



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:33 AM UTC

PDB ID : 1AX4 / pdb_00001ax4
Title : TRYPTOPHANASE FROM PROTEUS VULGARIS
Authors : Isupov, M.N.; Antson, A.A.; Dodson, E.J.; Dodson, G.G.; Dementieva, I.S.; Zakomirdina, L.N.; Wilson, K.S.; Dauter, Z.; Lebedev, A.A.; Harutyunyan, E.H.
Deposited on : 1997-10-28
Resolution : 2.10 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

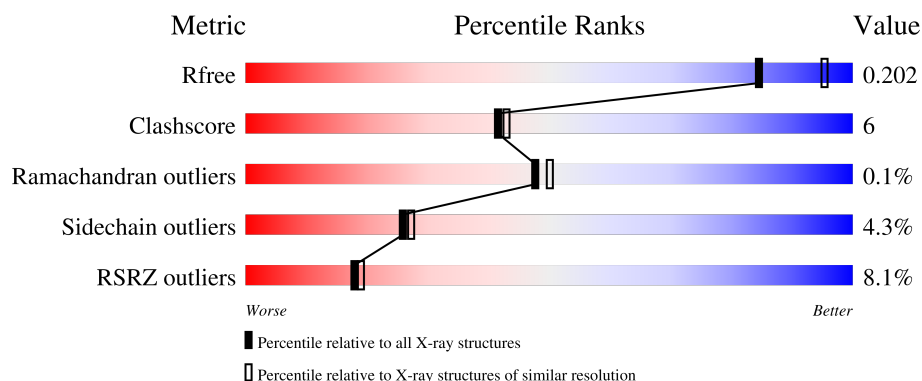
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	467	13% 75% 20% .
1	B	467	7% 81% 16% .
1	C	467	4% 82% 16% .
1	D	467	8% 76% 21% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15715 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 TRYPTOPHANASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	P	S	0	0	0
			3692	2356	627	690	1	18			
1	B	465	Total	C	N	O	P	S	0	0	0
			3693	2357	627	690	1	18			
1	C	465	Total	C	N	O	P	S	0	0	0
			3693	2357	627	690	1	18			
1	D	465	Total	C	N	O	P	S	0	0	0
			3693	2357	627	690	1	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	LLP	LYS	modified residue	UNP P28796
B	266	LLP	LYS	modified residue	UNP P28796
C	266	LLP	LYS	modified residue	UNP P28796
D	266	LLP	LYS	modified residue	UNP P28796

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		

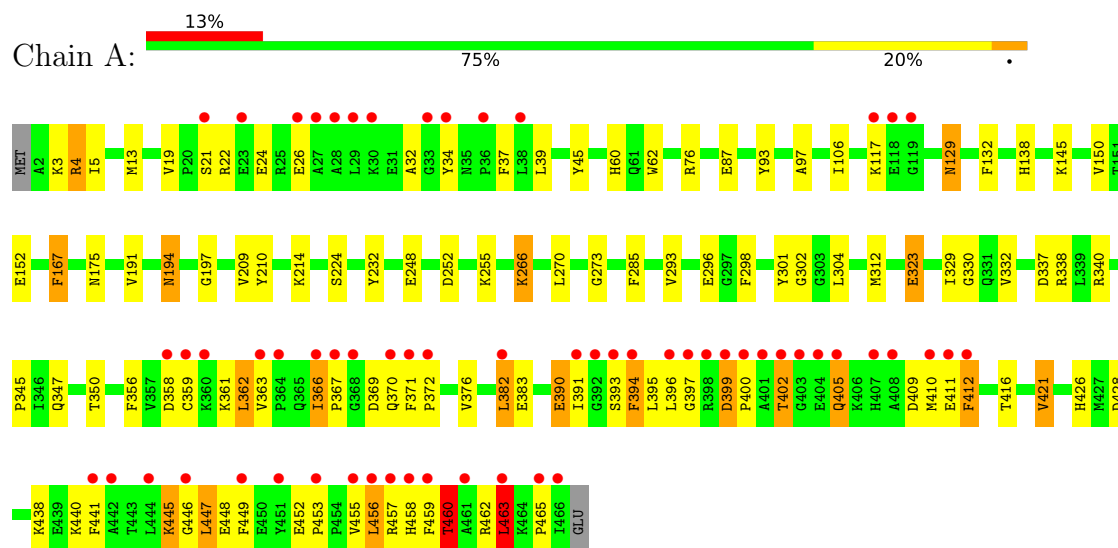
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	225	Total 225	O 225	0	0
3	B	240	Total 240	O 240	0	0
3	C	261	Total 261	O 261	0	0
3	D	214	Total 214	O 214	0	0

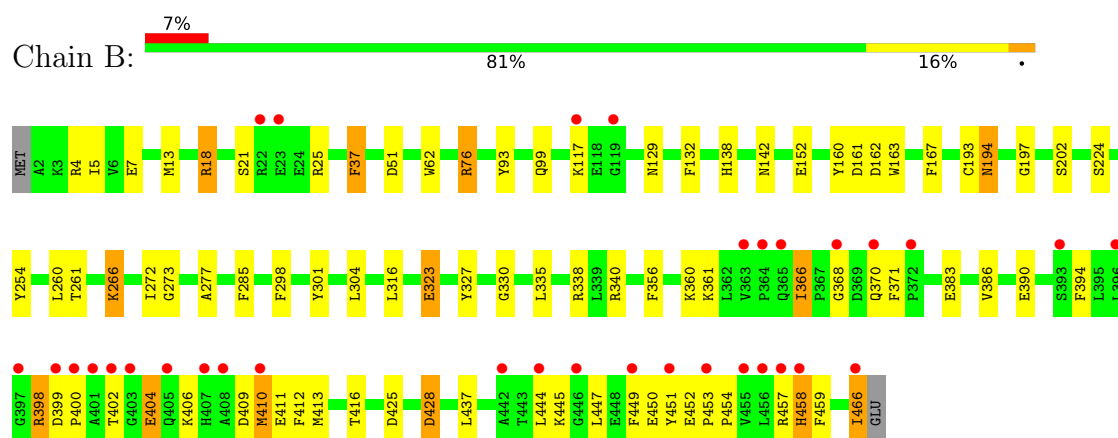
3 Residue-property plots [i](#)

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 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.

