
1:A:194:THR:HG21	1:A:460:PHE:N	2.23	0.53
2:B:276:VAL:HG11	3:C:62:VAL:HG23	1.91	0.53
2:B:375:LEU:HD23	2:B:404:MET:SD	2.49	0.52
3:C:69:ILE:O	3:C:69:ILE:HG22	2.08	0.52
1:A:361:LEU:HD13	3:C:35:ILE:CG2	2.39	0.52
2:B:385:ILE:HD13	2:B:404:MET:HE3	1.90	0.52
2:B:271:PRO:O	2:B:273:PRO:HD3	2.09	0.52
2:B:405:GLU:C	2:B:407:ASN:H	2.16	0.52
3:C:58:ASP:O	3:C:59:LEU:C	2.52	0.52
1:A:477:ASN:C	1:A:477:ASN:ND2	2.55	0.52
2:B:79:LYS:HE2	2:B:269:TYR:OH	2.09	0.52
2:B:307:LEU:HD21	2:B:337:VAL:CG1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:MET:HB3	2:B:99:ILE:HD11	1.91	0.52
2:B:241:ILE:HD13	2:B:242:GLY:N	2.25	0.52
1:A:380:LYS:HG2	3:C:50:VAL:HG13	1.91	0.52
1:A:8:VAL:HB	1:A:222:ASP:OD1	2.10	0.52
1:A:264:PRO:CB	1:A:299:LEU:HD22	2.40	0.52
2:B:175:GLN:NE2	2:B:322:GLU:OE2	2.42	0.52
2:B:307:LEU:HG	2:B:337:VAL:HG11	1.92	0.52
2:B:372:MET:O	2:B:376:ILE:HG13	2.09	0.52
2:B:365:THR:HG22	6:B:552:HOH:O	2.10	0.51
1:A:237:ASP:O	1:A:240:SER:OG	2.28	0.51
1:A:262:ALA:HB2	1:A:396:TYR:CG	2.46	0.51
2:B:154:GLU:HG3	2:B:155:PRO:HD2	1.91	0.51
3:C:32:LEU:HD12	3:C:36:LEU:HD22	1.92	0.51
2:B:136:TYR:N	2:B:136:TYR:CD1	2.79	0.51
2:B:344:LEU:HD13	2:B:348:VAL:HG11	1.92	0.51
2:B:307:LEU:O	2:B:307:LEU:CD2	2.59	0.51
1:A:188:VAL:HG13	1:A:217:THR:O	2.11	0.51
2:B:238:GLY:O	2:B:239:GLY:O	2.29	0.51
1:A:169:LEU:C	1:A:169:LEU:HD22	2.35	0.51
2:B:351:TYR:CE1	2:B:357:VAL:HG21	2.46	0.51
2:B:9:LEU:HD12	2:B:166:TYR:CD2	2.45	0.51
2:B:61:ARG:HD3	2:B:291:THR:CG2	2.41	0.51
2:B:83:TYR:CD2	2:B:85:ASP:CG	2.89	0.51
1:A:161:ALA:O	1:A:166:LEU:HB2	2.11	0.50
1:A:257:LYS:HD2	1:A:257:LYS:O	2.11	0.50
1:A:309:TYR:OH	4:A:511:ASN:HB2	2.11	0.50
2:B:63:ALA:HB2	2:B:121:LEU:HD13	1.93	0.50
2:B:247:ARG:CA	2:B:258:MET:HE2	2.41	0.50
1:A:322:SER:HB3	2:B:89:ALA:CB	2.40	0.50
2:B:98:PRO:HG2	2:B:101:GLU:HG3	1.92	0.50
2:B:338:LYS:O	2:B:341:SER:HB3	2.11	0.50
1:A:130:GLY:N	4:A:511:ASN:O	2.44	0.50
1:A:139:LYS:NZ	1:A:139:LYS:CB	2.73	0.50
2:B:309:LEU:CG	2:B:310:PRO:HD2	2.42	0.50
2:B:3:PHE:N	2:B:200:TYR:CD2	2.79	0.50
2:B:3:PHE:O	2:B:3:PHE:CG	2.61	0.50
2:B:169:LYS:HD3	2:B:169:LYS:C	2.37	0.50
1:A:14:LEU:O	1:A:20:ILE:HG22	2.12	0.50
1:A:90:THR:HA	1:A:96:LEU:HB3	1.93	0.50
2:B:288:VAL:CA	2:B:291:THR:HG22	2.42	0.50
2:B:392:GLU:OE2	2:B:396:LYS:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ILE:HG13	1:A:20:ILE:HG23	1.94	0.50
