



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:30 AM UTC

PDB ID : 1OAC / pdb_00001oac
Title : CRYSTAL STRUCTURE OF A QUINOENZYME: COPPER AMINE OXIDASE OF ESCHERICHIA COLI AT 2 ANGSTROMS RESOLUTION
Authors : Parsons, M.R.; Convery, M.A.; Wilmot, C.M.; Phillips, S.E.V.
Deposited on : 1995-09-27
Resolution : 2.00 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

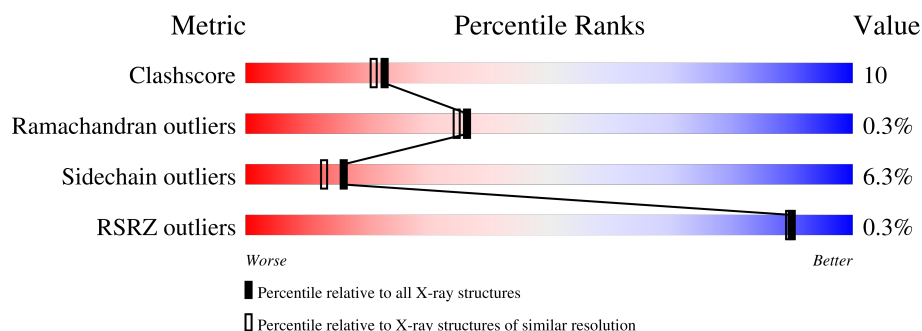
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	727	 64% 28% 6% ..
1	B	727	 62% 28% 8% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12358 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 COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	720	Total	C	N	O	S	0	0	0
			5679	3611	968	1078	22			
1	B	723	Total	C	N	O	S	0	0	0
			5705	3627	973	1083	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	466	TPQ	TYR	conflict	UNP P46883
B	466	TPQ	TYR	conflict	UNP P46883

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	489	Total	O	0	0
			489	489		

Continued on next page...

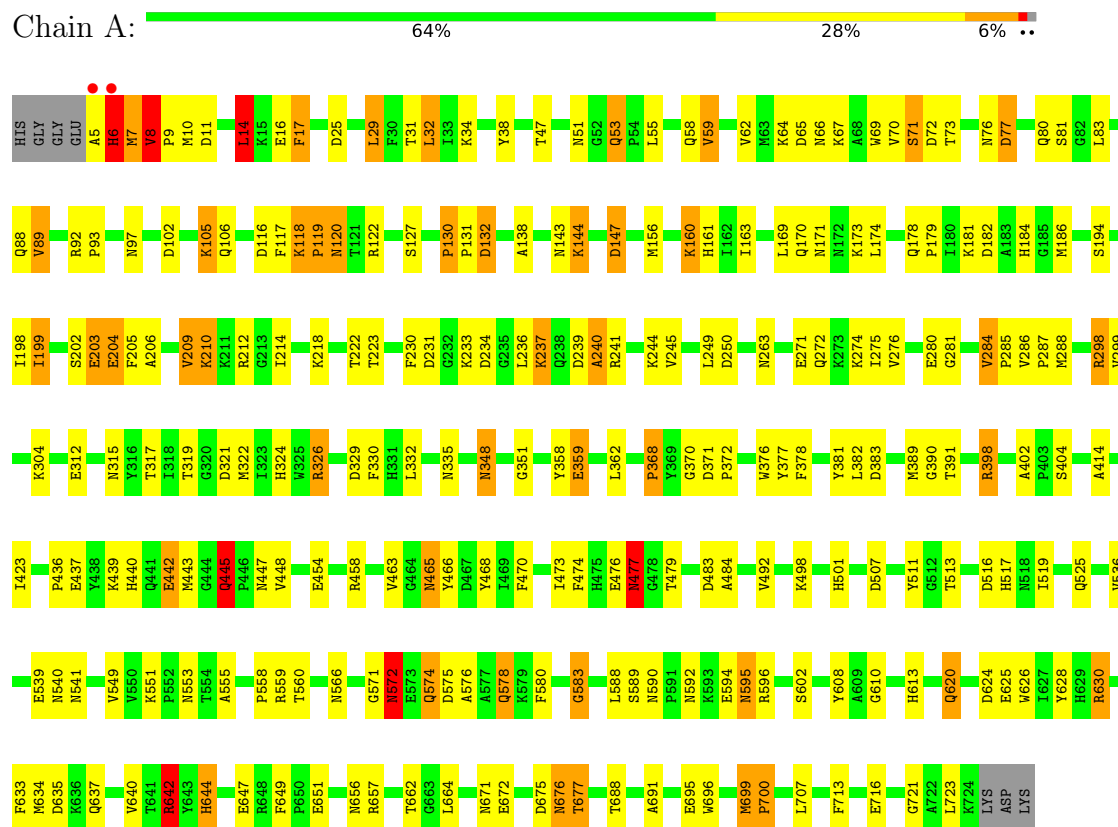
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	479	Total 479	O 479	0	0

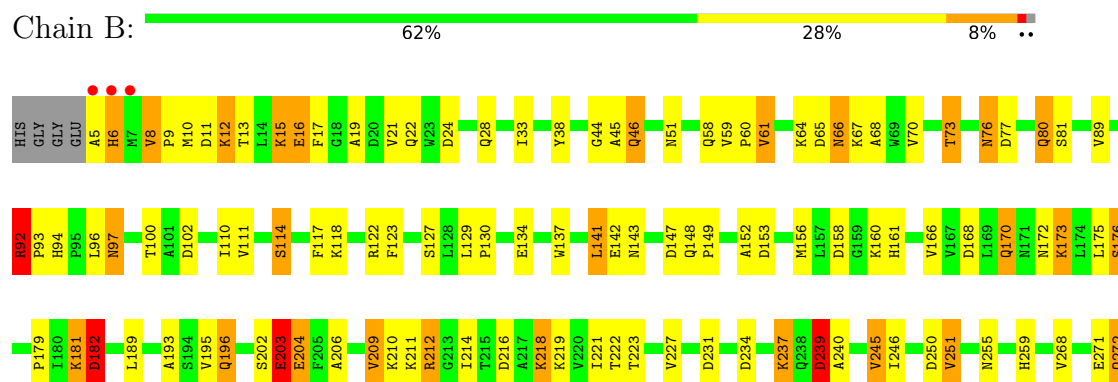
3 Residue-property plots

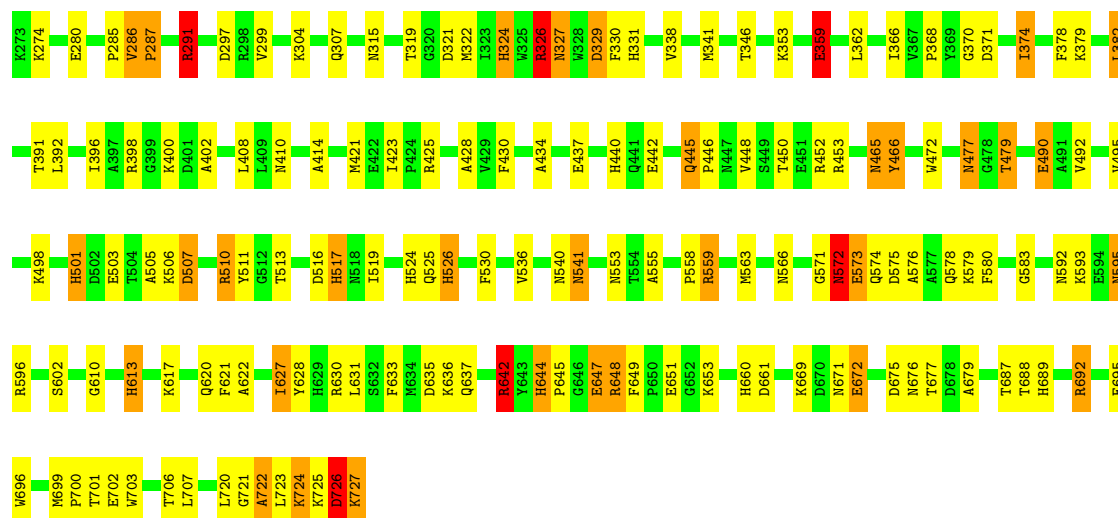
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: COPPER AMINE OXIDASE