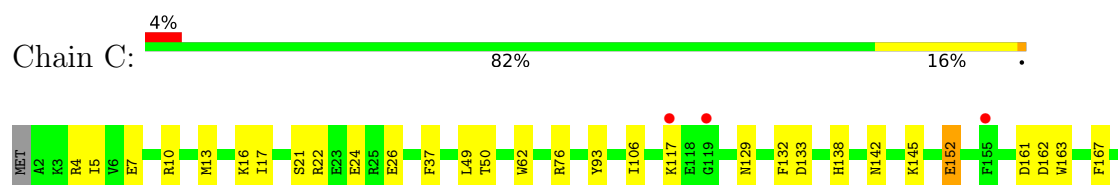
• Molecule 1: TRYPTOPHANASE

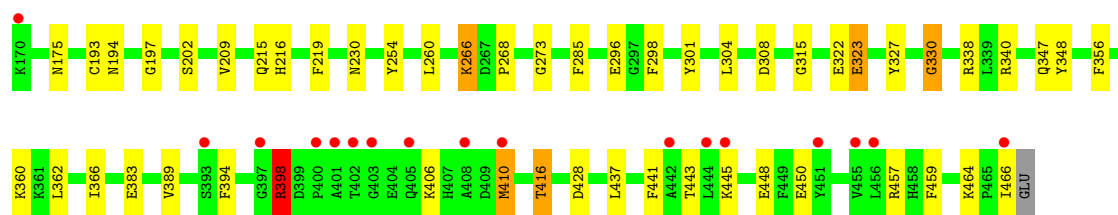


• Molecule 1: TRYPTOPHANASE

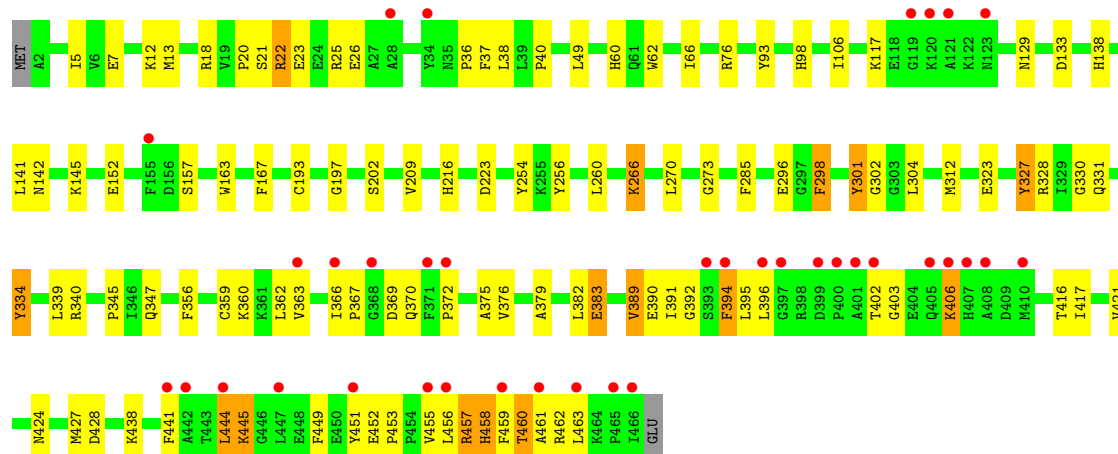
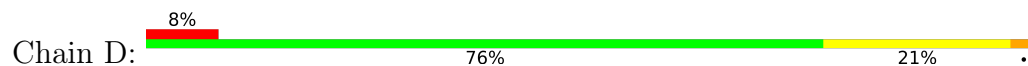


• Molecule 1: TRYPTOPHANASE





● Molecule 1: TRYPTOPHANASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.99Å 118.23Å 153.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.10 18.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (18.00-2.10) 96.8 (18.00-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 2.11Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.227 0.168 , 0.202	Depositor DCC
R_{free} test set	2364 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15715	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: LLP, K

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	0.84	0/3747	1.62	39/5060 (0.8%)
1	B	0.82	0/3747	1.56	32/5060 (0.6%)
1	C	0.79	0/3747	1.49	30/5060 (0.6%)
1	D	0.81	0/3747	1.61	36/5060 (0.7%)
All	All	0.82	0/14988	1.57	137/20240 (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	C	0	1

There are no bond length outliers.