1:A:72:PHE:O	1:A:115:ASN:O	2.29	0.50
1:A:261:VAL:HB	1:A:294:VAL:HG22	1.94	0.50
1:A:338:SER:HB2	3:C:100:ALA:OXT	2.12	0.50
1:A:105:SER:CB	1:A:202:GLY:HA3	2.42	0.49
2:B:306:GLU:O	2:B:307:LEU:HB3	2.10	0.49
2:B:176:TYR:CZ	2:B:296:PRO:HG3	2.46	0.49
2:B:229:LYS:N	2:B:229:LYS:HD2	2.27	0.49
2:B:331:ILE:HG22	2:B:332:GLU:N	2.28	0.49
2:B:348:VAL:CG2	2:B:349:ASN:N	2.75	0.49
1:A:368:SER:HA	6:A:531:HOH:O	2.12	0.49
2:B:259:ARG:HG3	2:B:259:ARG:NH1	2.26	0.49
2:B:298:GLU:CD	2:B:298:GLU:H	2.20	0.49
2:B:399:ASN:ND2	2:B:401:LYS:HB3	2.25	0.49
1:A:77:GLY:O	1:A:78:ILE:HD13	2.13	0.49
2:B:169:LYS:HD3	2:B:169:LYS:O	2.13	0.49
2:B:185:GLU:CD	2:B:185:GLU:H	2.19	0.49
2:B:331:ILE:HG22	2:B:332:GLU:H	1.78	0.49
2:B:340:THR:HG23	2:B:373:ILE:HD12	1.94	0.49
3:C:74:GLN:NE2	3:C:87:GLY:HA2	2.27	0.49
2:B:202:GLN:HG2	2:B:204:LYS:N	2.28	0.49
1:A:1:MET:O	1:A:4:ARG:HG2	2.13	0.49
1:A:174:ASP:HB2	1:A:179:ILE:HB	1.95	0.49
1:A:299:LEU:CD1	1:A:392:VAL:HG21	2.42	0.49
2:B:300:LYS:C	2:B:300:LYS:HD2	2.38	0.49
2:B:316:VAL:CG1	2:B:345:MET:HE2	2.42	0.49
2:B:356:GLN:O	2:B:358:GLU:HG2	2.13	0.49
1:A:125:ASP:CG	1:A:133:THR:HA	2.38	0.48
1:A:374:TYR:CE2	3:C:36:LEU:HG	2.47	0.48
2:B:93:SER:OG	2:B:94:GLN:N	2.46	0.48
2:B:363:LYS:CB	2:B:363:LYS:NZ	2.76	0.48
3:C:75:GLU:OE1	3:C:75:GLU:CA	2.58	0.48
2:B:288:VAL:HA	2:B:291:THR:CG2	2.42	0.48
2:B:343:TRP:CD1	2:B:373:ILE:HD13	2.48	0.48
2:B:356:GLN:HA	2:B:356:GLN:HE21	1.76	0.48
2:B:402:GLN:O	2:B:406:ASP:HB2	2.13	0.48
1:A:37:ASP:N	1:A:38:PRO:CD	2.77	0.48
1:A:192:LYS:NZ	1:A:193:PRO:O	2.36	0.48
2:B:7:ILE:HA	2:B:194:ASN:O	2.14	0.48
2:B:60:MET:HE3	2:B:70:ILE:HG21	1.95	0.48
2:B:309:LEU:HD12	2:B:310:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ALA:HA	3:C:59:LEU:HD11	1.95	0.48
2:B:7:ILE:HG22	2:B:195:ILE:CG1	2.44	0.48
1:A:22:PRO:HD2	1:A:59:ASP:OD1	2.14	0.48
2:B:86:ASN:HD21	2:B:90:TYR:N	2.12	0.48
2:B:234:GLU:O	2:B:239:GLY:HA3	2.14	0.48
2:B:260:VAL:HG12	2:B:260:VAL:O	2.14	0.48
2:B:276:VAL:HG22	2:B:277:PRO:HD2	1.95	0.48
2:B:278:LEU:HA	3:C:61:ASN:OD1	2.13	0.48
2:B:309:LEU:HD12	2:B:310:PRO:CD	2.44	0.48
2:B:137:SER:N	3:C:91:VAL:O	2.47	0.47
2:B:357:VAL:CG1	2:B:363:LYS:HE2	2.24	0.47
3:C:47:THR:HB	3:C:50:VAL:CG1	2.44	0.47
2:B:88:LYS:O	2:B:89:ALA:CB	2.63	0.47
2:B:352:LEU:O	2:B:356:GLN:N	2.47	0.47