• Molecule 1: COPPER AMINE OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.73Å 167.78Å 81.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.00) 86.6 (10.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.43 (at 2.00Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.162 , (Not available) 0.146 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 103.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12358	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: TPQ, CA, CU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.09	0/5809	2.07	188/7908 (2.4%)
1	B	1.10	4/5835 (0.1%)	2.07	202/7941 (2.5%)
All	All	1.09	4/11644 (0.0%)	2.07	390/15849 (2.5%)

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	8
1	B	0	5
All	All	0	13

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	391	THR	CA-CB	6.27	1.63	1.53
1	B	721	GLY	N-CA	6.08	1.50	1.45
1	B	259	HIS	CA-CB	5.32	1.59	1.53
1	B	513	THR	CA-CB	5.06	1.61	1.53

All (390) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	566	ASN	OD1-CG-ND2	15.70	138.30	122.60
1	B	566	ASN	OD1-CG-ND2	15.63	138.24	122.60
1	B	696	TRP	CA-C-O	-14.64	108.17	119.59
1	B	566	ASN	CA-CB-CG	-13.48	99.11	112.60
1	A	53	GLN	OE1-CD-NE2	13.34	135.94	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	696	TRP	CA-C-O	-13.20	109.29	119.59
1	B	695	GLU	O-C-N	12.97	138.31	122.35
1	B	182	ASP	CA-CB-CG	12.49	125.09	112.60
1	A	202	SER	CA-C-O	12.06	133.26	120.36
1	A	77	ASP	CA-CB-CG	11.83	124.43	112.60
1	A	8	VAL	N-CA-CB	-10.80	102.49	111.67
1	A	695	GLU	O-C-N	10.64	135.44	122.35
1	A	202	SER	CA-C-N	10.63	134.25	120.44
1	A	202	SER	C-N-CA	10.63	134.25	120.44
1	A	6	HIS	CA-CB-CG	-10.47	103.33	113.80
1	A	143	ASN	CA-CB-CG	-10.40	102.20	112.60
1	A	423	ILE	O-C-N	10.19	129.41	121.46
1	B	571	GLY	N-CA-C	9.97	127.02	114.66
1	B	501	HIS	CA-CB-CG	-9.74	104.06	113.80
1	B	696	TRP	O-C-N	9.72	132.22	121.23
1	B	675	ASP	CA-CB-CG	-9.62	102.98	112.60
1	B	425	ARG	NE-CZ-NH2	9.42	127.67	119.20
1	A	203	GLU	CB-CG-CD	9.03	127.94	112.60
1	B	410	ASN	CA-CB-CG	-9.01	103.59	112.60
1	A	116	ASP	CA-CB-CG	-8.88	103.72	112.60
1	B	143	ASN	CA-CB-CG	-8.86	103.74	112.60
1	A	700	PRO	CB-CA-C	8.79	122.80	111.46
1	A	161	HIS	CA-CB-CG	-8.71	105.09	113.80
1	B	202	SER	CA-C-O	8.69	130.42	120.60
1	A	6	HIS	CA-C-N	8.60	139.39	121.32
1	A	6	HIS	C-N-CA	8.60	139.39	121.32
1	A	132	ASP	N-CA-CB	8.58	122.53	110.17
1	B	6	HIS	CA-C-O	8.41	132.53	120.51
1	B	251	VAL	N-CA-CB	-8.33	101.52	112.26
1	A	539	GLU	CB-CG-CD	8.27	126.66	112.60
1	B	430	PHE	CA-CB-CG	8.27	122.07	113.80
1	B	179	PRO	CB-CA-C	8.26	122.20	111.21
1	A	574	GLN	CB-CG-CD	8.17	126.48	112.60
1	B	76	ASN	CA-CB-CG	-8.14	104.46	112.60
1	A	143	ASN	OD1-CG-ND2	8.12	130.72	122.60
1	A	675	ASP	CA-CB-CG	-8.11	104.49	112.60
1	B	129	LEU	CB-CA-C	8.10	118.59	110.33
1	A	171	ASN	CA-CB-CG	-8.09	104.51	112.60
1	B	202	SER	CA-C-N	7.84	131.68	120.79
1	B	202	SER	C-N-CA	7.84	131.68	120.79
1	A	122	ARG	NE-CZ-NH1	7.79	129.29	121.50
1	B	374	ILE	O-C-N	7.73	129.46	121.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	ALA	O-C-N	7.72	126.65	121.71
1	B	374	ILE	CB-CA-C	-7.69	101.97	112.04
1	A	371	ASP	CB-CA-C	7.68	118.76	109.31
1	B	19	ALA	CA-C-O	-7.67	112.15	121.36
1	B	5	ALA	CA-C-N	7.66	136.17	121.54
1	B	5	ALA	C-N-CA	7.66	136.17	121.54
1	A	620	GLN	OE1-CD-NE2	7.63	130.23	122.60
1	A	470	PHE	CA-CB-CG	-7.62	106.18	113.80
1	A	119	PRO	CA-C-N	-7.62	110.47	122.73
1	A	119	PRO	C-N-CA	-7.62	110.47	122.73
1	A	716	GLU	CA-C-O	-7.59	112.98	121.25
1	A	696	TRP	O-C-N	7.58	129.80	121.23
1	B	123	PHE	CA-C-O	-7.57	112.67	120.54
1	A	477	ASN	OD1-CG-ND2	-7.50	115.10	122.60
1	A	122	ARG	NE-CZ-NH2	-7.44	112.50	119.20
1	A	381	TYR	CA-C-N	7.41	132.37	122.06
1	A	381	TYR	C-N-CA	7.41	132.37	122.06
1	A	105	LYS	CA-CB-CG	-7.40	99.29	114.10
1	A	17	PHE	CA-CB-CG	7.38	121.18	113.80
1	B	147	ASP	CA-CB-CG	-7.38	105.22	112.60
1	B	578	GLN	N-CA-C	7.37	119.95	108.96
1	B	81	SER	N-CA-C	7.31	119.25	111.28
1	A	66	ASN	CB-CA-C	7.25	121.58	111.86
1	A	630	ARG	NE-CZ-NH1	7.24	128.74	121.50
1	A	378	PHE	CA-CB-CG	-7.21	106.59	113.80
1	B	326	ARG	CA-CB-CG	7.20	128.50	114.10
1	B	524	HIS	CA-C-O	-7.20	113.61	121.31
1	B	6	HIS	N-CA-C	7.15	126.03	110.80
1	B	6	HIS	CA-CB-CG	-7.13	106.67	113.80
1	B	122	ARG	CD-NE-CZ	7.12	134.36	124.40
1	B	695	GLU	N-CA-C	7.10	120.82	112.72
1	B	677	THR	CA-CB-OG1	-7.10	98.94	109.60
1	A	578	GLN	N-CA-C	7.08	119.52	108.96
1	B	102	ASP	O-C-N	7.04	129.70	122.09
1	B	227	VAL	CA-C-O	-7.03	112.45	119.20
1	B	203	GLU	CA-C-N	7.03	129.57	120.44
1	B	203	GLU	C-N-CA	7.03	129.57	120.44
1	A	389	MET	CA-C-N	7.00	127.72	119.94
1	A	389	MET	C-N-CA	7.00	127.72	119.94
1	B	324	HIS	CA-CB-CG	-7.00	106.80	113.80
1	B	706	THR	CA-CB-OG1	-6.99	99.11	109.60
1	B	648	ARG	NE-CZ-NH2	-6.96	112.94	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	507	ASP	CA-CB-CG	-6.95	105.65	112.60
1	A	390	GLY	N-CA-C	-6.93	104.46	112.50
1	B	583	GLY	N-CA-C	-6.93	104.85	115.66
1	A	6	HIS	CA-C-O	6.89	130.37	120.51
1	B	240	ALA	N-CA-C	6.84	119.65	110.35
1	B	378	PHE	CA-CB-CG	-6.84	106.96	113.80
1	A	572	ASN	O-C-N	6.82	131.56	122.96
1	A	513	THR	CA-C-O	-6.82	113.63	121.47
1	B	287	PRO	CB-CA-C	6.81	118.98	111.56
1	B	517	HIS	CA-CB-CG	-6.78	107.02	113.80
1	B	374	ILE	N-CA-CB	6.77	118.94	110.47
1	A	223	THR	CB-CA-C	6.76	118.43	109.65
1	A	66	ASN	CA-C-N	6.75	132.38	122.39
1	A	66	ASN	C-N-CA	6.75	132.38	122.39
1	A	713	PHE	N-CA-C	-6.75	103.39	111.69
1	B	649	PHE	O-C-N	6.74	127.39	121.39
1	B	490	GLU	O-C-N	6.73	130.56	122.96
1	A	458	ARG	NE-CZ-NH1	6.67	128.17	121.50
1	B	421	MET	CA-CB-CG	6.67	127.44	114.10
1	A	571	GLY	N-CA-C	6.63	126.00	115.66
1	A	8	VAL	CB-CA-C	6.62	120.38	110.97
1	A	414	ALA	CA-C-O	-6.62	113.50	121.05
1	A	613	HIS	CA-CB-CG	6.61	120.41	113.80
1	A	583	GLY	N-CA-C	-6.59	105.38	115.66
1	A	120	ASN	CB-CA-C	6.58	121.80	110.94
1	B	644	HIS	N-CA-CB	6.58	122.08	110.37
1	A	688	THR	N-CA-CB	6.55	121.00	110.65
1	A	330	PHE	CA-C-O	-6.55	114.26	121.33
1	B	204	GLU	O-C-N	6.53	128.79	122.07
1	B	725	LYS	CA-C-O	6.52	128.48	121.11
