



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:38 AM UTC

PDB ID : 1FP4 / pdb_00001fp4
Title : CRYSTAL STRUCTURE OF THE ALPHA-H195Q MUTANT OF NITRO-GENASE
Authors : Sorlie, M.; Christiansen, J.; Lemon, B.J.; Peters, J.W.; Dean, D.R.; Hales, B.J.
Deposited on : 2000-08-30
Resolution : 2.50 Å(reported)

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

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

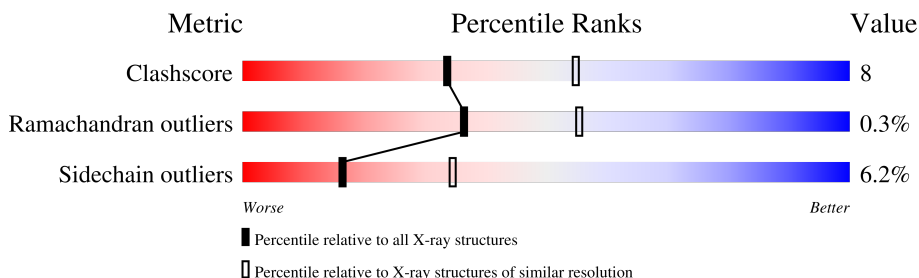
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	492	
1	C	492	
2	B	523	
2	D	523	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CFM	A	496	-	-	X	-
4	CFM	C	497	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16295 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 NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3708	2360	629	695	24			
1	C	468	Total	C	N	O	S	0	0	0
			3712	2363	630	695	24			

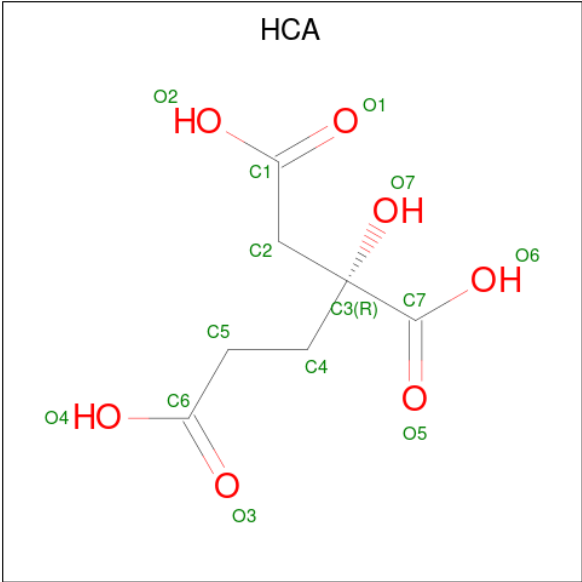
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	GLN	HIS	engineered mutation	UNP P07328
C	195	GLN	HIS	engineered mutation	UNP P07328

- Molecule 2 is a protein called NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN.

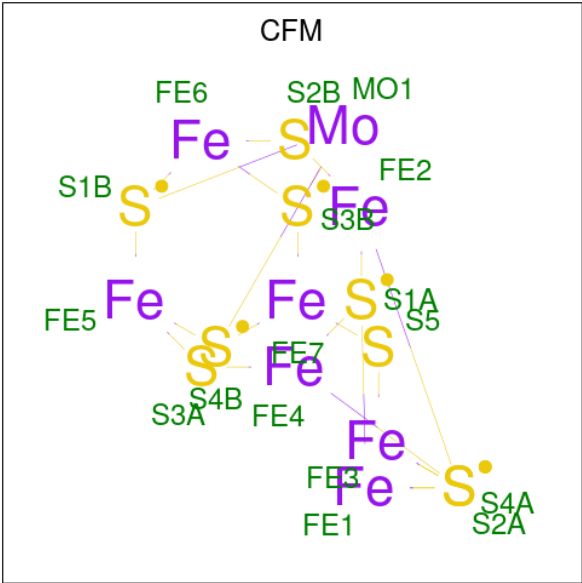
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: C₇H₁₀O₇).