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	ARG	CD-NE-CZ	13.72	143.61	124.40
1	D	424	ASN	CA-CB-CG	-8.69	103.91	112.60
1	B	167	PHE	CA-CB-CG	8.27	122.07	113.80
1	A	60	HIS	CA-CB-CG	-7.90	105.90	113.80
1	A	399	ASP	CA-CB-CG	7.75	120.35	112.60
1	B	450	GLU	N-CA-C	-7.70	104.02	113.41
1	B	193	CYS	CA-C-O	7.57	129.16	120.98
1	C	450	GLU	N-CA-C	-7.52	104.07	113.55
1	A	191	VAL	O-C-N	-7.34	115.33	123.26
1	C	398	ARG	CD-NE-CZ	7.28	134.59	124.40
1	B	458	HIS	CA-CB-CG	7.27	121.07	113.80
1	C	142	ASN	CA-CB-CG	-7.24	105.36	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	PHE	CA-CB-CG	7.11	120.91	113.80
1	D	457	ARG	CA-C-N	7.00	129.97	120.38
1	D	457	ARG	C-N-CA	7.00	129.97	120.38
1	C	50	THR	CA-C-O	-6.95	114.01	121.38
1	A	4	ARG	CD-NE-CZ	6.80	133.92	124.40
1	D	394	PHE	CA-CB-CG	6.80	120.60	113.80
1	D	129	ASN	N-CA-C	-6.70	103.98	111.28
1	A	350	THR	CA-C-N	-6.68	115.21	122.55
1	A	350	THR	C-N-CA	-6.68	115.21	122.55
1	B	398	ARG	CD-NE-CZ	6.63	133.68	124.40
1	C	175	ASN	CA-CB-CG	-6.54	106.06	112.60
1	D	40	PRO	CA-C-O	-6.54	114.01	122.12
1	D	339	LEU	CA-C-N	6.50	129.00	120.28
1	D	339	LEU	C-N-CA	6.50	129.00	120.28
1	D	403	GLY	N-CA-C	-6.36	105.91	115.32
1	D	328	ARG	CD-NE-CZ	6.33	133.26	124.40
1	B	447	LEU	N-CA-C	6.32	119.70	109.40
1	B	76	ARG	CB-CA-C	-6.26	100.41	110.79
1	A	458	HIS	N-CA-C	6.24	118.08	111.28
1	C	348	TYR	CB-CA-C	6.17	119.02	109.15
1	D	193	CYS	CA-C-O	6.14	127.61	120.98
1	C	308	ASP	CA-CB-CG	-6.13	106.47	112.60
1	D	327	TYR	CB-CG-CD2	6.12	129.97	120.80
1	D	445	LYS	N-CA-C	6.09	120.49	111.04
1	C	138	HIS	CA-CB-CG	-6.03	107.77	113.80
1	B	51	ASP	N-CA-C	-6.00	105.27	112.59
1	B	428	ASP	CA-C-O	6.00	126.91	120.55
1	A	446	GLY	CA-C-O	-6.00	117.99	122.37
1	C	129	ASN	CA-CB-CG	5.98	118.58	112.60
1	B	224	SER	N-CA-C	5.96	120.13	112.26
1	D	254	TYR	CA-CB-CG	-5.96	103.17	113.90
1	B	366	ILE	CA-C-O	5.88	125.27	119.62
1	C	193	CYS	CA-C-O	5.86	127.31	120.98
1	B	445	LYS	N-CA-C	5.85	117.35	110.97
1	D	427	MET	CA-CB-CG	5.84	125.77	114.10
1	B	18	ARG	CA-C-N	-5.82	118.64	122.60
1	B	18	ARG	C-N-CA	-5.82	118.64	122.60
1	C	216	HIS	CA-CB-CG	-5.82	107.98	113.80
1	D	142	ASN	CA-CB-CG	-5.82	106.78	112.60
1	A	394	PHE	CA-CB-CG	5.81	119.61	113.80
1	A	138	HIS	CA-CB-CG	-5.79	108.01	113.80
1	C	76	ARG	CB-CA-C	-5.79	100.85	110.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	VAL	CA-C-O	5.77	126.45	120.39
1	C	129	ASN	N-CA-C	-5.75	104.92	111.07
1	B	138	HIS	CA-CB-CG	-5.74	108.06	113.80
1	A	224	SER	N-CA-C	5.74	119.59	112.59
1	A	460	THR	N-CA-C	5.69	120.88	113.88
1	D	302	GLY	O-C-N	-5.65	117.94	122.51
1	A	129	ASN	N-CA-C	-5.64	105.13	111.28
1	D	421	VAL	CB-CA-C	-5.64	105.89	111.30
1	D	417	ILE	N-CA-C	5.62	115.95	107.80
1	D	12	LYS	N-CA-C	-5.61	107.08	114.04
1	A	302	GLY	O-C-N	-5.61	117.97	122.51
1	B	194	ASN	CA-CB-CG	-5.61	106.99	112.60
1	B	413	MET	N-CA-CB	5.60	119.38	110.65
1	A	446	GLY	N-CA-C	-5.58	106.44	112.08
1	B	272	ILE	CA-C-O	-5.57	116.52	121.09
1	C	322	GLU	N-CA-C	5.55	117.33	111.28
1	D	157	SER	N-CA-C	5.53	117.77	111.02
1	C	416	THR	CA-C-O	-5.50	114.44	120.43
1	A	76	ARG	CB-CA-C	-5.49	101.35	110.68
1	A	175	ASN	CA-CB-CG	-5.46	107.14	112.60
1	C	330	GLY	O-C-N	-5.46	116.33	122.28
1	B	161	ASP	CA-CB-CG	-5.42	107.18	112.60
1	C	394	PHE	CA-CB-CG	5.42	119.22	113.80
1	C	161	ASP	CA-CB-CG	-5.42	107.18	112.60
1	A	337	ASP	CA-CB-CG	-5.41	107.19	112.60
1	D	76	ARG	CA-CB-CG	5.41	124.91	114.10
1	A	371	PHE	CA-C-N	5.40	124.86	119.24
1	A	371	PHE	C-N-CA	5.40	124.86	119.24
1	D	379	ALA	N-CA-C	-5.40	105.29	111.07
1	D	98	HIS	CA-C-O	-5.39	113.77	119.97
1	D	347	GLN	N-CA-C	-5.38	102.32	110.28
1	A	395	LEU	CB-CA-C	-5.38	102.41	110.90
1	D	76	ARG	CB-CA-C	-5.37	101.88	110.79
1	B	412	PHE	N-CA-C	5.37	118.47	110.52
1	A	421	VAL	CB-CA-C	-5.37	106.15	111.30
1	A	440	LYS	N-CA-C	5.36	118.92	112.38
1	D	389	VAL	N-CA-C	5.34	115.58	108.11
1	D	347	GLN	CA-C-O	-5.32	115.20	121.16
1	C	268	PRO	O-C-N	-5.31	115.48	122.64
1	C	254	TYR	CA-CB-CG	-5.30	104.35	113.90
1	B	445	LYS	CA-C-O	-5.30	115.43	121.00
1	D	216	HIS	CA-CB-CG	-5.30	108.50	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	ASN	CA-CB-CG	-5.30	107.30	112.60
1	B	99	GLN	CG-CD-NE2	5.29	124.33	116.40
1	C	445	LYS	N-CA-C	5.28	119.64	112.04
1	B	335	LEU	O-C-N	5.28	128.17	122.15
1	C	347	GLN	CB-CA-C	5.28	118.34	109.89
1	B	425	ASP	CA-CB-CG	-5.27	107.33	112.60
1	C	175	ASN	OD1-CG-ND2	5.26	127.86	122.60
1	C	315	GLY	O-C-N	-5.26	117.14	122.19
1	D	60	HIS	CA-CB-CG	-5.23	108.57	113.80
1	C	219	PHE	CA-C-N	-5.23	116.70	123.19
1	C	219	PHE	C-N-CA	-5.23	116.70	123.19
1	A	248	GLU	CG-CD-OE1	5.20	130.36	118.40
1	A	463	LEU	CA-CB-CG	5.20	134.50	116.30
1	A	445	LYS	N-CA-C	5.18	119.50	112.04
1	A	455	VAL	CB-CA-C	5.18	115.83	110.70
1	B	386	VAL	CA-C-O	-5.18	114.95	121.11
1	A	347	GLN	N-CA-C	-5.17	102.21	109.96
1	C	215	GLN	OE1-CD-NE2	5.15	127.75	122.60
1	D	256	TYR	CA-CB-CG	-5.14	104.66	113.90
1	D	331	GLN	CA-C-O	5.14	125.86	120.42
1	D	301	TYR	N-CA-C	-5.13	108.77	114.62
1	A	97	ALA	CA-C-O	-5.12	115.61	121.40
1	C	366	ILE	CA-C-O	5.11	122.93	119.20
1	A	332	VAL	O-C-N	5.09	127.07	121.83
1	C	459	PHE	N-CA-C	5.09	116.63	111.14
1	A	402	THR	N-CA-C	-5.07	107.16	113.55
1	A	167	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	34	TYR	CA-CB-CG	-5.06	104.80	113.90
1	B	254	TYR	CA-C-O	5.06	125.75	119.12
1	B	37	PHE	CA-CB-CG	-5.06	108.74	113.80
1	D	334	TYR	CA-C-O	5.06	125.91	120.70
1	A	426	HIS	N-CA-C	-5.04	105.86	111.36
1	B	261	THR	N-CA-C	-5.04	101.19	109.40
1	B	316	LEU	CA-C-N	5.04	127.29	120.44
1	B	316	LEU	C-N-CA	5.04	127.29	120.44
1	C	230	ASN	CA-CB-CG	-5.04	107.56	112.60
1	A	194	ASN	CA-CB-CG	-5.03	107.57	112.60
1	A	412	PHE	N-CA-C	5.03	117.75	109.76
1	B	129	ASN	CA-CB-CG	5.01	117.61	112.60
1	D	138	HIS	CA-CB-CG	-5.01	108.79	113.80
1	D	298	PHE	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	162	ASP	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3692	0	3659	66	0
1	B	3693	0	3659	39	0
1	C	3693	0	3660	42	0
1	D	3693	0	3659	60	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	225	0	0	4	0
3	B	240	0	0	4	0
3	C	261	0	0	4	0
3	D	214	0	0	5	0
All	All	15715	0	14637	189	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 6.