1:A:90:THR:O	1:A:91:CYS:HB2	2.14	0.47
2:B:307:LEU:HD21	2:B:337:VAL:HG11	1.96	0.47
2:B:176:TYR:HE2	2:B:299:ARG:CD	2.27	0.47
2:B:209:ALA:HA	2:B:244:GLU:O	2.15	0.47
1:A:325:ASP:HB3	1:A:343:TYR:HE1	1.79	0.47
2:B:259:ARG:HG3	2:B:260:VAL:N	2.29	0.47
2:B:388:LYS:C	2:B:391:PRO:HD2	2.39	0.47
2:B:169:LYS:HE2	2:B:173:ILE:HD11	1.97	0.47
2:B:257:LEU:C	2:B:257:LEU:HD13	2.40	0.47
2:B:405:GLU:C	2:B:407:ASN:N	2.73	0.47
2:B:7:ILE:HG22	2:B:195:ILE:CB	2.45	0.46
1:A:78:ILE:HG21	1:A:108:MET:HE3	1.96	0.46
2:B:245:THR:OG1	2:B:261:LYS:HE2	2.15	0.46
2:B:378:ASP:CG	2:B:379:GLY:N	2.73	0.46
1:A:280:VAL:O	1:A:283:ALA:HB3	2.14	0.46
2:B:295:LEU:HB3	2:B:296:PRO:HD2	1.96	0.46
1:A:78:ILE:CD1	1:A:108:MET:HE1	2.45	0.46
1:A:242:PRO:CD	3:C:59:LEU:HD11	2.45	0.46
2:B:129:LYS:HE2	2:B:143:ARG:NH2	2.31	0.46
1:A:261:VAL:HG22	1:A:398:VAL:CG2	2.45	0.46
1:A:361:LEU:HD13	3:C:35:ILE:HG22	1.96	0.46
1:A:439:ILE:O	1:A:454:GLN:HA	2.16	0.46
2:B:64:MET:C	2:B:66:LEU:N	2.71	0.46
2:B:64:MET:C	2:B:66:LEU:H	2.23	0.46
2:B:307:LEU:O	2:B:309:LEU:N	2.49	0.46
1:A:15:ILE:HG21	1:A:72:PHE:HD2	1.81	0.46
3:C:26:GLU:HA	3:C:26:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:GLU:O	3:C:31:THR:CG2	2.60	0.46
1:A:61:LEU:N	1:A:61:LEU:HD22	2.31	0.46
2:B:220:VAL:HG23	2:B:221:ARG:N	2.31	0.46
2:B:401:LYS:HG2	2:B:401:LYS:O	2.16	0.46
1:A:11:LEU:O	1:A:15:ILE:HD12	2.15	0.46
2:B:317:LEU:HG	2:B:345:MET:CE	2.45	0.46
2:B:129:LYS:CE	2:B:143:ARG:HH21	2.28	0.46
2:B:294:GLU:O	2:B:299:ARG:HD2	2.16	0.45
3:C:47:THR:HB	3:C:50:VAL:HG12	1.98	0.45
1:A:268:LEU:O	1:A:277:LYS:HE2	2.16	0.45
2:B:214:LEU:HB3	2:B:220:VAL:HG12	1.98	0.45
2:B:371:GLY:HA2	2:B:374:LYS:HE2	1.99	0.45
1:A:111:LEU:HD12	1:A:111:LEU:HA	1.79	0.45
1:A:311:VAL:HG11	1:A:374:TYR:O	2.16	0.45
2:B:167:LEU:CD2	2:B:220:VAL:HG21	2.46	0.45
2:B:389:VAL:HG23	2:B:390:PHE:N	2.31	0.45
1:A:426:LEU:HG	1:A:427:LEU:HD13	1.98	0.45
2:B:138:LEU:N	2:B:138:LEU:HD22	2.31	0.45
2:B:198:ARG:HG3	2:B:198:ARG:HH11	1.81	0.45
1:A:61:LEU:CD2	1:A:61:LEU:H	2.30	0.45
1:A:221:LYS:HZ2	1:A:252:ILE:CG2	2.28	0.45
2:B:330:THR:CG2	2:B:340:THR:HG21	2.46	0.45
3:C:4:VAL:O	3:C:4:VAL:HG12	2.16	0.45
2:B:121:LEU:HA	2:B:150:GLU:O	2.16	0.45
2:B:226:TYR:CD1	2:B:226:TYR:C	2.95	0.45
2:B:300:LYS:O	2:B:304:VAL:HG23	2.16	0.45
1:A:84:THR:CG2	1:A:121:LYS:CE	2.95	0.45
2:B:5:THR:HG22	2:B:197:LEU:CD1	2.47	0.45