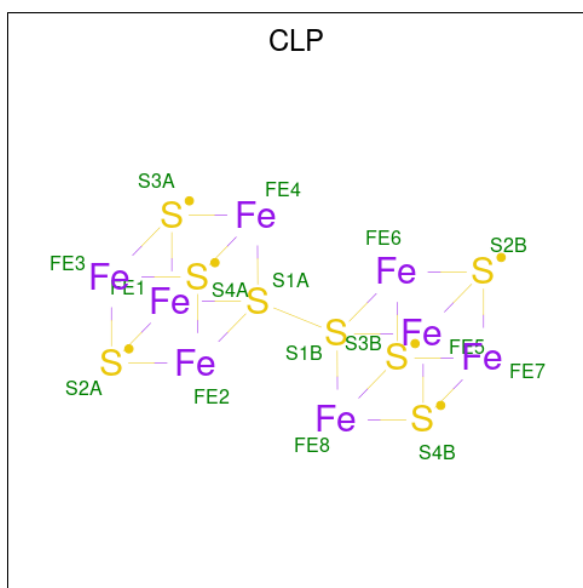
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	7	7		
3	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 4 is FE-MO-S CLUSTER (CCD ID: CFM) (formula: Fe₇MoS₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
4	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 5 is FE-S CLUSTER (CCD ID: CLP) (formula: Fe_8S_8).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			15	8	7		
5	C	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		

- Molecule 7 is water.

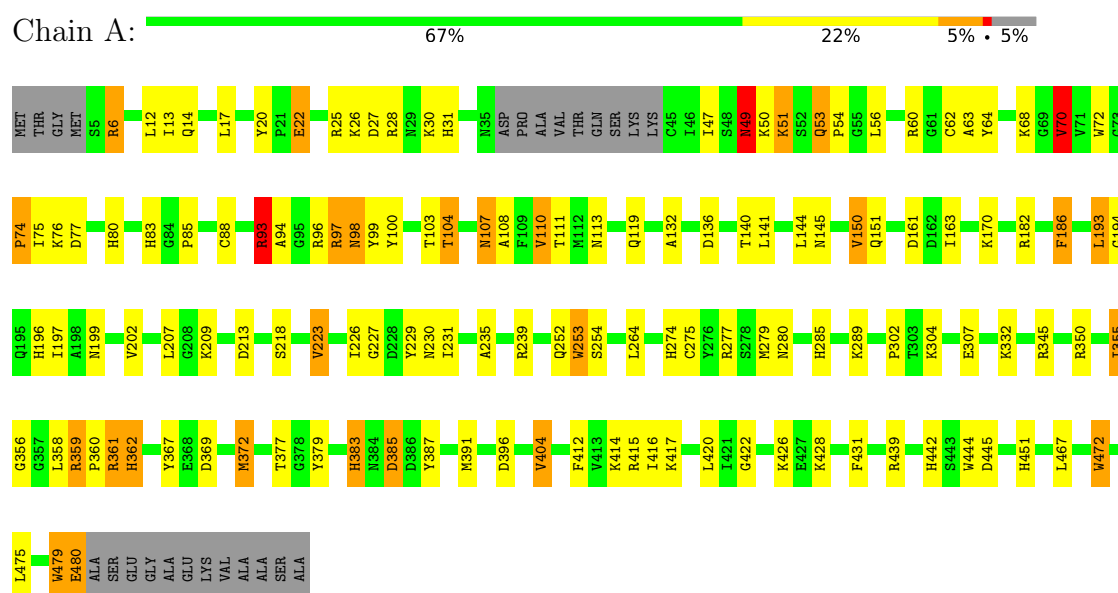
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	102	Total	O	0	0
			102	102		
7	B	114	Total	O	0	0
			114	114		
7	C	74	Total	O	0	0
			74	74		
7	D	143	Total	O	0	0
			143	143		