1	B	8	VAL	N-CA-CB	-6.51	102.10	111.21
1	B	595	ASN	CA-CB-CG	6.50	119.10	112.60
1	B	526	HIS	CA-C-O	-6.49	113.58	120.40
1	A	47	THR	CA-CB-OG1	-6.48	99.87	109.60
1	A	578	GLN	N-CA-CB	-6.48	101.32	111.56
1	B	379	LYS	CA-C-O	6.48	128.33	120.62
1	A	127	SER	CA-C-O	-6.47	114.08	121.40
1	A	250	ASP	CA-C-O	-6.47	113.28	120.60
1	B	203	GLU	CB-CG-CD	6.46	123.58	112.60
1	A	322	MET	CA-CB-CG	-6.45	101.20	114.10
1	B	726	ASP	CA-CB-CG	-6.42	106.18	112.60
1	A	14	LEU	O-C-N	6.41	129.01	122.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	625	GLU	CB-CG-CD	6.40	123.48	112.60
1	B	702	GLU	CA-C-O	-6.40	113.79	120.70
1	B	196	GLN	OE1-CD-NE2	-6.40	116.20	122.60
1	B	6	HIS	CA-C-N	6.39	133.56	122.82
1	B	6	HIS	C-N-CA	6.39	133.56	122.82
1	A	179	PRO	CB-CA-C	6.39	119.70	111.21
1	B	196	GLN	CB-CG-CD	6.38	123.45	112.60
1	A	29	LEU	O-C-N	6.38	131.05	123.33
1	B	143	ASN	CA-C-N	6.37	130.12	121.20
1	B	143	ASN	C-N-CA	6.37	130.12	121.20
1	A	66	ASN	CA-CB-CG	-6.37	106.23	112.60
1	A	391	THR	CA-CB-OG1	-6.34	100.10	109.60
1	B	329	ASP	CA-CB-CG	-6.33	106.27	112.60
1	B	81	SER	CA-C-O	-6.31	113.86	120.55
1	A	102	ASP	CA-CB-CG	-6.31	106.29	112.60
1	A	218	LYS	N-CA-C	-6.28	105.10	112.89
1	B	720	LEU	CA-C-N	-6.28	114.22	122.63
1	B	720	LEU	C-N-CA	-6.28	114.22	122.63
1	A	539	GLU	N-CA-C	6.28	119.41	111.69
1	B	129	LEU	N-CA-C	-6.25	96.07	109.01
1	B	251	VAL	CB-CA-C	6.25	118.96	111.20
1	A	721	GLY	O-C-N	6.25	129.29	123.35
1	A	16	GLU	CB-CG-CD	6.25	123.22	112.60
1	A	178	GLN	O-C-N	6.25	126.63	121.44
1	A	516	ASP	CA-C-O	-6.24	114.76	121.38
1	B	660	HIS	CA-CB-CG	-6.23	107.57	113.80
1	B	58	GLN	CA-C-O	6.22	127.11	120.70
1	A	440	HIS	N-CA-CB	6.21	120.83	110.59
1	A	178	GLN	CB-CA-C	-6.19	102.47	111.01
1	B	93	PRO	N-CA-CB	6.19	108.84	103.27
1	B	707	LEU	N-CA-CB	-6.18	100.03	111.52
1	A	240	ALA	N-CA-C	6.17	119.21	110.50
1	A	677	THR	CA-CB-OG1	-6.17	100.35	109.60
1	A	118	LYS	CA-C-O	6.16	126.98	120.64
1	B	100	THR	CA-CB-OG1	-6.16	100.37	109.60
1	B	77	ASP	O-C-N	6.15	128.73	122.09
1	A	184	HIS	N-CA-CB	6.14	120.68	110.85
1	B	695	GLU	CB-CG-CD	6.14	123.04	112.60
1	A	676	ASN	CA-CB-CG	-6.11	106.49	112.60
1	B	541	ASN	CA-CB-CG	6.11	118.71	112.60
1	B	503	GLU	CA-CB-CG	6.10	126.30	114.10
1	A	144	LYS	CA-C-O	6.09	123.82	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	661	ASP	CA-C-O	6.08	127.47	120.60
1	B	701	THR	CA-CB-OG1	-6.08	100.48	109.60
1	A	620	GLN	CB-CA-C	-6.07	103.67	111.50
1	A	624	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	72	ASP	CA-C-N	6.07	133.36	122.38
1	A	72	ASP	C-N-CA	6.07	133.36	122.38
1	B	374	ILE	CA-C-O	-6.06	114.75	121.05
1	A	695	GLU	N-CA-C	6.04	119.61	112.72
1	B	16	GLU	CB-CG-CD	6.04	122.87	112.60
1	B	453	ARG	CD-NE-CZ	6.03	132.84	124.40
1	B	700	PRO	CB-CA-C	6.01	119.20	111.56
1	A	25	ASP	CA-CB-CG	-6.01	106.59	112.60
1	A	317	THR	CA-CB-OG1	-6.00	100.59	109.60
1	A	572	ASN	CA-C-O	-6.00	114.79	121.51
1	A	448	VAL	CA-C-O	-6.00	114.15	120.39
1	A	117	PHE	CA-CB-CG	-5.99	107.81	113.80
1	B	239	ASP	N-CA-CB	-5.98	101.31	109.98
1	B	414	ALA	CA-C-O	-5.96	114.06	120.92
1	B	692	ARG	CA-C-N	5.96	128.87	120.28
1	B	692	ARG	C-N-CA	5.96	128.87	120.28
1	A	284	VAL	N-CA-C	-5.96	100.52	107.61
1	A	382	LEU	N-CA-C	-5.96	101.30	109.71
1	A	484	ALA	CA-C-O	-5.92	113.96	120.24
1	B	61	VAL	N-CA-C	-5.92	101.94	109.58
1	A	161	HIS	CA-C-O	-5.92	114.23	120.80
1	B	330	PHE	CA-CB-CG	5.92	119.72	113.80
1	B	286	VAL	O-C-N	5.88	127.54	121.07
1	A	398	ARG	O-C-N	-5.88	116.52	123.11
1	A	633	PHE	CA-C-N	5.88	128.75	120.28
1	A	633	PHE	C-N-CA	5.88	128.75	120.28
1	A	161	HIS	O-C-N	5.87	130.06	123.19
1	B	526	HIS	CA-CB-CG	-5.86	107.94	113.80
1	B	193	ALA	O-C-N	5.86	128.42	122.09
1	B	212	ARG	NE-CZ-NH2	-5.86	113.92	119.20
1	B	559	ARG	O-C-N	5.86	130.04	122.89
1	B	329	ASP	CA-C-O	-5.85	113.83	120.32
1	A	330	PHE	CA-CB-CG	5.85	119.65	113.80
1	B	633	PHE	CA-C-N	5.85	128.70	120.28
1	B	633	PHE	C-N-CA	5.85	128.70	120.28
1	B	479	THR	CA-CB-OG1	-5.84	100.84	109.60
1	B	622	ALA	CB-CA-C	5.84	118.67	109.27
1	B	495	VAL	CA-C-O	-5.84	115.85	121.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	ASN	OD1-CG-ND2	5.82	128.42	122.60
1	A	620	GLN	CA-C-N	5.81	131.88	122.29
1	A	620	GLN	C-N-CA	5.81	131.88	122.29
1	A	359	GLU	CB-CA-C	-5.81	98.18	109.68
1	A	89	VAL	O-C-N	5.81	129.56	122.83
1	B	68	ALA	CB-CA-C	5.81	119.11	109.53
1	A	66	ASN	N-CA-C	-5.80	103.40	111.52
1	A	391	THR	O-C-N	5.79	128.26	122.12
1	A	88	GLN	N-CA-CB	5.79	120.57	111.20
1	A	329	ASP	CA-C-O	-5.78	113.17	120.28
1	A	376	TRP	N-CA-C	5.77	123.09	110.80
1	B	353	LYS	N-CA-CB	5.76	119.16	109.94
1	A	644	HIS	CA-CB-CG	-5.76	108.04	113.80
1	B	202	SER	N-CA-C	5.73	117.55	108.67
1	A	324	HIS	CA-CB-CG	-5.72	108.08	113.80
1	B	223	THR	CB-CA-C	5.72	117.09	109.65
1	B	445	GLN	O-C-N	5.72	126.22	121.35
1	B	672	GLU	CG-CD-OE1	5.72	131.55	118.40
1	B	572	ASN	CB-CG-ND2	5.71	124.97	116.40
1	B	400	LYS	O-C-N	5.71	128.63	121.95
1	B	595	ASN	N-CA-C	-5.71	102.47	110.35
1	B	234	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	205	PHE	CA-CB-CG	-5.70	108.10	113.80
1	B	147	ASP	CB-CA-C	5.70	118.75	111.40
1	A	473	ILE	CA-C-O	-5.69	114.44	120.53
1	A	662	THR	CA-CB-OG1	-5.69	101.06	109.60
1	A	664	LEU	CA-C-O	-5.68	114.53	120.55
1	B	114	SER	N-CA-CB	5.67	118.31	109.97
1	B	153	ASP	CA-C-O	-5.67	114.29	120.36
1	A	59	VAL	O-C-N	5.67	126.84	121.11
1	A	440	HIS	CA-CB-CG	-5.67	108.13	113.80
1	B	530	PHE	CA-CB-CG	-5.66	108.14	113.80
1	B	695	GLU	CA-C-O	-5.65	113.06	119.78
1	B	576	ALA	CA-C-O	-5.63	112.33	119.31
1	A	483	ASP	CA-C-O	-5.63	114.75	120.71
1	A	404	SER	CA-C-O	-5.62	112.68	119.49
1	A	628	TYR	CA-C-O	5.60	126.70	120.82
1	A	707	LEU	N-CA-CB	-5.60	101.11	111.52
1	B	80	GLN	CB-CG-CD	5.60	122.11	112.60
1	A	362	LEU	N-CA-C	-5.59	102.12	110.23
1	A	319	THR	CA-CB-OG1	-5.58	101.22	109.60
1	B	76	ASN	OD1-CG-ND2	5.58	128.18	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	448	VAL	N-CA-CB	5.57	118.92	111.90
1	B	17	PHE	CA-CB-CG	5.57	119.37	113.80
1	A	445	GLN	O-C-N	5.56	127.72	121.32
1	B	227	VAL	O-C-N	5.56	127.68	122.23
1	B	573	GLU	N-CA-C	5.55	118.09	111.71