2:B:202:GLN:HE21	2:B:202:GLN:HB3	1.49	0.45
1:A:206:PHE:CD1	1:A:317:ALA:HB2	2.52	0.45
1:A:376:LYS:HE2	3:C:52:PRO:HG2	1.99	0.45
2:B:56:VAL:CG2	2:B:123:MET:HE1	2.35	0.44
1:A:84:THR:HB	6:A:547:HOH:O	2.15	0.44
2:B:138:LEU:CD2	2:B:138:LEU:N	2.80	0.44
3:C:93:THR:HG23	3:C:93:THR:O	2.15	0.44
2:B:53:LYS:HB2	3:C:63:LEU:HB3	2.00	0.44
3:C:78:LEU:HD22	3:C:84:THR:CG2	2.48	0.44
1:A:103:TYR:CD1	2:B:39:VAL:HG11	2.52	0.44
2:B:363:LYS:NZ	2:B:363:LYS:HB3	2.32	0.44
2:B:364:LEU:CD1	2:B:368:ASN:ND2	2.81	0.44
2:B:286:GLU:O	2:B:287:ARG:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:LEU:CD1	2:B:348:VAL:HG11	2.47	0.44
3:C:28:MET:O	3:C:32:LEU:HB2	2.16	0.44
1:A:215:PRO:HG2	1:A:223:ASN:OD1	2.18	0.44
1:A:257:LYS:HA	1:A:291:GLY:HA3	1.98	0.44
2:B:373:ILE:O	2:B:377:GLU:HB3	2.17	0.44
1:A:40:ILE:HA	1:A:142:VAL:HG22	2.00	0.44
1:A:400:VAL:HG22	1:A:401:GLY:N	2.32	0.44
3:C:74:GLN:HE21	3:C:87:GLY:HA2	1.83	0.43
1:A:169:LEU:C	1:A:169:LEU:CD2	2.91	0.43
2:B:198:ARG:HB3	2:B:205:PHE:CD2	2.53	0.43
2:B:351:TYR:HE1	2:B:357:VAL:HG21	1.81	0.43
1:A:63:ALA:C	1:A:65:ASP:H	2.24	0.43
2:B:174:ILE:HG21	2:B:182:VAL:HG11	2.00	0.43
1:A:62:GLN:HB2	1:A:67:MET:HE3	2.00	0.43
2:B:240:GLU:HA	2:B:240:GLU:OE1	2.18	0.43
1:A:7:SER:HB2	1:A:222:ASP:OD2	2.17	0.43
2:B:333:HIS:ND1	2:B:370:ALA:HB2	2.33	0.43
2:B:21:MET:N	2:B:147:PRO:HD3	2.33	0.43
1:A:208:SER:HB3	2:B:274:ASP:OD1	2.19	0.43
1:A:257:LYS:O	1:A:257:LYS:CD	2.67	0.43
1:A:264:PRO:HG2	1:A:267:TYR:CD2	2.54	0.43
2:B:64:MET:SD	2:B:289:ARG:HD2	2.58	0.43
2:B:309:LEU:HD12	2:B:309:LEU:HA	1.62	0.43
2:B:216:SER:OG	2:B:219:TYR:HB2	2.17	0.43
2:B:286:GLU:O	2:B:289:ARG:N	2.51	0.43
2:B:371:GLY:O	2:B:372:MET:C	2.62	0.43
1:A:186:CYS:O	1:A:188:VAL:HG23	2.18	0.43
2:B:7:ILE:CG2	2:B:195:ILE:HG13	2.48	0.43
2:B:332:GLU:O	2:B:333:HIS:C	2.62	0.43
1:A:48:LYS:HG2	1:A:52:ILE:HD12	2.00	0.43
1:A:418:PRO:HA	1:A:421:MET:HB3	2.01	0.43
1:A:1:MET:CG	1:A:4:ARG:HD2	2.42	0.42
1:A:44:LEU:HD22	1:A:123:ASN:HA	2.00	0.42
1:A:181:GLN:HB3	1:A:182:PRO:HD3	2.01	0.42
2:B:114:LYS:HE2	2:B:162:GLU:OE1	2.19	0.42
2:B:330:THR:HG22	2:B:340:THR:HG21	2.01	0.42
3:C:20:ILE:CD1	3:C:24:GLU:HB3	2.48	0.42
1:A:128:ALA:HA	1:A:154:SER:CB	2.49	0.42
1:A:221:LYS:NZ	1:A:252:ILE:HB	2.34	0.42
3:C:21:SER:O	3:C:24:GLU:N	2.50	0.42