3 Residue-property plots

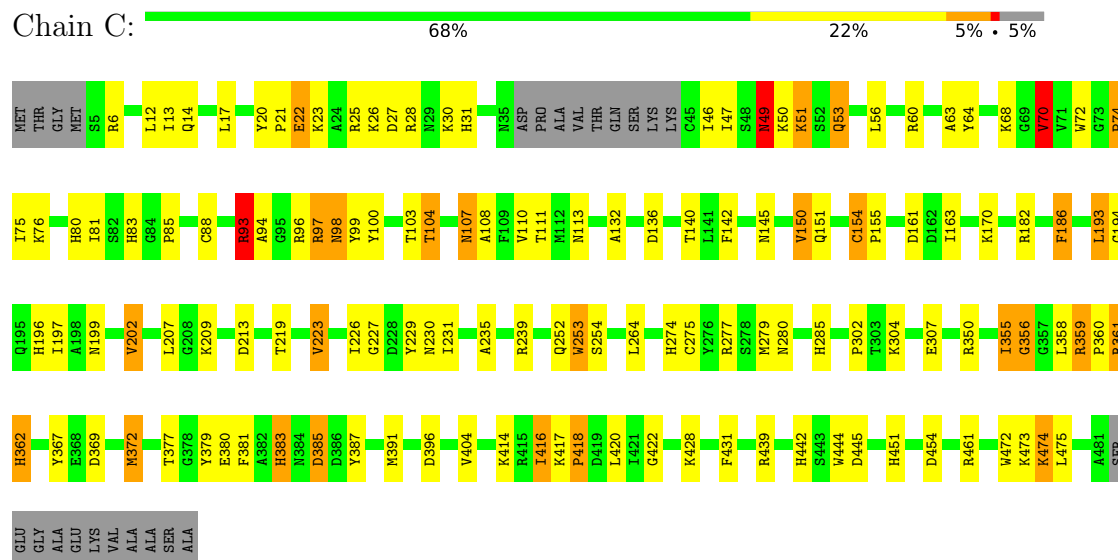
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN

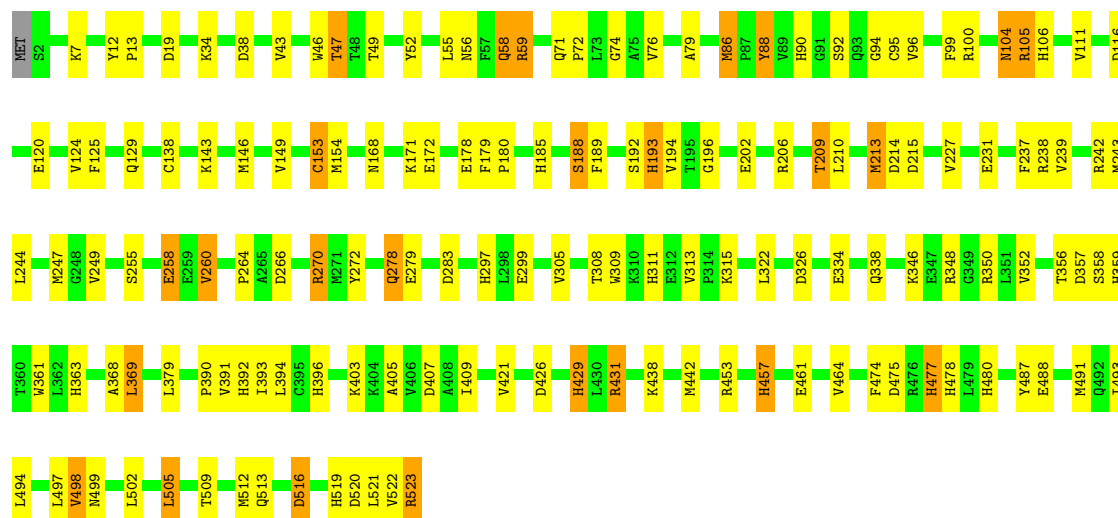


• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN



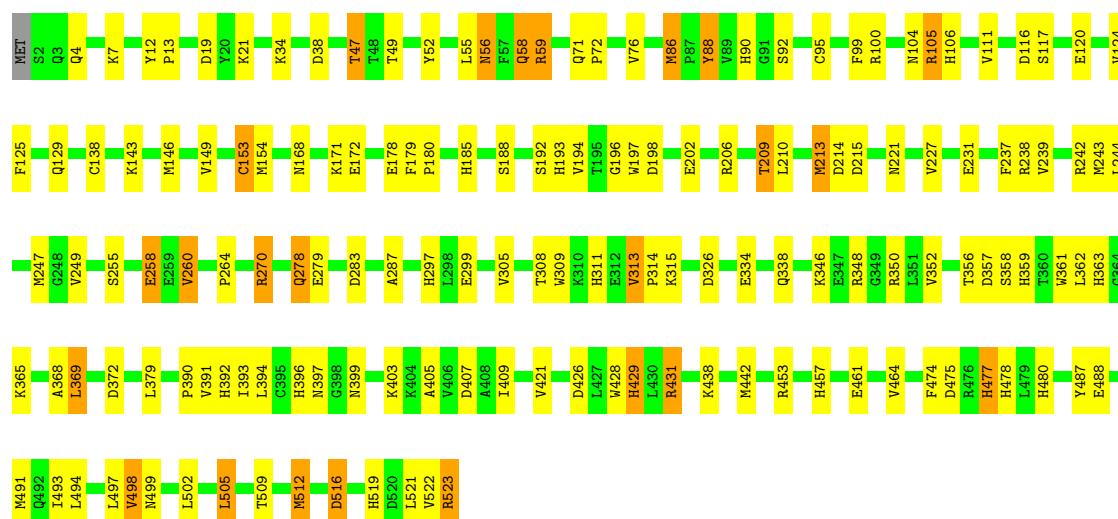
• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