1	A	445	GLN	OE1-CD-NE2	5.54	128.14	122.60
1	B	647	GLU	CA-C-O	-5.54	115.16	120.92
1	B	423	ILE	O-C-N	5.54	125.78	121.46
1	A	566	ASN	N-CA-CB	-5.53	101.41	110.21
1	B	148	GLN	CB-CA-C	5.53	118.00	109.15
1	B	440	HIS	N-CA-CB	5.52	119.70	110.59
1	B	440	HIS	CA-CB-CG	-5.51	108.28	113.80
1	A	174	LEU	O-C-N	5.51	129.79	123.02
1	A	695	GLU	CB-CG-CD	5.50	121.95	112.60
1	A	716	GLU	CB-CG-CD	5.49	121.94	112.60
1	A	59	VAL	CB-CA-C	-5.49	104.80	110.13
1	B	141	LEU	CA-C-O	-5.49	113.04	119.24
1	A	76	ASN	OD1-CG-ND2	5.49	128.09	122.60
1	B	695	GLU	CG-CD-OE2	5.48	131.00	118.40
1	B	636	LYS	CA-C-O	-5.47	114.93	121.11
1	B	97	ASN	CA-C-O	-5.47	115.13	121.15
1	A	479	THR	CA-CB-OG1	-5.46	101.41	109.60
1	B	160	LYS	N-CA-C	-5.45	105.28	113.89
1	A	312	GLU	CG-CD-OE2	-5.45	105.86	118.40
1	A	127	SER	O-C-N	5.43	129.74	123.17
1	A	335	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	B	649	PHE	CA-CB-CG	-5.41	108.39	113.80
1	A	691	ALA	N-CA-C	5.41	117.85	110.55
1	B	434	ALA	N-CA-CB	-5.41	103.51	111.51
1	B	566	ASN	N-CA-CB	-5.40	102.30	110.35
1	A	501	HIS	CA-CB-CG	-5.39	108.41	113.80
1	A	590	ASN	O-C-N	5.38	126.29	120.85
1	B	579	LYS	N-CA-C	-5.38	102.52	110.48
1	B	73	THR	CA-CB-CG2	5.37	119.63	110.50
1	B	696	TRP	N-CA-C	5.37	118.91	107.91
1	B	299	VAL	CA-C-O	-5.36	114.74	120.59
1	B	642	ARG	CB-CA-C	5.34	118.56	109.53
1	A	312	GLU	CA-CB-CG	-5.34	103.41	114.10
1	B	122	ARG	NE-CZ-NH2	-5.34	114.40	119.20
1	B	362	LEU	N-CA-C	-5.34	102.49	110.23
1	B	566	ASN	CB-CG-ND2	-5.33	108.40	116.40
1	B	359	GLU	CA-CB-CG	5.33	124.77	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	725	LYS	N-CA-C	5.33	118.25	109.72
1	A	66	ASN	CA-C-O	5.33	127.88	121.65
1	B	206	ALA	CA-C-O	5.33	126.20	120.55
1	A	476	GLU	CG-CD-OE1	-5.32	106.16	118.40
1	A	436	PRO	CB-CA-C	5.32	118.28	111.21
1	A	588	LEU	N-CA-C	-5.32	98.58	107.99
1	B	382	LEU	N-CA-C	-5.32	98.61	108.24
1	B	402	ALA	CA-C-O	-5.32	115.61	120.50
1	A	186	MET	N-CA-CB	-5.31	103.06	110.29
1	A	677	THR	N-CA-CB	-5.30	103.04	111.62
1	B	117	PHE	CA-CB-CG	-5.30	108.50	113.80
1	B	319	THR	CA-CB-OG1	-5.29	101.66	109.60
1	B	338	VAL	N-CA-C	5.29	118.07	112.83
1	B	130	PRO	O-C-N	5.29	127.70	121.46
1	B	572	ASN	CA-CB-CG	-5.29	107.31	112.60
1	A	468	TYR	CA-CB-CG	-5.28	104.39	113.90
1	B	450	THR	CA-CB-CG2	5.28	119.48	110.50
1	A	602	SER	N-CA-C	5.28	117.00	109.14
1	B	231	ASP	N-CA-CB	-5.27	104.17	112.13
1	A	83	LEU	N-CA-C	-5.27	106.70	113.23
1	A	402	ALA	O-C-N	5.27	125.54	121.85
1	B	268	VAL	O-C-N	5.26	128.87	123.18
1	A	640	VAL	N-CA-CB	5.25	119.77	111.99
1	B	635	ASP	CA-C-O	-5.25	113.16	119.15
1	A	651	GLU	CG-CD-OE1	5.24	130.46	118.40
1	A	97	ASN	CB-CG-ND2	5.24	124.26	116.40
1	A	589	SER	CB-CA-C	-5.23	99.80	109.37
1	B	374	ILE	N-CA-C	5.22	116.57	110.62
1	B	699	MET	N-CA-C	5.22	116.49	109.24
1	A	32	LEU	CA-C-N	-5.21	116.31	123.14
1	A	32	LEU	C-N-CA	-5.21	116.31	123.14
1	A	170	GLN	CB-CG-CD	-5.21	103.74	112.60
1	B	321	ASP	O-C-N	5.21	128.55	122.24
1	B	722	ALA	CA-C-O	5.20	126.99	121.16
1	B	505	ALA	N-CA-C	5.20	117.35	111.11
1	A	118	LYS	CA-C-N	5.20	125.00	119.28
1	A	118	LYS	C-N-CA	5.20	125.00	119.28
1	A	699	MET	N-CA-C	5.18	116.44	109.24
1	A	281	GLY	O-C-N	5.17	126.94	121.77
1	B	127	SER	N-CA-C	5.17	117.24	109.23
1	B	307	GLN	OE1-CD-NE2	5.17	127.77	122.60
1	A	206	ALA	CA-C-N	5.17	127.47	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	ALA	C-N-CA	5.17	127.47	120.44
1	B	166	VAL	CA-C-O	-5.16	114.97	120.39
1	A	275	ILE	N-CA-CB	5.16	116.54	110.82
1	A	474	PHE	CA-CB-CG	-5.15	108.65	113.80
1	A	234	ASP	CA-C-N	5.14	129.24	120.91
1	A	234	ASP	C-N-CA	5.14	129.24	120.91
1	B	688	THR	CA-CB-OG1	-5.14	101.89	109.60
1	B	703	TRP	N-CA-C	5.14	117.94	109.72
1	B	110	ILE	CA-C-O	-5.14	115.72	121.17
1	B	245	VAL	O-C-N	5.13	128.52	123.18
1	B	173	LYS	CA-CB-CG	5.13	124.36	114.10
1	B	602	SER	N-CA-C	5.13	116.79	109.14
1	A	507	ASP	CA-CB-CG	-5.13	107.47	112.60
1	A	635	ASP	N-CA-CB	-5.13	102.41	110.46
1	B	173	LYS	O-C-N	5.13	129.13	123.33
1	A	263	ASN	OD1-CG-ND2	5.13	127.73	122.60
1	A	437	GLU	N-CA-C	-5.12	105.78	111.36
1	B	176	SER	O-C-N	5.12	128.99	123.56
1	B	371	ASP	CB-CA-C	5.12	115.61	109.31
1	B	700	PRO	O-C-N	-5.12	116.39	122.89
1	A	656	ASN	CB-CA-C	5.11	117.93	110.26
1	B	442	GLU	CB-CG-CD	5.10	121.27	112.60
1	A	558	PRO	N-CA-C	5.09	120.22	113.86
1	A	442	GLU	CA-C-O	-5.08	114.97	120.81
1	A	31	THR	N-CA-CB	5.08	118.57	110.65
1	A	371	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	511	TYR	CA-C-O	-5.07	113.61	119.59
1	A	144	LYS	CA-CB-CG	5.06	124.22	114.10
1	B	285	PRO	CB-CA-C	5.06	117.94	111.21
1	B	593	LYS	CA-C-O	-5.06	114.84	120.66
1	A	130	PRO	N-CA-C	5.05	116.87	110.70
1	A	454	GLU	CA-C-O	-5.05	115.25	120.70
1	B	689	HIS	CA-C-N	5.05	129.36	122.90
1	B	689	HIS	C-N-CA	5.05	129.36	122.90
1	B	44	GLY	CA-C-O	-5.04	114.21	119.20
1	A	199	ILE	O-C-N	5.04	126.76	121.87
1	B	644	HIS	CA-CB-CG	-5.03	108.77	113.80
1	B	327	ASN	OD1-CG-ND2	5.03	127.63	122.60
1	A	163	ILE	N-CA-CB	5.03	119.68	111.44
1	B	152	ALA	CA-C-N	5.03	129.46	122.77
1	B	152	ALA	C-N-CA	5.03	129.46	122.77
1	B	67	LYS	O-C-N	5.02	128.94	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	651	GLU	CA-C-O	-5.01	113.21	119.28
1	B	77	ASP	CA-C-O	-5.01	115.54	120.70
1	B	425	ARG	NH1-CZ-NH2	-5.01	112.79	119.30
1	B	92	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	B	653	LYS	CA-C-O	-5.01	115.56	120.82
1	B	472	TRP	N-CA-C	-5.01	100.36	108.52
1	B	648	ARG	NH1-CZ-NH2	5.01	125.81	119.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	298	ARG	Sidechain
1	A	326	ARG	Sidechain
1	A	398	ARG	Sidechain
1	A	596	ARG	Sidechain
1	A	630	ARG	Sidechain
1	A	642	ARG	Sidechain
1	A	657	ARG	Sidechain
1	A	92	ARG	Sidechain
1	B	291	ARG	Sidechain
1	B	630	ARG	Sidechain
1	B	642	ARG	Sidechain
1	B	692	ARG	Sidechain
1	B	92	ARG	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	5679	0	5550	116	0
1	B	5705	0	5580	132	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	489	0	0	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	479	0	0	23	0
All	All	12358	0	11130	235	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 10.