1:A:78:ILE:O	1:A:121:LYS:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:LYS:HE3	1:A:390:ASP:OD2	2.19	0.42
1:A:484:LYS:O	1:A:485:LEU:CB	2.67	0.42
1:A:256:ILE:HD12	1:A:292:ALA:HB2	2.01	0.42
2:B:338:LYS:HZ2	2:B:338:LYS:HB3	1.83	0.42
2:B:343:TRP:CE3	2:B:343:TRP:HA	2.54	0.42
3:C:96:ASN:CG	3:C:97:GLU:H	2.24	0.42
1:A:1:MET:H1	1:A:28:ASP:HA	1.84	0.42
1:A:203:LEU:HD21	1:A:211:ASP:HB3	2.01	0.42
2:B:363:LYS:HB3	2:B:363:LYS:HZ3	1.84	0.42
3:C:50:VAL:HG13	3:C:50:VAL:O	2.18	0.42
1:A:105:SER:HB2	1:A:202:GLY:HA3	2.00	0.42
1:A:187:GLY:HA2	6:A:549:HOH:O	2.19	0.42
2:B:197:LEU:CD1	2:B:197:LEU:N	2.83	0.42
2:B:313:ASP:HA	2:B:345:MET:CE	2.49	0.42
1:A:419:LEU:HD13	1:A:419:LEU:HA	1.76	0.42
2:B:344:LEU:O	2:B:348:VAL:HG22	2.19	0.42
1:A:188:VAL:HG12	1:A:217:THR:O	2.19	0.42
1:A:299:LEU:HD13	1:A:392:VAL:HG21	2.00	0.42
1:A:410:ASN:HB2	1:A:413:GLU:HB2	2.02	0.42
2:B:119:THR:HG22	2:B:154:GLU:CA	2.50	0.42
2:B:212:LYS:HD2	2:B:212:LYS:HA	1.60	0.42
2:B:322:GLU:CD	2:B:322:GLU:H	2.27	0.42
1:A:85:ASN:HD22	1:A:86:GLY:N	2.18	0.42
1:A:107:VAL:HG23	1:A:108:MET:HE2	2.01	0.42
1:A:425:ASP:HB3	1:A:429:THR:HG23	2.02	0.42
2:B:7:ILE:HD11	2:B:157:ILE:CG2	2.50	0.42
2:B:119:THR:HG22	2:B:154:GLU:HA	2.01	0.42
2:B:297:ASP:HB2	2:B:298:GLU:OE2	2.19	0.42
1:A:97:GLU:CD	1:A:138:PHE:HE1	2.28	0.41
1:A:231:SER:O	1:A:232:GLY:O	2.38	0.41
1:A:339:LEU:HD21	2:B:84:PRO:HD3	2.02	0.41
3:C:28:MET:HA	3:C:31:THR:CG2	2.46	0.41
1:A:91:CYS:SG	1:A:204:VAL:HG11	2.60	0.41
1:A:169:LEU:HG	1:A:226:VAL:HG21	2.03	0.41
2:B:64:MET:HE1	2:B:288:VAL:HG23	2.01	0.41
2:B:316:VAL:HA	2:B:319:LEU:HD13	2.01	0.41
3:C:12:ILE:N	3:C:12:ILE:HD13	2.35	0.41
2:B:113:THR:HG22	2:B:114:LYS:N	2.35	0.41
2:B:164:TYR:CD1	2:B:164:TYR:C	2.98	0.41
2:B:176:TYR:HE2	2:B:299:ARG:HD3	1.85	0.41
2:B:216:SER:O	2:B:217:PHE:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:LEU:HB3	2:B:296:PRO:CD	2.50	0.41
2:B:3:PHE:HB2	6:B:524:HOH:O	2.20	0.41
2:B:60:MET:HB3	2:B:99:ILE:CD1	2.50	0.41
2:B:363:LYS:HB2	2:B:394:ALA:O	2.21	0.41
1:A:75:PRO:HB3	1:A:119:ILE:CD1	2.50	0.41
1:A:247:ASP:OD2	1:A:250:SER:CB	2.62	0.41
2:B:230:ARG:CZ	2:B:246:ARG:HE	2.33	0.41
2:B:255:THR:C	2:B:256:ILE:HD12	2.45	0.41
2:B:276:VAL:HG22	2:B:277:PRO:CD	2.51	0.41
2:B:335:ALA:HB1	2:B:340:THR:HG23	2.03	0.41
2:B:336:ASP:O	2:B:337:VAL:C	2.64	0.41
2:B:60:MET:O	2:B:64:MET:HG3	2.19	0.41