Chain B:  71% 24% 5%



• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

Chain D:  70% 25% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.20Å 130.20Å 80.40Å 90.00° 111.20° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.184 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16295	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CLP, CFM, HCA

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	0.91	18/3793 (0.5%)	1.68	58/5114 (1.1%)
1	C	0.99	18/3797 (0.5%)	1.71	73/5120 (1.4%)
2	B	0.89	18/4280 (0.4%)	1.57	63/5786 (1.1%)
2	D	0.89	19/4280 (0.4%)	1.57	66/5786 (1.1%)
All	All	0.92	73/16150 (0.5%)	1.63	260/21806 (1.2%)

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	418	PRO	N-CD	-26.90	1.10	1.47
1	A	70	VAL	CA-CB	8.54	1.64	1.55
2	D	297	HIS	CD2-NE2	-7.60	1.29	1.37
2	B	297	HIS	CD2-NE2	-7.51	1.29	1.37
2	B	457	HIS	CD2-NE2	-7.14	1.29	1.37
1	C	70	VAL	CA-CB	7.12	1.62	1.55
2	B	480	HIS	CD2-NE2	-7.04	1.30	1.37
2	B	193	HIS	CD2-NE2	-6.91	1.30	1.37
2	B	429	HIS	CD2-NE2	-6.88	1.30	1.37
2	B	185	HIS	CD2-NE2	-6.78	1.30	1.37
2	D	311	HIS	CD2-NE2	-6.77	1.30	1.37
2	D	193	HIS	CD2-NE2	-6.72	1.30	1.37
2	D	429	HIS	CD2-NE2	-6.72	1.30	1.37
2	D	480	HIS	CD2-NE2	-6.63	1.30	1.37
2	D	457	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	274	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	442	HIS	CD2-NE2	-6.53	1.30	1.37
2	D	90	HIS	CD2-NE2	-6.53	1.30	1.37
2	B	477	HIS	CD2-NE2	-6.52	1.30	1.37
2	D	519	HIS	CD2-NE2	-6.49	1.30	1.37
2	D	185	HIS	CD2-NE2	-6.47	1.30	1.37
2	D	477	HIS	CD2-NE2	-6.47	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	HIS	CD2-NE2	-6.46	1.30	1.37
2	B	396	HIS	CD2-NE2	-6.44	1.30	1.37
1	C	80	HIS	CD2-NE2	-6.40	1.30	1.37
2	B	519	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	83	HIS	CD2-NE2	-6.38	1.30	1.37
1	C	362	HIS	CD2-NE2	-6.38	1.30	1.37
2	D	478	HIS	CD2-NE2	-6.38	1.30	1.37
1	C	31	HIS	CD2-NE2	-6.28	1.30	1.37
1	C	274	HIS	CD2-NE2	-6.28	1.30	1.37
1	C	442	HIS	CD2-NE2	-6.28	1.30	1.37
2	B	311	HIS	CD2-NE2	-6.27	1.30	1.37
1	C	383	HIS	CD2-NE2	-6.27	1.30	1.37
1	A	362	HIS	CD2-NE2	-6.25	1.30	1.37
2	B	90	HIS	CD2-NE2	-6.25	1.30	1.37
1	C	451	HIS	CD2-NE2	-6.23	1.31	1.37
1	A	451	HIS	CD2-NE2	-6.22	1.31	1.37
2	D	396	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	196	HIS	CG-ND1	-6.17	1.31	1.38
1	A	80	HIS	CD2-NE2	-6.14	1.31	1.37
2	D	359	HIS	CD2-NE2	-6.12	1.31	1.37
2	B	392	HIS	CD2-NE2	-6.07	1.31	1.37
2	D	363	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	31	HIS	CD2-NE2	-5.97	1.31	1.37
2	B	106	HIS	CD2-NE2	-5.94	1.31	1.37
2	B	478	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	417	LYS	N-CA	5.93	1.54	1.46
1	C	196	HIS	CG-ND1	-5.92	1.31	1.38
2	B	359	HIS	CD2-NE2	-5.91	1.31	1.37
1	C	83	HIS	CD2-NE2	-5.86	1.31	1.37
2	B	363	HIS	CD2-NE2	-5.82	1.31	1.37
2	D	106	HIS	CD2-NE2	-5.79	1.31	1.37
2	D	392	HIS	CD2-NE2	-5.72	1.31	1.37
1	C	285	HIS	CD2-NE2	-5.58	1.31	1.37
1	C	418	PRO	N-CA	5.55	1.53	1.47
1	A	31	HIS	CG-ND1	-5.46	1.32	1.38
1	C	150	VAL	CA-CB	5.44	1.61	1.53
1	A	196	HIS	CD2-NE2	-5.44	1.31	1.37
1	A	285	HIS	CD2-NE2	-5.39	1.31	1.37
1	A	404	VAL	CA-CB	5.28	1.59	1.54
1	A	150	VAL	CA-CB	5.27	1.60	1.53
2	D	185	HIS	CG-ND1	-5.26	1.32	1.38
1	C	196	HIS	CD2-NE2	-5.23	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	106	HIS	CG-ND1	-5.21	1.32	1.38
1	C	31	HIS	CG-ND1	-5.19	1.32	1.38
1	C	219	THR	CA-CB	5.17	1.60	1.53
1	C	80	HIS	CG-ND1	-5.13	1.32	1.38
1	A	83	HIS	CG-ND1	-5.11	1.32	1.38
2	D	359	HIS	CG-ND1	-5.06	1.32	1.38
2	B	193	HIS	CG-ND1	-5.02	1.32	1.38
1	A	80	HIS	CG-ND1	-5.02	1.32	1.38
2	B	396	HIS	CG-ND1	-5.00	1.32	1.38