All (235) 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:93:PRO:HG2	4:A:1172:HOH:O	1.49	1.11
1:A:249:LEU:HD23	1:A:288:MET:HE1	1.43	0.98
1:A:315:ASN:HD21	1:B:304:LYS:H	1.08	0.97
1:B:216:ASP:HB3	1:B:219:LYS:HD2	1.46	0.97
1:A:304:LYS:H	1:B:315:ASN:HD21	1.17	0.92
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.52	0.91
1:B:94:HIS:HD2	1:B:96:LEU:H	1.23	0.86
1:B:580:PHE:H	1:B:637:GLN:HE21	1.21	0.86
1:B:613:HIS:HB2	4:B:1221:HOH:O	1.77	0.85
1:B:221:ILE:CD1	1:B:250:ASP:HB2	2.08	0.83
1:A:7:MET:HE1	1:A:59:VAL:HG11	1.61	0.81
1:A:443:MET:CE	4:B:1146:HOH:O	2.29	0.79
1:B:272:GLN:NE2	1:B:274:LYS:HD2	1.98	0.79
1:B:592:ASN:HD21	1:B:676:ASN:HD21	1.30	0.79
1:B:322:MET:HG3	4:B:1195:HOH:O	1.82	0.79
1:A:572:ASN:ND2	1:A:575:ASP:H	1.82	0.77
1:A:580:PHE:H	1:A:637:GLN:HE21	1.32	0.77
1:A:443:MET:HE3	4:B:1146:HOH:O	1.85	0.76
1:A:62:VAL:HG23	1:A:69:TRP:HB2	1.68	0.74
1:A:553:ASN:ND2	1:A:555:ALA:H	1.85	0.74
1:A:574:GLN:H	1:A:671:ASN:ND2	1.86	0.73
1:A:592:ASN:HD21	1:A:676:ASN:HD21	1.34	0.73
1:B:574:GLN:H	1:B:671:ASN:ND2	1.87	0.73
1:B:272:GLN:HE21	1:B:274:LYS:HD2	1.53	0.73
1:B:642:ARG:CB	1:B:642:ARG:HH11	2.03	0.72
1:A:642:ARG:HB2	1:A:642:ARG:HH11	1.54	0.72
1:A:203:GLU:HG2	1:A:204:GLU:HG3	1.70	0.72
1:B:525:GLN:HE22	1:B:620:GLN:H	1.38	0.72
1:A:377:TYR:CE1	1:B:558:PRO:HG2	2.26	0.71
1:B:511:TYR:HB3	4:B:926:HOH:O	1.91	0.69
1:A:536:VAL:H	1:A:541:ASN:HD21	1.41	0.68
1:B:168:ASP:HB2	1:B:175:LEU:HD11	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:GLN:NE2	1:B:620:GLN:H	1.90	0.68
1:B:553:ASN:HD21	1:B:555:ALA:HB3	1.58	0.68
1:A:203:GLU:HG2	1:A:204:GLU:H	1.59	0.67
1:B:642:ARG:HH11	1:B:642:ARG:HB2	1.60	0.67
1:A:212:ARG:HH21	1:A:280:GLU:HB3	1.60	0.67
1:A:181:LYS:O	1:A:182:ASP:HB2	1.95	0.66
1:A:272:GLN:HB3	1:A:274:LYS:HD3	1.78	0.66
1:B:209:VAL:HG13	1:B:214:ILE:HB	1.78	0.66
1:A:288:MET:HE2	1:A:288:MET:HA	1.77	0.65
1:A:212:ARG:NH2	1:A:280:GLU:HB3	2.11	0.65
1:A:551:LYS:HE3	4:A:1225:HOH:O	1.95	0.64
1:B:498:LYS:O	1:B:517:HIS:HD2	1.79	0.64
1:A:465:ASN:HD22	1:A:465:ASN:H	1.44	0.64
1:B:33:ILE:HD12	4:B:1232:HOH:O	1.97	0.64
1:A:348:ASN:HD22	1:A:348:ASN:C	2.06	0.64
1:A:572:ASN:HD22	1:A:575:ASP:H	1.44	0.64
1:B:181:LYS:O	1:B:182:ASP:HB2	1.98	0.63
1:A:38:TYR:H	1:A:51:ASN:ND2	1.96	0.63
1:B:580:PHE:H	1:B:637:GLN:NE2	1.94	0.63
1:B:466:TPQ:C5	4:B:1192:HOH:O	2.48	0.62
1:A:5:ALA:O	1:A:6:HIS:HB2	1.97	0.62
1:A:517:HIS:CE1	1:B:596:ARG:HH11	2.18	0.61
1:A:38:TYR:H	1:A:51:ASN:HD21	1.47	0.61
1:B:506:LYS:HE3	1:B:510:ARG:HH12	1.64	0.61
1:B:506:LYS:HE2	1:B:510:ARG:HH22	1.66	0.60
1:A:10:MET:HG3	1:A:14:LEU:HD23	1.84	0.60
1:B:12:LYS:O	1:B:16:GLU:HG2	2.02	0.60
1:B:465:ASN:HD22	1:B:465:ASN:H	1.48	0.60
1:A:498:LYS:O	1:A:517:HIS:HD2	1.84	0.59
1:B:445:GLN:HB3	1:B:446:PRO:HD2	1.85	0.59
1:A:17:PHE:CE2	1:A:34:LYS:HD2	2.37	0.59
1:A:272:GLN:HE21	1:A:274:LYS:HD3	1.68	0.58
1:B:368:PRO:HB2	1:B:621:PHE:HZ	1.69	0.58
1:B:65:ASP:O	1:B:66:ASN:HB2	2.02	0.58
1:B:216:ASP:OD1	1:B:218:LYS:HB2	2.04	0.57
1:B:506:LYS:CE	1:B:510:ARG:HH22	2.17	0.57
1:A:73:THR:HG23	1:A:77:ASP:OD2	2.05	0.57
1:B:38:TYR:H	1:B:51:ASN:ND2	2.01	0.57
1:A:298:ARG:HA	1:B:722:ALA:O	2.05	0.57
1:A:642:ARG:HH11	1:A:642:ARG:CB	2.16	0.57
1:B:645:PRO:O	4:B:1040:HOH:O	2.17	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:SER:OG	1:A:73:THR:HG22	2.04	0.57
1:A:549:VAL:CG2	1:A:551:LYS:HE2	2.35	0.57
1:A:203:GLU:HG2	1:A:204:GLU:N	2.20	0.56
1:B:574:GLN:H	1:B:671:ASN:HD22	1.52	0.56
1:B:572:ASN:ND2	1:B:575:ASP:H	2.02	0.56
1:A:230:PHE:O	1:A:233:LYS:HG2	2.07	0.55
1:B:94:HIS:CD2	1:B:96:LEU:H	2.13	0.55
1:A:583:GLY:HA3	1:B:617:LYS:HE2	1.87	0.55
1:B:8:VAL:HG23	1:B:9:PRO:HD2	1.88	0.55
1:A:147:ASP:HB3	4:A:1226:HOH:O	2.05	0.55
1:B:396:ILE:HD13	1:B:428:ALA:HB2	1.88	0.55
1:A:209:VAL:HG13	1:A:214:ILE:HB	1.88	0.54
1:B:141:LEU:HD21	1:B:346:THR:HG21	1.88	0.54
1:B:477:ASN:HD22	1:B:477:ASN:C	2.15	0.54
1:B:536:VAL:H	1:B:541:ASN:HD21	1.54	0.54
1:A:93:PRO:CG	4:A:1172:HOH:O	2.28	0.54
1:A:540:ASN:HB3	1:A:676:ASN:ND2	2.23	0.54
1:A:160:LYS:HE3	1:A:271:GLU:OE1	2.08	0.54
1:B:466:TPQ:C3	1:B:526:HIS:HE1	2.20	0.54
1:B:38:TYR:H	1:B:51:ASN:HD21	1.56	0.54
1:B:94:HIS:HB3	1:B:97:ASN:ND2	2.23	0.54
1:A:580:PHE:H	1:A:637:GLN:NE2	2.04	0.53
1:A:574:GLN:HG2	1:A:671:ASN:CG	2.33	0.53
1:B:203:GLU:OE2	1:B:204:GLU:HG3	2.08	0.53
1:B:8:VAL:HG22	1:B:13:THR:OG1	2.09	0.53
1:A:477:ASN:C	1:A:477:ASN:HD22	2.17	0.52
1:A:644:HIS:HE1	1:A:672:GLU:OE1	1.92	0.52
1:B:134:GLU:HB2	4:B:1137:HOH:O	2.08	0.52
1:B:341:MET:HE2	4:B:919:HOH:O	2.08	0.52
1:B:322:MET:HE3	1:B:331:HIS:HB2	1.92	0.52
1:A:465:ASN:H	1:A:465:ASN:ND2	2.07	0.52
1:B:573:GLU:HG3	1:B:672:GLU:O	2.10	0.52
1:B:10:MET:HG3	1:B:70:VAL:HG11	1.91	0.51
1:A:65:ASP:HB3	1:A:67:LYS:HD2	1.92	0.51
1:A:368:PRO:HG3	1:A:634:MET:CE	2.41	0.51
1:A:439:LYS:NZ	1:A:447:ASN:ND2	2.59	0.51
1:A:525:GLN:HE22	1:A:620:GLN:H	1.57	0.51
1:B:507:ASP:OD1	1:B:510:ARG:NH2	2.37	0.51
1:B:553:ASN:ND2	1:B:555:ALA:H	2.08	0.51
1:A:723:LEU:HD23	1:B:297:ASP:O	2.11	0.51
1:B:368:PRO:HB2	1:B:621:PHE:CZ	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLN:NE2	1:A:73:THR:HG21	2.26	0.50
1:B:324:HIS:ND1	4:B:1035:HOH:O	2.30	0.50
1:B:359:GLU:CD	1:B:648:ARG:HH22	2.20	0.50
1:B:329:ASP:OD1	4:B:1035:HOH:O	2.20	0.50
1:A:236:LEU:HD11	1:A:244:LYS:HE3	1.92	0.50
1:A:348:ASN:ND2	1:A:351:GLY:H	2.09	0.50