All (189) 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:4:ARG:HH21	1:C:4:ARG:NH2	1.11	1.48
1:A:4:ARG:NH2	1:C:4:ARG:NH2	1.67	1.41
1:A:4:ARG:NH2	1:C:4:ARG:HH21	1.16	1.36
1:A:266:LLP:NZ	1:A:266:LLP:C4	2.34	0.90
1:A:26:GLU:HG3	1:A:382:LEU:HD21	1.52	0.89
1:C:383:GLU:HG2	1:C:437:LEU:HD21	1.56	0.85
1:A:4:ARG:NH2	1:C:4:ARG:CZ	2.43	0.81
1:B:453:PRO:HG2	1:B:457:ARG:HA	1.64	0.78
1:D:145:LYS:HE3	3:D:615:HOH:O	1.85	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:LEU:HG	3:D:692:HOH:O	1.85	0.76
1:A:4:ARG:CZ	1:C:4:ARG:NH2	2.49	0.75
1:B:13:MET:HE2	1:D:62:TRP:CD1	2.25	0.71
1:A:399:ASP:HB3	1:A:402:THR:OG1	1.94	0.68
1:A:453:PRO:HG2	1:A:460:THR:HB	1.74	0.68
1:A:410:MET:HB2	3:A:723:HOH:O	1.94	0.67
1:B:383:GLU:HG3	1:B:437:LEU:HD21	1.74	0.67
1:D:453:PRO:HG2	1:D:457:ARG:HA	1.76	0.67
1:D:375:ALA:HB1	1:D:444:LEU:HD22	1.76	0.65
1:B:266:LLP:H4'1	3:B:583:HOH:O	1.97	0.65
1:A:197:GLY:HA2	1:A:356:PHE:CE1	2.32	0.65
1:B:197:GLY:HA2	1:B:356:PHE:CE1	2.32	0.64
1:D:367:PRO:HG2	1:D:370:GLN:HG3	1.80	0.63
1:D:390:GLU:O	1:D:391:ILE:HD13	1.98	0.63
1:A:62:TRP:CD1	1:C:13:MET:HE2	2.34	0.62
1:C:145:LYS:HE3	3:C:698:HOH:O	1.99	0.62
1:A:87:GLU:HB2	3:A:643:HOH:O	2.00	0.62
1:D:197:GLY:HA2	1:D:356:PHE:CE1	2.35	0.62
1:D:366:ILE:HD11	1:D:444:LEU:HB3	1.83	0.61
1:B:383:GLU:HG2	3:B:668:HOH:O	2.00	0.61
1:D:445:LYS:HD2	1:D:445:LYS:H	1.65	0.61
1:B:62:TRP:CD1	1:D:13:MET:HE2	2.36	0.60
1:C:197:GLY:HA2	1:C:356:PHE:CE1	2.37	0.60
1:C:266:LLP:H4'1	3:C:589:HOH:O	2.00	0.60
1:A:399:ASP:OD1	1:A:400:PRO:HD2	2.02	0.60
1:D:20:PRO:HG2	1:D:25:ARG:HG2	1.82	0.60
1:A:359:CYS:HA	1:A:362:LEU:HG	1.84	0.59
1:B:402:THR:HB	1:B:404:GLU:HG2	1.84	0.59
1:D:458:HIS:H	1:D:458:HIS:CD2	2.20	0.59
1:C:448:GLU:HG3	1:C:466:ILE:HG13	1.84	0.59
1:B:410:MET:SD	3:B:705:HOH:O	2.57	0.59
1:B:370:GLN:NE2	1:B:466:ILE:HD13	2.18	0.58
1:D:21:SER:O	1:D:25:ARG:HG3	2.04	0.58
1:A:13:MET:HE2	1:C:62:TRP:CD1	2.39	0.57
1:A:4:ARG:CZ	1:C:4:ARG:CZ	2.82	0.57
1:C:152:GLU:HG2	3:C:646:HOH:O	2.05	0.56
1:A:32:ALA:HB2	1:A:39:LEU:HD23	1.88	0.56
1:A:323:GLU:H	1:A:323:GLU:CD	2.14	0.55
1:D:26:GLU:HG2	1:D:382:LEU:HD22	1.89	0.55
1:A:394:PHE:CZ	1:A:463:LEU:HD21	2.42	0.55
1:A:21:SER:OG	1:A:24:GLU:HG3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:LEU:HD23	1:D:406:LYS:HB3	1.89	0.54
1:D:438:LYS:HA	1:D:441:PHE:CD2	2.42	0.54
1:C:340:ARG:HD3	3:C:645:HOH:O	2.06	0.53
1:D:345:PRO:HD2	1:D:362:LEU:HD21	1.90	0.53
1:A:4:ARG:HH21	1:C:4:ARG:HH21	0.75	0.53
1:A:4:ARG:NH1	1:A:428:ASP:OD2	2.41	0.53
1:C:22:ARG:O	1:C:26:GLU:HG3	2.09	0.53
1:B:323:GLU:H	1:B:323:GLU:CD	2.16	0.53
1:D:93:TYR:HB3	1:D:285:PHE:CD1	2.44	0.53
1:D:451:TYR:HB3	1:D:462:ARG:HG3	1.91	0.53
1:D:362:LEU:O	1:D:441:PHE:HB3	2.09	0.52
1:A:5:ILE:HD12	1:A:330:GLY:HA3	1.91	0.52
1:A:438:LYS:HA	1:A:441:PHE:CD2	2.43	0.52
1:C:448:GLU:HG3	1:C:466:ILE:CG1	2.39	0.52
1:D:340:ARG:HD3	3:D:676:HOH:O	2.10	0.52
1:A:397:GLY:HA2	1:A:457:ARG:HH11	1.74	0.52
1:B:266:LLP:H2'2	3:B:516:HOH:O	2.09	0.52
1:A:390:GLU:O	1:A:391:ILE:HD13	2.09	0.52
1:D:5:ILE:HD12	1:D:330:GLY:HA3	1.92	0.51
1:A:145:LYS:HE3	3:A:671:HOH:O	2.11	0.51
1:A:456:LEU:HD23	1:A:460:THR:OG1	2.10	0.51
1:A:447:LEU:HD23	1:A:465:PRO:HA	1.93	0.50
1:C:398:ARG:HG2	1:C:398:ARG:HH11	1.76	0.50
1:D:38:LEU:HD21	1:D:460:THR:HA	1.93	0.50
1:A:366:ILE:HG22	1:A:372:PRO:HD3	1.94	0.49
1:B:7:GLU:HG3	1:B:327:TYR:CZ	2.47	0.49
1:B:398:ARG:HG2	1:B:398:ARG:HH11	1.77	0.49
1:A:359:CYS:HB3	1:A:376:VAL:HG21	1.94	0.49
1:A:449:PHE:CD1	1:A:463:LEU:HD22	2.46	0.49
1:A:22:ARG:HH21	1:A:382:LEU:HD22	1.77	0.49
1:B:93:TYR:HB3	1:B:285:PHE:CD1	2.48	0.49
1:C:93:TYR:HB3	1:C:285:PHE:CD1	2.47	0.49
1:D:395:LEU:HG	1:D:395:LEU:O	2.12	0.49
1:B:21:SER:O	1:B:25:ARG:HG3	2.13	0.49
1:D:334:TYR:OH	1:D:428:ASP:OD1	2.29	0.48
1:B:197:GLY:HA2	1:B:356:PHE:CZ	2.48	0.48
1:B:13:MET:HE2	1:D:62:TRP:CG	2.48	0.48
1:C:7:GLU:HG3	1:C:327:TYR:CZ	2.49	0.48
1:A:345:PRO:HD2	1:A:362:LEU:HD21	1.95	0.48
1:B:451:TYR:OH	1:B:453:PRO:HB3	2.13	0.48
1:C:5:ILE:HD12	1:C:330:GLY:HA3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:GLU:H	1:C:323:GLU:CD	2.22	0.48
1:D:7:GLU:HG3	1:D:327:TYR:CZ	2.48	0.48
1:A:369:ASP:HA	1:A:405:GLN:HE21	1.78	0.48
1:D:106:ILE:HD11	1:D:296:GLU:HG3	1.96	0.48
1:A:453:PRO:CG	1:A:460:THR:HB	2.43	0.48
1:D:21:SER:HG	1:D:23:GLU:HG2	1.79	0.48
1:D:451:TYR:HB3	1:D:462:ARG:HB2	1.96	0.48