3:C:31:THR:O	3:C:32:LEU:C	2.62	0.41
1:A:1:MET:HG2	1:A:4:ARG:CD	2.39	0.41
1:A:306:ILE:N	1:A:307:PRO:HD2	2.35	0.41
2:B:249:ASP:HB2	2:B:256:ILE:CD1	2.49	0.41
1:A:43:PHE:O	1:A:139:LYS:HE3	2.21	0.41
1:A:57:GLU:O	1:A:60:GLU:HB2	2.21	0.41
2:B:174:ILE:CG2	2:B:182:VAL:HG11	2.51	0.41
1:A:53:LYS:HE2	1:A:57:GLU:OE2	2.21	0.41
1:A:200:ARG:NH2	2:B:274:ASP:OD1	2.39	0.41
1:A:322:SER:CB	2:B:89:ALA:HB3	2.50	0.41
1:A:477:ASN:ND2	1:A:479:HIS:H	2.18	0.41
2:B:29:PHE:CD1	2:B:29:PHE:N	2.89	0.41
2:B:105:ILE:HD11	2:B:166:TYR:CE1	2.56	0.41
2:B:121:LEU:C	2:B:121:LEU:CD2	2.94	0.41
2:B:135:GLU:OE1	2:B:135:GLU:HA	2.20	0.41
2:B:202:GLN:CG	2:B:203:GLU:N	2.82	0.41
2:B:202:GLN:CG	2:B:204:LYS:H	2.33	0.41
1:A:15:ILE:HD11	1:A:25:VAL:HG21	2.03	0.41
1:A:132:SER:O	1:A:133:THR:CB	2.66	0.41
1:A:192:LYS:O	1:A:192:LYS:CG	2.67	0.41
1:A:312:ILE:HG13	1:A:378:SER:HB3	2.03	0.41
2:B:285:LYS:O	2:B:289:ARG:HB2	2.21	0.41
2:B:307:LEU:CG	2:B:337:VAL:HG11	2.49	0.41
1:A:1:MET:O	1:A:2:SER:C	2.63	0.40
2:B:192:ASP:OD2	2:B:212:LYS:CD	2.52	0.40
2:B:295:LEU:HD22	2:B:295:LEU:H	1.84	0.40
1:A:166:LEU:HA	1:A:166:LEU:HD12	1.86	0.40
1:A:483:GLU:HB2	6:A:564:HOH:O	2.20	0.40
2:B:160:PRO:HG3	2:B:225:GLU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:LEU:HG	2:B:345:MET:HE1	2.01	0.40
3:C:36:LEU:O	3:C:39:ALA:HB3	2.21	0.40
1:A:44:LEU:HD23	1:A:80:ASP:OD2	2.21	0.40
1:A:106:THR:HB	1:A:199:SER:OG	2.22	0.40
1:A:376:LYS:CE	3:C:52:PRO:HG2	2.52	0.40
1:A:15:ILE:HG13	1:A:20:ILE:CG2	2.51	0.40
1:A:399:VAL:HB	1:A:456:ILE:HB	2.03	0.40
2:B:32:GLU:HB3	6:B:515:HOH:O	2.21	0.40
1:A:103:TYR:HB3	2:B:39:VAL:HG11	2.02	0.40
2:B:326:PHE:CZ	2:B:364:LEU:HG	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	483/485 (100%)	462 (96%)	20 (4%)	1 (0%)	43	56
2	B	403/483 (83%)	364 (90%)	28 (7%)	11 (3%)	4	3
3	C	96/100 (96%)	89 (93%)	5 (5%)	2 (2%)	5	5
All	All	982/1068 (92%)	915 (93%)	53 (5%)	14 (1%)	9	11

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	GLY
2	B	239	GLY
2	B	308	GLY
2	B	381	MET
2	B	383	SER
2	B	110	ASP
2	B	379	GLY

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Mol	Chain	Res	Type
2	B	102	ASN
2	B	310	PRO
2	B	337	VAL
2	B	384	LYS
3	C	95	MET
2	B	293	PRO
3	C	94	ILE

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	406/406 (100%)	353 (87%)	53 (13%)	4	4
2	B	352/419 (84%)	302 (86%)	50 (14%)	3	3