1:A:439:LYS:HZ2	1:A:447:ASN:HD21	1.59	0.49
1:B:158:ASP:O	1:B:161:HIS:HD2	1.95	0.49
1:A:106:GLN:NE2	1:A:169:LEU:O	2.41	0.49
1:A:644:HIS:HB2	1:A:647:GLU:HG3	1.93	0.49
1:A:358:TYR:CD2	1:A:359:GLU:HG3	2.47	0.49
1:B:620:GLN:HG3	4:B:992:HOH:O	2.11	0.49
1:A:160:LYS:HG2	1:A:271:GLU:CD	2.38	0.49
1:A:549:VAL:HG21	1:A:551:LYS:HE2	1.95	0.49
1:A:368:PRO:HG3	1:A:634:MET:HE1	1.95	0.49
1:B:46:GLN:HA	1:B:46:GLN:OE1	2.12	0.49
1:B:237:LYS:HE2	1:B:239:ASP:CG	2.37	0.49
1:A:58:GLN:HE21	1:A:73:THR:HG21	1.78	0.48
1:B:540:ASN:HB3	1:B:676:ASN:ND2	2.28	0.48
1:A:105:LYS:HD3	4:A:1271:HOH:O	2.14	0.48
1:B:466:TPQ:C6	4:B:1192:HOH:O	2.60	0.48
1:B:149:PRO:HB3	1:B:170:GLN:HB2	1.95	0.48
1:B:11:ASP:O	1:B:15:LYS:HD2	2.14	0.48
1:B:627:ILE:HG22	4:B:994:HOH:O	2.12	0.48
1:B:642:ARG:HB2	1:B:642:ARG:NH1	2.28	0.48
1:B:465:ASN:H	1:B:465:ASN:ND2	2.12	0.48
1:B:648:ARG:NH1	4:B:1040:HOH:O	2.43	0.48
1:B:642:ARG:HH11	1:B:642:ARG:CG	2.26	0.48
1:A:321:ASP:HB3	1:A:332:LEU:O	2.15	0.47
1:A:10:MET:HE3	1:A:70:VAL:CG1	2.45	0.47
1:A:620:GLN:HB2	1:B:563:MET:HE2	1.97	0.47
1:B:111:VAL:O	1:B:114:SER:HB3	2.15	0.47
1:B:222:THR:HB	1:B:245:VAL:HG13	1.97	0.47
1:A:525:GLN:NE2	1:A:620:GLN:H	2.13	0.47
1:B:8:VAL:CG2	1:B:9:PRO:HD2	2.46	0.46
1:B:366:ILE:HD11	1:B:627:ILE:HD11	1.96	0.46
1:A:553:ASN:HD21	1:A:555:ALA:HB3	1.79	0.46
1:B:97:ASN:ND2	1:B:331:HIS:NE2	2.61	0.46
1:A:286:VAL:HG12	1:A:288:MET:HE3	1.98	0.46
1:B:209:VAL:CG1	1:B:214:ILE:HB	2.46	0.46
1:A:348:ASN:HD21	1:A:351:GLY:H	1.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:GLU:OE1	1:B:501:HIS:HE1	1.98	0.46
1:A:237:LYS:HD3	1:A:240:ALA:HB2	1.98	0.45
1:A:77:ASP:O	1:A:81:SER:HB3	2.16	0.45
1:A:576:ALA:O	1:A:578:GLN:HG2	2.16	0.45
1:A:118:LYS:HB3	1:A:119:PRO:HD2	1.98	0.45
1:A:348:ASN:HD21	1:A:351:GLY:CA	2.30	0.45
1:A:160:LYS:HB3	1:A:241:ARG:HB2	1.98	0.45
1:A:549:VAL:HG23	1:A:551:LYS:HE2	1.98	0.45
1:B:553:ASN:ND2	1:B:555:ALA:HB3	2.30	0.45
1:A:610:GLY:HA3	1:B:610:GLY:HA3	1.98	0.45
1:B:613:HIS:HD2	4:B:988:HOH:O	1.99	0.45
1:B:627:ILE:HG13	1:B:631:LEU:HD12	2.00	0.44
1:A:17:PHE:O	1:A:34:LYS:HE3	2.17	0.44
1:A:130:PRO:HA	1:A:131:PRO:HD3	1.85	0.44
1:B:214:ILE:HD11	1:B:286:VAL:HG21	1.99	0.44
1:B:644:HIS:HB2	1:B:647:GLU:HG3	1.99	0.44
1:B:506:LYS:HD3	1:B:510:ARG:HH22	1.82	0.44
1:B:398:ARG:HG2	1:B:408:LEU:HD11	1.99	0.44
1:B:59:VAL:HA	1:B:60:PRO:HD3	1.84	0.44
1:A:138:ALA:HB1	1:A:144:LYS:HE2	2.00	0.43
1:A:147:ASP:CB	4:A:1226:HOH:O	2.65	0.43
1:A:286:VAL:HA	1:A:287:PRO:HD3	1.83	0.43
1:A:560:THR:HG23	4:B:1182:HOH:O	2.18	0.43
1:A:608:TYR:HE1	4:A:1058:HOH:O	2.00	0.43
1:B:723:LEU:HD12	1:B:723:LEU:HA	1.82	0.43
1:A:204:GLU:HG3	1:A:204:GLU:H	1.66	0.43
1:A:649:PHE:HD2	4:A:1231:HOH:O	1.99	0.43
1:A:194:SER:O	1:A:198:ILE:HG13	2.19	0.43
1:A:442:GLU:HB3	1:A:445:GLN:HB2	2.01	0.43
1:B:382:LEU:HD23	1:B:651:GLU:HG3	2.01	0.43
1:B:572:ASN:HD22	1:B:575:ASP:H	1.66	0.43
1:A:284:VAL:HA	1:A:285:PRO:HD3	1.84	0.43
1:B:492:VAL:HB	1:B:519:ILE:HG23	2.01	0.43
1:A:572:ASN:HB2	1:A:671:ASN:ND2	2.34	0.43
1:B:15:LYS:NZ	1:B:21:VAL:HB	2.34	0.43
1:B:181:LYS:O	1:B:182:ASP:CB	2.64	0.43
1:B:286:VAL:HA	1:B:287:PRO:HD3	1.89	0.43
1:B:445:GLN:HB3	1:B:446:PRO:CD	2.48	0.42
1:B:687:THR:HG21	4:B:1221:HOH:O	2.19	0.42
1:B:726:ASP:HB3	1:B:727:LYS:H	1.49	0.42
1:A:231:ASP:HB2	1:A:626:TRP:CZ2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:GLU:HB3	4:B:1132:HOH:O	2.19	0.42
1:A:8:VAL:HA	1:A:9:PRO:HD3	1.84	0.42
1:B:10:MET:HG3	1:B:70:VAL:CG1	2.49	0.42
1:A:560:THR:CG2	4:B:1182:HOH:O	2.67	0.42
1:A:595:ASN:HD22	1:A:595:ASN:C	2.26	0.42
1:A:699:MET:HA	1:A:700:PRO:HD3	1.88	0.42
1:B:45:ALA:O	1:B:60:PRO:HB3	2.20	0.42
1:B:149:PRO:HB3	1:B:170:GLN:CB	2.49	0.42
1:B:222:THR:HB	1:B:245:VAL:CG1	2.50	0.42
1:B:246:ILE:HD13	1:B:246:ILE:HA	1.84	0.42
1:A:492:VAL:HB	1:A:519:ILE:HG23	2.02	0.42
1:A:64:LYS:HB3	1:A:65:ASP:H	1.46	0.42
1:A:299:VAL:HG23	1:B:724:LYS:HG3	2.03	0.41
1:B:679:ALA:HB2	4:B:1215:HOH:O	2.20	0.41
1:A:559:ARG:HH22	1:B:370:GLY:HA2	1.84	0.41
1:A:383:ASP:HB3	1:A:463:VAL:HG21	2.03	0.41
1:A:595:ASN:C	1:A:595:ASN:ND2	2.78	0.41
1:B:61:VAL:HG22	1:B:70:VAL:HG12	2.02	0.41
1:A:370:GLY:HA2	1:B:559:ARG:HH22	1.86	0.41
1:A:222:THR:HB	1:A:245:VAL:CG1	2.51	0.41
1:A:439:LYS:NZ	1:A:447:ASN:HD21	2.19	0.41
1:B:237:LYS:HE2	1:B:239:ASP:HB3	2.03	0.41
1:B:175:LEU:O	1:B:176:SER:HB3	2.20	0.41
1:B:326:ARG:HB2	1:B:327:ASN:H	1.70	0.41
1:B:572:ASN:ND2	1:B:671:ASN:HD21	2.19	0.41
1:B:189:LEU:HD21	1:B:392:LEU:HD21	2.03	0.40
1:B:196:GLN:HE22	1:B:222:THR:H	1.69	0.40
1:B:212:ARG:NH2	1:B:280:GLU:HB3	2.36	0.40
1:B:477:ASN:HD22	1:B:479:THR:H	1.69	0.40
1:B:24:ASP:O	1:B:28:GLN:N	2.52	0.40
1:B:76:ASN:O	1:B:80:GLN:HB2	2.21	0.40
1:B:437:GLU:HA	1:B:452:ARG:HB2	2.03	0.40
1:A:210:LYS:HA	1:A:214:ILE:O	2.21	0.40
1:A:274:LYS:HZ3	1:A:276:VAL:HG12	1.86	0.40
1:A:443:MET:HE3	4:B:807:HOH:O	2.20	0.40
1:B:212:ARG:HH21	1:B:280:GLU:HB3	1.86	0.40
1:B:272:GLN:HG2	1:B:274:LYS:HB3	2.03	0.40
1:B:291:ARG:NH1	1:B:516:ASP:OD2	2.55	0.40
1:B:628:TYR:C	1:B:628:TYR:CD1	3.00	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	717/727 (99%)	696 (97%)	20 (3%)	1 (0%)	48	46
1	B	720/727 (99%)	697 (97%)	19 (3%)	4 (1%)	21	17
All	All	1437/1454 (99%)	1393 (97%)	39 (3%)	5 (0%)	36	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	6	HIS
1	A	6	HIS
1	B	726	ASP
1	B	182	ASP
1	B	66	ASN