1:A:210:TYR:CE1	1:A:214:LYS:HE3	2.49	0.47
1:B:5:ILE:HD12	1:B:330:GLY:HA3	1.95	0.47
1:D:323:GLU:H	1:D:323:GLU:CD	2.21	0.47
1:D:390:GLU:OE1	1:D:392:GLY:N	2.45	0.47
1:A:421:VAL:CG1	1:C:10:ARG:HD2	2.44	0.47
1:B:163:TRP:CD2	1:B:202:SER:HB3	2.49	0.47
1:B:360:LYS:HD2	1:B:411:GLU:HG2	1.97	0.47
1:D:449:PHE:CD1	1:D:452:GLU:HB2	2.49	0.47
1:B:260:LEU:HG	1:B:277:ALA:HB3	1.96	0.46
1:C:106:ILE:HD11	1:C:296:GLU:HG3	1.96	0.46
1:C:410:MET:HA	1:C:410:MET:HE2	1.97	0.46
1:D:22:ARG:HH21	1:D:382:LEU:HD13	1.81	0.46
1:D:167:PHE:CD1	1:D:209:VAL:HG21	2.50	0.46
1:C:383:GLU:HG2	1:C:437:LEU:CD2	2.38	0.46
1:A:19:VAL:HG22	1:A:45:TYR:CD2	2.50	0.46
1:C:16:LYS:HG2	1:C:17:ILE:N	2.30	0.46
1:B:260:LEU:C	1:B:260:LEU:HD12	2.41	0.46
1:D:260:LEU:HD12	1:D:260:LEU:C	2.41	0.46
1:A:273:GLY:HA2	1:A:304:LEU:HD21	1.97	0.46
1:D:359:CYS:HB3	1:D:376:VAL:HG21	1.97	0.45
1:A:197:GLY:HA2	1:A:356:PHE:CZ	2.52	0.45
1:D:163:TRP:CD2	1:D:202:SER:HB3	2.50	0.45
1:B:371:PHE:CE1	1:B:394:PHE:HA	2.51	0.45
1:D:36:PRO:HB2	3:D:610:HOH:O	2.16	0.45
1:A:106:ILE:HD11	1:A:296:GLU:HG3	1.98	0.45
1:A:132:PHE:HD1	1:A:194:ASN:HD22	1.65	0.45
1:C:21:SER:OG	1:C:24:GLU:HG3	2.17	0.45
1:C:260:LEU:C	1:C:260:LEU:HD12	2.42	0.45
1:A:167:PHE:CD1	1:A:209:VAL:HG21	2.52	0.44
1:D:394:PHE:CZ	1:D:463:LEU:HD21	2.52	0.44
1:B:366:ILE:HD11	1:B:444:LEU:O	2.16	0.44
1:B:4:ARG:NH1	1:B:428:ASP:OD2	2.49	0.44
1:D:21:SER:OG	1:D:23:GLU:HG2	2.18	0.44
1:A:372:PRO:HG3	1:A:411:GLU:HG3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:LEU:HD12	1:A:396:LEU:HA	1.83	0.44
1:A:448:GLU:O	1:A:463:LEU:HB3	2.18	0.44
1:B:399:ASP:OD1	1:B:400:PRO:HD2	2.18	0.44
1:C:49:LEU:HD12	1:C:389:VAL:HB	1.99	0.44
1:C:163:TRP:CD2	1:C:202:SER:HB3	2.53	0.44
1:C:197:GLY:HA2	1:C:356:PHE:CZ	2.52	0.44
1:A:62:TRP:CG	1:C:13:MET:HE2	2.52	0.43
1:D:372:PRO:O	1:D:376:VAL:HG23	2.18	0.43
1:D:273:GLY:HA2	1:D:304:LEU:HD21	1.99	0.43
1:A:293:VAL:HG11	1:B:459:PHE:CE2	2.54	0.43
1:A:358:ASP:O	1:A:362:LEU:HG	2.19	0.43
1:B:132:PHE:HD1	1:B:194:ASN:HD22	1.65	0.43
1:A:13:MET:HE3	1:C:13:MET:HE3	1.99	0.43
1:A:298:PHE:HB3	1:A:301:TYR:CE2	2.54	0.42
1:B:449:PHE:CZ	1:B:457:ARG:NH1	2.87	0.42
1:B:449:PHE:CZ	1:B:457:ARG:HD2	2.54	0.42
1:D:22:ARG:NH2	1:D:382:LEU:HB3	2.34	0.42
1:B:273:GLY:HA2	1:B:304:LEU:HD21	2.01	0.42
1:A:93:TYR:HB3	1:A:285:PHE:CD1	2.54	0.42
1:C:273:GLY:HA2	1:C:304:LEU:HD21	2.00	0.42
1:D:340:ARG:HD3	1:D:340:ARG:HH11	1.64	0.42
1:D:457:ARG:O	1:D:461:ALA:N	2.39	0.42
1:A:232:TYR:CD2	1:A:329:ILE:HD13	2.54	0.42
1:C:298:PHE:HB3	1:C:301:TYR:CE2	2.54	0.42
1:D:456:LEU:HD22	1:D:459:PHE:HD2	1.84	0.42
1:A:397:GLY:HA2	1:A:457:ARG:NH1	2.34	0.42
1:B:449:PHE:CD1	1:B:452:GLU:HB2	2.54	0.42
1:A:393:SER:HB2	1:A:405:GLN:HE22	1.85	0.42
1:A:449:PHE:CD1	1:A:452:GLU:HB2	2.55	0.42
1:D:223:ASP:OD1	1:D:223:ASP:C	2.63	0.42
1:D:266:LLP:O3	1:D:266:LLP:NZ	2.50	0.42
1:B:13:MET:HE3	1:D:13:MET:HE3	2.02	0.41
1:D:22:ARG:NH1	1:D:383:GLU:OE2	2.49	0.41
1:D:49:LEU:HD12	1:D:389:VAL:HB	2.02	0.41
1:D:298:PHE:HB3	1:D:301:TYR:CE2	2.55	0.41
1:A:367:PRO:O	1:A:372:PRO:HD3	2.21	0.41
1:A:252:ASP:O	1:A:255:LYS:HB2	2.21	0.41
1:A:369:ASP:HA	1:A:405:GLN:NE2	2.35	0.41
1:B:453:PRO:HA	1:B:454:PRO:HD3	1.88	0.41
1:A:367:PRO:HG2	1:A:370:GLN:HG3	2.02	0.41
1:C:132:PHE:HD1	1:C:194:ASN:HD22	1.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:PHE:HB3	1:B:301:TYR:CE1	2.56	0.41
1:C:4:ARG:NH1	1:C:428:ASP:OD2	2.53	0.41
1:D:394:PHE:CE1	1:D:463:LEU:HD21	2.56	0.41
1:D:396:LEU:HD12	1:D:396:LEU:HA	1.96	0.41
1:C:62:TRP:CZ3	1:D:66:ILE:HD13	2.56	0.41
1:C:167:PHE:CD1	1:C:209:VAL:HG21	2.56	0.41
1:A:129:ASN:O	1:A:150:VAL:HB	2.22	0.40
1:A:270:LEU:HD11	1:A:312:MET:HA	2.02	0.40
1:B:160:TYR:OH	1:B:162:ASP:OD1	2.35	0.40
1:D:266:LLP:H2'2	3:D:521:HOH:O	2.22	0.40
1:D:270:LEU:HD11	1:D:312:MET:HA	2.03	0.40
1:A:3:LYS:CE	3:A:651:HOH:O	2.69	0.40
1:A:340:ARG:HH11	1:A:340:ARG:HD3	1.68	0.40
1:B:76:ARG:HH11	1:B:76:ARG:HG3	1.85	0.40
1:C:362:LEU:HD13	1:C:441:PHE:CZ	2.57	0.40
1:D:367:PRO:HG2	1:D:369:ASP:OD1	2.22	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	462/467 (99%)	440 (95%)	22 (5%)	0	100	100
1	B	462/467 (99%)	439 (95%)	21 (4%)	2 (0%)	30	28
1	C	462/467 (99%)	446 (96%)	16 (4%)	0	100	100
1	D	462/467 (99%)	442 (96%)	20 (4%)	0	100	100
All	All	1848/1868 (99%)	1767 (96%)	79 (4%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	409	ASP
1	B	368	GLY