3	C	86/88 (98%)	64 (74%)	22 (26%)	0	0
All	All	844/913 (92%)	719 (85%)	125 (15%)	3	2

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ILE
1	A	13	THR
1	A	15	ILE
1	A	37	ASP
1	A	38	PRO
1	A	44	LEU
1	A	46	LEU
1	A	52	ILE
1	A	53	LYS
1	A	56	GLN
1	A	61	LEU
1	A	64	LYS
1	A	65	ASP
1	A	71	LEU

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Mol	Chain	Res	Type
1	A	83	ILE
1	A	96	LEU
1	A	102	ILE
1	A	111	LEU
1	A	121	LYS
1	A	122	LEU
1	A	139	LYS
1	A	144	PRO
1	A	166	LEU
1	A	169	LEU
1	A	171	LEU
1	A	179	ILE
1	A	192	LYS
1	A	194	THR
1	A	206	PHE
1	A	216	LEU
1	A	221	LYS
1	A	245	ASP
1	A	246	VAL
1	A	257	LYS
1	A	268	LEU
1	A	287	LEU
1	A	290	LEU
1	A	299	LEU
1	A	325	ASP
1	A	335	GLU
1	A	366	LEU
1	A	376	LYS
1	A	384	LEU
1	A	411	LEU
1	A	419	LEU
1	A	427	LEU
1	A	433	LEU
1	A	436	LEU
1	A	465	LEU
1	A	477	ASN
1	A	478	LEU
1	A	485	LEU
2	B	4	GLU
2	B	50	VAL
2	B	66	LEU
2	B	73	GLU

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Mol	Chain	Res	Type
2	B	108	GLU
2	B	109	VAL
2	B	114	LYS
2	B	119	THR
2	B	129	LYS
2	B	136	TYR
2	B	141	LEU
2	B	167	LEU
2	B	169	LYS
2	B	185	GLU
2	B	197	LEU
2	B	202	GLN
2	B	212	LYS
2	B	241	ILE
2	B	254	LYS
2	B	256	ILE
2	B	260	VAL
2	B	290	GLN
2	B	316	VAL
2	B	319	LEU
2	B	322	GLU
2	B	331	ILE
2	B	338	LYS
2	B	340	THR
2	B	344	LEU
2	B	345	MET
2	B	348	VAL
2	B	353	ASN
2	B	354	LYS
2	B	355	ASN
2	B	357	VAL
2	B	358	GLU
2	B	360	LEU
2	B	362	THR
2	B	363	LYS
2	B	364	LEU
2	B	368	ASN
2	B	369	LEU
2	B	373	ILE
2	B	377	GLU
2	B	378	ASP
2	B	385	ILE

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Mol	Chain	Res	Type
2	B	392	GLU
2	B	402	GLN
2	B	406	ASP
2	B	407	ASN
3	C	3	LYS
3	C	4	VAL
3	C	12	ILE
3	C	14	ASN
3	C	18	LEU
3	C	19	GLN
3	C	23	GLU
3	C	31	THR
3	C	32	LEU
3	C	33	GLU
3	C	35	ILE
3	C	36	LEU
3	C	56	VAL
3	C	57	LEU
3	C	59	LEU
3	C	63	LEU
3	C	67	LYS
3	C	69	ILE
3	C	75	GLU
3	C	94	ILE
3	C	97	GLU
3	C	98	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	85	ASN
1	A	115	ASN
1	A	212	GLN
1	A	337	HIS
1	A	379	GLN
1	A	387	ASN
1	A	445	GLN
1	A	447	ASN
1	A	471	GLN
1	A	477	ASN
2	B	86	ASN

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Mol	Chain	Res	Type
2	B	144	GLN
2	B	194	ASN
2	B	202	GLN
2	B	290	GLN
2	B	315	HIS
2	B	342	ASN
2	B	368	ASN
2	B	399	ASN
2	B	402	GLN
3	C	60	GLN
3	C	74	GLN
3	C	80	ASN