All (260) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	51	LYS	N-CA-C	17.52	133.02	110.24
1	A	49	ASN	CB-CA-C	-14.36	81.84	110.42
1	C	49	ASN	CB-CA-C	-14.01	82.54	110.42
1	C	418	PRO	CA-N-CD	13.44	130.82	112.00
1	A	51	LYS	N-CA-C	12.20	126.94	110.35
1	C	418	PRO	N-CA-CB	-12.00	90.78	103.38
2	B	58	GLN	OE1-CD-NE2	-11.86	110.74	122.60
2	D	58	GLN	OE1-CD-NE2	-11.07	111.53	122.60
1	C	50	LYS	N-CA-CB	-10.91	92.05	110.49
1	A	50	LYS	N-CA-CB	-10.70	92.40	110.49
1	C	454	ASP	CA-CB-CG	10.18	122.78	112.60
1	C	253	TRP	O-C-N	10.04	134.97	122.93
1	A	253	TRP	O-C-N	9.66	134.52	122.93
1	A	385	ASP	CA-CB-CG	9.29	121.89	112.60
1	C	385	ASP	CA-CB-CG	8.95	121.55	112.60
1	A	417	LYS	N-CA-CB	8.73	125.90	110.37
1	C	362	HIS	N-CA-C	8.51	121.69	111.82
1	C	98	ASN	OD1-CG-ND2	-8.44	114.16	122.60
2	B	116	ASP	CA-CB-CG	8.37	120.97	112.60
1	A	362	HIS	N-CA-C	8.36	121.52	111.82
2	D	116	ASP	CA-CB-CG	8.27	120.87	112.60
1	A	22	GLU	N-CA-C	7.81	119.43	111.07
2	B	278	GLN	OE1-CD-NE2	-7.72	114.88	122.60
1	C	428	LYS	N-CA-C	7.71	120.42	111.02
1	A	76	LYS	N-CA-C	7.70	120.42	111.02
1	A	428	LYS	N-CA-C	7.70	120.42	111.02
1	C	76	LYS	N-CA-C	7.68	120.38	111.02
2	D	260	VAL	CB-CA-C	-7.65	101.82	112.14
2	D	297	HIS	CA-CB-CG	7.63	121.43	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	297	HIS	CA-CB-CG	7.61	121.41	113.80
2	B	58	GLN	CG-CD-NE2	7.54	127.72	116.40
1	A	98	ASN	OD1-CG-ND2	-7.52	115.08	122.60
1	C	22	GLU	N-CA-C	7.42	119.01	111.07
2	B	299	GLU	CA-CB-CG	-7.40	99.30	114.10
2	D	213	MET	N-CA-C	7.33	120.32	111.82
2	B	260	VAL	CB-CA-C	-7.32	102.25	112.14
2	B	213	MET	N-CA-C	7.28	120.27	111.82
2	D	299	GLU	CA-CB-CG	-7.22	99.65	114.10
2	D	391	VAL	N-CA-C	7.22	117.98	110.62
2	D	478	HIS	N-CA-C	7.22	121.67	112.86
2	B	516	ASP	CA-CB-CG	7.12	119.72	112.60
2	D	153	CYS	CB-CA-C	-7.07	98.66	110.68
1	A	50	LYS	N-CA-C	-6.98	95.94	110.80
1	C	383	HIS	CB-CG-CD2	-6.97	122.14	131.20
2	D	516	ASP	CA-CB-CG	6.91	119.51	112.60
2	B	153	CYS	CB-CA-C	-6.89	98.96	110.68
1	A	383	HIS	CB-CG-CD2	-6.88	122.26	131.20
2	D	58	GLN	CG-CD-NE2	6.84	126.67	116.40