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	383/385 (100%)	362 (94%)	21 (6%)	19	18
1	B	383/385 (100%)	368 (96%)	15 (4%)	28	31
1	C	383/385 (100%)	369 (96%)	14 (4%)	30	33
1	D	383/385 (100%)	367 (96%)	16 (4%)	26	28
All	All	1532/1540 (100%)	1466 (96%)	66 (4%)	26	27

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	PHE
1	A	117	LYS
1	A	152	GLU
1	A	323	GLU
1	A	361	LYS
1	A	362	LEU
1	A	363	VAL
1	A	366	ILE
1	A	382	LEU
1	A	383	GLU
1	A	390	GLU
1	A	405	GLN
1	A	409	ASP
1	A	412	PHE
1	A	416	THR
1	A	445	LYS
1	A	447	LEU
1	A	456	LEU
1	A	460	THR
1	A	462	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	463	LEU
1	B	18	ARG
1	B	37	PHE
1	B	117	LYS
1	B	152	GLU
1	B	323	GLU
1	B	338	ARG
1	B	340	ARG
1	B	361	LYS
1	B	390	GLU
1	B	404	GLU
1	B	406	LYS
1	B	410	MET
1	B	416	THR
1	B	458	HIS
1	B	466	ILE
1	C	37	PHE
1	C	117	LYS
1	C	133	ASP
1	C	152	GLU
1	C	323	GLU
1	C	338	ARG
1	C	360	LYS
1	C	398	ARG
1	C	406	LYS
1	C	410	MET
1	C	416	THR
1	C	443	THR
1	C	457	ARG
1	C	464	LYS
1	D	18	ARG
1	D	22	ARG
1	D	37	PHE
1	D	117	LYS
1	D	133	ASP
1	D	152	GLU
1	D	360	LYS
1	D	363	VAL
1	D	383	GLU
1	D	402	THR
1	D	406	LYS
1	D	416	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	444	LEU
1	D	455	VAL
1	D	458	HIS
1	D	460	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	A	194	ASN
1	A	243	ASN
1	A	374	GLN
1	A	378	ASN
1	B	175	ASN
1	B	194	ASN
1	B	243	ASN
1	B	365	GLN
1	C	175	ASN
1	C	194	ASN
1	C	243	ASN
1	D	175	ASN
1	D	194	ASN
1	D	243	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	LLP	D	266	1	23,24,25	1.39	3 (13%)	25,32,34	1.84	7 (28%)
1	LLP	B	266	1	23,24,25	1.44	2 (8%)	25,32,34	1.86	9 (36%)
1	LLP	C	266	1	23,24,25	1.46	3 (13%)	25,32,34	2.32	5 (20%)
1	LLP	A	266	1	20,22,25	1.81	7 (35%)	20,28,34	2.03	5 (25%)