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	610/615 (99%)	576 (94%)	34 (6%)	19	16
1	B	613/615 (100%)	570 (93%)	43 (7%)	14	10
All	All	1223/1230 (99%)	1146 (94%)	77 (6%)	16	13

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	8	VAL
1	A	11	ASP
1	A	14	LEU
1	A	29	LEU
1	A	32	LEU
1	A	53	GLN
1	A	55	LEU
1	A	71	SER
1	A	80	GLN
1	A	89	VAL
1	A	120	ASN
1	A	132	ASP
1	A	147	ASP
1	A	156	MET
1	A	160	LYS
1	A	173	LYS
1	A	199	ILE
1	A	204	GLU
1	A	209	VAL
1	A	210	LYS
1	A	237	LYS
1	A	239	ASP
1	A	326	ARG
1	A	348	ASN
1	A	368	PRO
1	A	372	PRO
1	A	445	GLN
1	A	465	ASN
1	A	477	ASN
1	A	572	ASN
1	A	595	ASN
1	A	642	ARG
1	A	677	THR
1	B	12	LYS
1	B	15	LYS
1	B	22	GLN
1	B	46	GLN
1	B	64	LYS
1	B	73	THR
1	B	89	VAL
1	B	92	ARG
1	B	118	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	137	TRP
1	B	142	GLU
1	B	156	MET
1	B	170	GLN
1	B	172	ASN
1	B	173	LYS
1	B	181	LYS
1	B	195	VAL
1	B	203	GLU
1	B	209	VAL
1	B	210	LYS
1	B	211	LYS
1	B	218	LYS
1	B	237	LYS
1	B	239	ASP
1	B	251	VAL
1	B	271	GLU
1	B	272	GLN
1	B	291	ARG
1	B	326	ARG
1	B	359	GLU
1	B	374	ILE
1	B	465	ASN
1	B	477	ASN
1	B	490	GLU
1	B	510	ARG
1	B	572	ASN
1	B	595	ASN
1	B	613	HIS
1	B	627	ILE
1	B	642	ARG
1	B	669	LYS
1	B	724	LYS
1	B	727	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	51	ASN
1	A	53	GLN
1	A	58	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	80	GLN
1	A	97	ASN
1	A	120	ASN
1	A	148	GLN
1	A	170	GLN
1	A	178	GLN
1	A	196	GLN
1	A	263	ASN
1	A	272	GLN
1	A	307	GLN
1	A	315	ASN
1	A	324	HIS
1	A	327	ASN
1	A	348	ASN
1	A	447	ASN
1	A	465	ASN
1	A	477	ASN
1	A	517	HIS
1	A	525	GLN
1	A	541	ASN
1	A	553	ASN
1	A	566	ASN
1	A	567	GLN
1	A	572	ASN
1	A	592	ASN
1	A	595	ASN
1	A	599	ASN
1	A	637	GLN
1	A	644	HIS
1	A	660	HIS
1	A	671	ASN
1	A	676	ASN
1	B	51	ASN
1	B	76	ASN
1	B	80	GLN
1	B	94	HIS
1	B	97	ASN
1	B	161	HIS
1	B	170	GLN
1	B	196	GLN
1	B	197	ASN
1	B	200	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	238	GLN
1	B	263	ASN
1	B	315	ASN
1	B	327	ASN
1	B	350	ASN
1	B	447	ASN
1	B	465	ASN
1	B	477	ASN
1	B	501	HIS
1	B	517	HIS
1	B	525	GLN
1	B	541	ASN
1	B	553	ASN
1	B	567	GLN
1	B	572	ASN
1	B	595	ASN
1	B	599	ASN
1	B	604	GLN
1	B	637	GLN
1	B	671	ASN
1	B	676	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPQ	A	466	2,1	13,14,15	2.06	5 (38%)	13,19,21	1.22	1 (7%)
1	TPQ	B	466	2,1	13,14,15	1.92	2 (15%)	13,19,21	1.67	2 (15%)