1	C	50	LYS	N-CA-C	-6.82	96.27	110.80
2	B	478	HIS	N-CA-C	6.77	121.11	112.86
1	A	99	TYR	N-CA-C	6.76	119.55	110.35
2	D	278	GLN	OE1-CD-NE2	-6.68	115.92	122.60
2	B	391	VAL	N-CA-C	6.62	117.37	110.62
2	D	168	ASN	OD1-CG-ND2	-6.60	116.00	122.60
2	D	59	ARG	NE-CZ-NH2	6.59	125.13	119.20
2	D	209	THR	N-CA-C	6.58	121.14	112.72
1	A	253	TRP	N-CA-C	6.49	118.86	108.41
2	B	168	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	C	253	TRP	N-CA-C	6.46	118.81	108.41
2	D	270	ARG	NE-CZ-NH2	6.46	125.01	119.20
2	B	270	ARG	NE-CZ-NH2	6.44	125.00	119.20
1	A	253	TRP	CA-C-O	6.40	127.43	120.58
2	D	326	ASP	CA-CB-CG	6.40	119.00	112.60
2	B	326	ASP	CA-CB-CG	6.38	118.98	112.60
2	B	59	ARG	NE-CZ-NH2	6.37	124.94	119.20
2	B	357	ASP	CA-CB-CG	6.37	118.97	112.60
2	D	105	ARG	NE-CZ-NH2	6.34	124.91	119.20
1	A	49	ASN	N-CA-C	6.31	124.25	110.80
2	D	283	ASP	CA-CB-CG	6.31	118.91	112.60
1	C	49	ASN	N-CA-C	6.28	124.17	110.80
1	A	75	ILE	CA-C-N	6.26	129.49	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ILE	C-N-CA	6.26	129.49	120.79
2	B	209	THR	N-CA-C	6.26	120.73	112.72
2	D	210	LEU	N-CA-C	6.25	118.89	111.33
1	A	223	VAL	N-CA-CB	-6.21	103.10	112.35
2	B	359	HIS	N-CA-C	6.20	118.84	111.71
1	A	207	LEU	N-CA-C	6.19	118.03	111.28
1	C	98	ASN	CA-CB-CG	6.17	118.77	112.60
2	D	214	ASP	CA-CB-CG	6.14	118.74	112.60
2	D	357	ASP	CA-CB-CG	6.14	118.74	112.60
1	C	207	LEU	N-CA-C	6.14	117.97	111.28
1	C	53	GLN	CA-C-N	6.12	126.07	119.76
1	C	53	GLN	C-N-CA	6.12	126.07	119.76
1	C	253	TRP	CA-C-O	6.11	127.12	120.58
1	C	6	ARG	N-CA-C	6.11	119.57	111.75
2	D	143	LYS	O-C-N	-6.11	118.72	121.53
2	B	429	HIS	CB-CG-CD2	-6.08	123.29	131.20
2	D	19	ASP	CA-CB-CG	6.06	118.66	112.60
2	D	464	VAL	CA-C-N	6.04	125.98	119.76
2	D	464	VAL	C-N-CA	6.04	125.98	119.76
2	B	464	VAL	CA-C-N	6.03	125.97	119.76
2	B	464	VAL	C-N-CA	6.03	125.97	119.76
1	C	75	ILE	CA-C-N	6.02	129.15	120.79
1	C	75	ILE	C-N-CA	6.02	129.15	120.79
1	A	145	ASN	CA-CB-CG	6.01	118.61	112.60
2	D	429	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	A	186	PHE	CA-CB-CG	5.96	119.76	113.80