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	LLP	D	266	1	-	4/16/17/19	0/1/1/1
1	LLP	B	266	1	-	4/16/17/19	0/1/1/1
1	LLP	C	266	1	-	4/16/17/19	0/1/1/1
1	LLP	A	266	1	-	3/12/13/19	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	266	LLP	O3-C3	-4.13	1.27	1.36
1	B	266	LLP	C2'-C2	4.03	1.56	1.50
1	A	266	LLP	C4-C3	3.75	1.44	1.38
1	B	266	LLP	O3-C3	-3.53	1.28	1.36
1	A	266	LLP	C2'-C2	3.31	1.55	1.50
1	A	266	LLP	O3-C3	-3.05	1.30	1.36
1	D	266	LLP	C2'-C2	2.92	1.55	1.50
1	C	266	LLP	C2-N1	2.84	1.38	1.33
1	D	266	LLP	O3-C3	-2.76	1.30	1.36
1	C	266	LLP	C2'-C2	2.69	1.54	1.50
1	D	266	LLP	C2-N1	2.51	1.38	1.33
1	A	266	LLP	C2-N1	2.37	1.38	1.33
1	A	266	LLP	C4-C5	2.35	1.43	1.39
1	A	266	LLP	P-OP1	2.34	1.57	1.50
1	A	266	LLP	P-OP3	-2.27	1.46	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	266	LLP	C4-C3-C2	6.95	124.05	120.14
1	A	266	LLP	C3-C4-C5	-5.30	115.31	120.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	266	LLP	C3-C4-C5	-5.16	114.13	118.28
1	C	266	LLP	CE-NZ-C4'	4.61	133.47	118.72
1	A	266	LLP	C4-C5-C6	4.37	120.94	116.90
1	B	266	LLP	CE-NZ-C4'	3.97	131.45	118.72
1	B	266	LLP	C6-N1-C2	3.68	125.86	119.20
1	B	266	LLP	C5-C6-N1	-3.56	118.04	123.83
1	D	266	LLP	C4-C3-C2	3.32	122.01	120.14
1	D	266	LLP	C5-C6-N1	-3.27	118.52	123.83
1	C	266	LLP	OP3-P-OP4	3.17	114.94	106.67
1	D	266	LLP	C3-C2-N1	-3.08	117.07	120.96
1	D	266	LLP	C6-N1-C2	3.00	124.63	119.20
1	A	266	LLP	OP3-P-OP2	2.97	118.96	107.80
1	B	266	LLP	C3-C2-N1	-2.94	117.25	120.96
1	D	266	LLP	CE-NZ-C4'	2.74	127.51	118.72
1	C	266	LLP	C3-C2-N1	-2.73	117.52	120.96
1	B	266	LLP	C4-C4'-NZ	-2.48	112.60	124.04
1	A	266	LLP	C5-C6-N1	-2.44	120.36	123.99
1	D	266	LLP	OP3-P-OP2	2.43	116.93	107.80
1	A	266	LLP	OP3-P-OP4	2.38	112.89	106.67
1	B	266	LLP	OP2-P-OP4	-2.26	100.79	106.67
1	B	266	LLP	OP3-P-OP2	2.19	116.03	107.80
1	B	266	LLP	C4-C3-C2	2.12	121.34	120.14
1	D	266	LLP	OP3-P-OP1	-2.08	102.75	110.83
1	B	266	LLP	OP3-P-OP4	2.02	111.93	106.67

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	266	LLP	O-C-CA-CB
1	B	266	LLP	O-C-CA-CB
1	C	266	LLP	O-C-CA-CB
1	D	266	LLP	O-C-CA-CB
1	B	266	LLP	CG-CD-CE-NZ
1	C	266	LLP	CG-CD-CE-NZ
1	D	266	LLP	CG-CD-CE-NZ
1	B	266	LLP	C3-C4-C4'-NZ
1	A	266	LLP	CG-CD-CE-NZ
1	C	266	LLP	C3-C4-C4'-NZ
1	D	266	LLP	C3-C4-C4'-NZ
1	A	266	LLP	C-CA-CB-CG
1	B	266	LLP	C-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	C	266	LLP	C-CA-CB-CG
1	D	266	LLP	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	266	LLP	2	0
1	B	266	LLP	2	0
1	C	266	LLP	1	0
1	A	266	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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