3	C	88	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ASN	A	511	-	7,8,8	0.73	0	6,10,10	3.76	1 (16%)

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
4	ASN	A	511	-	-	2/8/8/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	511	ASN	CA-CB-CG	8.95	130.19	112.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	511	ASN	CA-CB-CG-OD1
4	A	511	ASN	CA-CB-CG-ND2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	511	ASN	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	485/485 (100%)	-0.23	5 (1%) 79 80	24, 38, 58, 80	0
2	B	405/483 (83%)	0.98	64 (15%) 5 4	30, 67, 95, 95	0
3	C	98/100 (98%)	0.68	11 (11%) 10 9	42, 62, 95, 95	0
All	All	988/1068 (92%)	0.36	80 (8%) 18 17	24, 49, 95, 95	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	400	ALA	6.3
1	A	1	MET	5.5
2	B	359	LEU	5.5
2	B	382	SER	5.3
2	B	403	ILE	5.3
2	B	363	LYS	4.8
2	B	397	GLY	4.3
2	B	335	ALA	3.9
2	B	361	ASP	3.9
3	C	95	MET	3.8
2	B	401	LYS	3.7
2	B	381	MET	3.6
2	B	404	MET	3.6
2	B	362	THR	3.5
2	B	329	SER	3.5
2	B	390	PHE	3.4
2	B	385	ILE	3.4
3	C	96	ASN	3.3
2	B	364	LEU	3.3
2	B	370	ALA	3.3
2	B	398	GLY	3.3
2	B	360	LEU	3.2
3	C	94	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	99	ASP	3.2
3	C	92	PRO	3.1
2	B	340	THR	3.1
2	B	339	LEU	3.1
2	B	337	VAL	3.0
2	B	372	MET	3.0
2	B	405	GLU	3.0
2	B	373	ILE	2.9
2	B	260	VAL	2.9
2	B	113	THR	2.9
2	B	290	GLN	2.9
2	B	5	THR	2.8
2	B	238	GLY	2.8
2	B	333	HIS	2.8
2	B	237	ASN	2.8
2	B	375	LEU	2.8
2	B	310	PRO	2.7
2	B	376	ILE	2.7
2	B	393	LEU	2.6
2	B	258	MET	2.6
1	A	485	LEU	2.6
2	B	389	VAL	2.6
2	B	379	GLY	2.6
3	C	38	PHE	2.5
3	C	100	ALA	2.5
2	B	243	GLN	2.5
2	B	28	HIS	2.5
2	B	109	VAL	2.5
2	B	316	VAL	2.4
2	B	358	GLU	2.4
2	B	368	ASN	2.4
2	B	136	TYR	2.4
2	B	202	GLN	2.3
2	B	212	LYS	2.3
1	A	411	LEU	2.3
2	B	305	ASN	2.3
2	B	338	LYS	2.2
2	B	374	LYS	2.2
2	B	378	ASP	2.2
3	C	3	LYS	2.2
2	B	309	LEU	2.1
2	B	380	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	97	GLU	2.1
1	A	417	ASP	2.1
3	C	22	PRO	2.1
2	B	248	PHE	2.1
3	C	23	GLU	2.1
2	B	253	GLY	2.1
2	B	307	LEU	2.1
2	B	331	ILE	2.0
2	B	387	LYS	2.0
2	B	226	TYR	2.0
2	B	247	ARG	2.0
2	B	36	ASN	2.0
2	B	349	ASN	2.0
2	B	345	MET	2.0
1	A	231	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	B	501	1/1	0.87	0.14	33,33,33,33	0
4	ASN	A	511	9/9	0.95	0.08	32,36,39,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.