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
1	TPQ	A	466	2,1	-	4/5/22/24	0/1/1/1
1	TPQ	B	466	2,1	-	3/5/22/24	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466	TPQ	C1-C2	-5.06	1.42	1.49
1	A	466	TPQ	C1-C2	-5.04	1.42	1.49
1	B	466	TPQ	C4-C5	-2.35	1.40	1.47
1	A	466	TPQ	C4-C5	-2.26	1.40	1.47
1	A	466	TPQ	C3-C4	2.14	1.39	1.36
1	A	466	TPQ	C6-C1	2.14	1.40	1.34
1	A	466	TPQ	C6-C5	-2.00	1.39	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	TPQ	O2-C2-C3	-3.44	114.00	121.83
1	B	466	TPQ	C6-C1-C2	-2.64	116.77	118.66
1	A	466	TPQ	O2-C2-C3	-2.58	115.97	121.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	466	TPQ	C-CA-CB-C1
1	A	466	TPQ	C2-C1-CB-CA
1	B	466	TPQ	C-CA-CB-C1
1	A	466	TPQ	N-CA-CB-C1
1	B	466	TPQ	N-CA-CB-C1
1	B	466	TPQ	C2-C1-CB-CA
1	A	466	TPQ	C6-C1-CB-CA

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	466	TPQ	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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	719/727 (98%)	-0.97	2 (0%)	90 89	11, 22, 56, 100	0
1	B	722/727 (99%)	-0.86	3 (0%)	88 88	10, 25, 61, 100	0
All	All	1441/1454 (99%)	-0.92	5 (0%)	90 89	10, 24, 59, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	ALA	5.1
1	A	6	HIS	2.5
1	B	6	HIS	2.1
1	B	7	MET	2.1
1	B	5	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q < 0.9
1	TPQ	A	466	14/15	0.93	0.08	16,41,47,60	0
1	TPQ	B	466	14/15	0.94	0.07	15,37,48,58	0

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(Å ²)	Q<0.9
3	CA	A	803	1/1	0.98	0.02	20,20,20,20	0
3	CA	B	803	1/1	0.98	0.03	22,22,22,22	0
3	CA	B	802	1/1	0.99	0.02	18,18,18,18	0
3	CA	A	802	1/1	0.99	0.01	16,16,16,16	0
2	CU	A	801	1/1	1.00	0.02	19,19,19,19	0
2	CU	B	801	1/1	1.00	0.01	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.