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	464/467 (99%)	0.13	61 (13%) 7 7	8, 21, 64, 89	0
1	B	464/467 (99%)	-0.12	33 (7%) 22 23	8, 21, 64, 89	0
1	C	464/467 (99%)	-0.19	20 (4%) 40 41	8, 21, 64, 88	0
1	D	464/467 (99%)	0.00	37 (7%) 18 19	7, 22, 64, 89	0
All	All	1856/1868 (99%)	-0.05	151 (8%) 18 19	7, 21, 65, 89	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	401	ALA	7.3
1	D	401	ALA	6.0
1	A	372	PRO	5.6
1	D	456	LEU	5.1
1	A	408	ALA	4.6
1	A	451	TYR	4.6
1	A	400	PRO	4.4
1	A	456	LEU	4.3
1	A	371	PHE	4.1
1	D	119	GLY	4.1
1	B	365	GLN	4.0
1	A	366	ILE	3.9
1	B	456	LEU	3.9
1	A	393	SER	3.8
1	D	455	VAL	3.8
1	B	403	GLY	3.8
1	D	451	TYR	3.7
1	C	402	THR	3.7
1	D	121	ALA	3.6
1	A	396	LEU	3.6
1	A	34	TYR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	397	GLY	3.6
1	D	372	PRO	3.5
1	A	399	ASP	3.5
1	D	405	GLN	3.5
1	A	407	HIS	3.5
1	C	401	ALA	3.4
1	C	408	ALA	3.4
1	A	368	GLY	3.4
1	D	368	GLY	3.3
1	B	401	ALA	3.3
1	A	117	LYS	3.3
1	B	397	GLY	3.3
1	B	410	MET	3.3
1	D	393	SER	3.2
1	B	400	PRO	3.2
1	C	400	PRO	3.2
1	A	391	ILE	3.2
1	A	397	GLY	3.2
1	D	402	THR	3.2
1	D	466	ILE	3.1
1	B	396	LEU	3.1
1	C	403	GLY	3.0
1	A	402	THR	3.0
1	B	364	PRO	3.0
1	D	465	PRO	3.0
1	A	33	GLY	3.0
1	B	368	GLY	3.0
1	B	119	GLY	3.0
1	B	407	HIS	3.0
1	B	446	GLY	2.9
1	C	466	ILE	2.9
1	A	370	GLN	2.9
1	B	408	ALA	2.9
1	A	403	GLY	2.9
1	A	26	GLU	2.9
1	A	394	PHE	2.9
1	C	445	LYS	2.9
1	D	441	PHE	2.9
1	A	457	ARG	2.8
1	A	455	VAL	2.8
1	A	358	ASP	2.8
1	A	28	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	118	GLU	2.8
1	A	359	CYS	2.8
1	C	117	LYS	2.8
1	C	397	GLY	2.8
1	D	442	ALA	2.8
1	A	29	LEU	2.8
1	D	463	LEU	2.8
1	C	455	VAL	2.8
1	B	399	ASP	2.7
1	B	22	ARG	2.7
1	C	393	SER	2.7
1	A	449	PHE	2.7
1	D	410	MET	2.7
1	C	119	GLY	2.7
1	A	465	PRO	2.6
1	D	363	VAL	2.6
1	A	461	ALA	2.6
1	B	402	THR	2.6
1	D	408	ALA	2.6
1	D	400	PRO	2.6
1	D	366	ILE	2.5
1	A	119	GLY	2.5
1	C	170	LYS	2.5
1	A	441	PHE	2.5
1	A	410	MET	2.5
1	B	455	VAL	2.5
1	B	453	PRO	2.5
1	A	382	LEU	2.5
1	D	444	LEU	2.5
1	D	407	HIS	2.5
1	B	442	ALA	2.4
1	B	117	LYS	2.4
1	A	446	GLY	2.4
1	A	466	ILE	2.4
1	A	444	LEU	2.4
1	A	458	HIS	2.4
1	A	392	GLY	2.4
1	A	27	ALA	2.4
1	D	155	PHE	2.4
1	A	364	PRO	2.4
1	A	463	LEU	2.3
1	D	123	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	442	ALA	2.3
1	C	456	LEU	2.3
1	B	449	PHE	2.3
1	B	23	GLU	2.3
1	A	23	GLU	2.3
1	B	393	SER	2.3
1	A	405	GLN	2.3
1	B	405	GLN	2.3
1	B	466	ILE	2.3
1	D	447	LEU	2.3
1	A	363	VAL	2.2
1	B	457	ARG	2.2
1	A	360	LYS	2.2
1	A	412	PHE	2.2
1	A	36	PRO	2.2
1	A	367	PRO	2.2
1	D	120	LYS	2.2
1	A	38	LEU	2.2
1	C	451	TYR	2.2
1	C	155	PHE	2.2
1	D	371	PHE	2.2
1	C	410	MET	2.2
1	B	363	VAL	2.2
1	A	442	ALA	2.2
1	A	459	PHE	2.1
1	B	458	HIS	2.1
1	B	451	TYR	2.1
1	B	370	GLN	2.1
1	A	398	ARG	2.1
1	D	459	PHE	2.1
1	D	406	LYS	2.1
1	B	444	LEU	2.1
1	C	444	LEU	2.1
1	A	404	GLU	2.1
1	C	405	GLN	2.1
1	A	453	PRO	2.1
1	B	372	PRO	2.1
1	A	21	SER	2.1
1	A	411	GLU	2.0
1	A	30	LYS	2.0
1	D	394	PHE	2.0
1	D	28	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	461	ALA	2.0
1	D	396	LEU	2.0
1	D	399	ASP	2.0
1	D	34	TYR	2.0

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	LLP	A	266	23/25	0.97	0.06	7,12,17,19	0
1	LLP	C	266	24/25	0.97	0.06	7,12,18,21	0
1	LLP	B	266	24/25	0.98	0.04	7,12,18,21	0
1	LLP	D	266	24/25	0.98	0.05	7,12,18,22	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
2	K	A	500	1/1	1.00	0.04	12,12,12,12	0
2	K	B	500	1/1	1.00	0.05	10,10,10,10	0
2	K	C	500	1/1	1.00	0.02	10,10,10,10	0
2	K	D	500	1/1	1.00	0.02	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.