2	D	358	SER	N-CA-C	5.94	120.69	113.38
1	C	99	TYR	N-CA-C	5.92	118.85	110.50
1	A	53	GLN	CA-C-N	5.91	125.85	119.76
1	A	53	GLN	C-N-CA	5.91	125.85	119.76
2	B	19	ASP	CA-CB-CG	5.91	118.51	112.60
2	D	59	ARG	NE-CZ-NH1	-5.88	115.62	121.50
1	A	75	ILE	O-C-N	5.88	129.92	122.57
1	C	60	ARG	N-CA-C	5.85	118.72	110.23
2	B	283	ASP	CA-CB-CG	5.85	118.45	112.60
2	B	214	ASP	CA-CB-CG	5.83	118.43	112.60
2	D	227	VAL	CA-C-N	5.82	125.20	118.85
2	D	227	VAL	C-N-CA	5.82	125.20	118.85
1	C	377	THR	CA-CB-OG1	-5.80	100.90	109.60
2	D	129	GLN	OE1-CD-NE2	-5.79	116.81	122.60
2	B	457	HIS	CB-CG-CD2	-5.78	123.69	131.20
2	B	474	PHE	CA-CB-CG	5.74	119.54	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ARG	N-CA-C	5.73	118.53	110.23
1	A	6	ARG	N-CA-C	5.73	123.00	110.80
2	D	153	CYS	N-CA-CB	5.70	118.61	110.06
1	C	145	ASN	CA-CB-CG	5.69	118.29	112.60
2	D	359	HIS	N-CA-C	5.69	118.25	111.71
2	D	399	ASN	CA-CB-CG	5.68	118.28	112.60
2	B	129	GLN	OE1-CD-NE2	-5.67	116.93	122.60
1	A	98	ASN	CA-CB-CG	5.67	118.27	112.60
2	B	179	PHE	N-CA-C	-5.64	102.54	109.65
2	B	392	HIS	CB-CG-CD2	-5.64	123.86	131.20
2	B	513	GLN	OE1-CD-NE2	-5.63	116.97	122.60
2	B	210	LEU	N-CA-C	5.63	118.14	111.33
2	B	104	ASN	CA-CB-CG	5.61	118.21	112.60
2	B	523	ARG	NE-CZ-NH2	5.61	124.25	119.20
2	B	227	VAL	CA-C-N	5.60	125.13	119.19
2	B	227	VAL	C-N-CA	5.60	125.13	119.19
2	B	153	CYS	N-CA-CB	5.60	118.46	110.06
2	D	523	ARG	NE-CZ-NH1	-5.60	115.90	121.50
2	B	79	ALA	N-CA-C	5.59	117.38	111.28
1	A	104	THR	CA-CB-OG1	-5.59	101.21	109.60
2	B	215	ASP	CA-CB-CG	5.59	118.19	112.60
1	C	74	PRO	N-CA-C	5.59	121.10	113.84
1	A	110	VAL	N-CA-C	5.57	116.97	110.62
1	A	479	TRP	CA-C-N	5.55	131.69	121.70
1	A	479	TRP	C-N-CA	5.55	131.69	121.70
1	A	74	PRO	N-CA-C	5.55	121.05	113.84
2	B	59	ARG	NE-CZ-NH1	-5.54	115.96	121.50
2	D	258	GLU	N-CA-C	5.54	118.08	111.71
2	D	391	VAL	N-CA-CB	-5.54	103.01	110.54
2	B	105	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	C	280	ASN	CA-CB-CG	5.53	118.13	112.60
1	C	161	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	93	ARG	NE-CZ-NH2	5.51	124.16	119.20
2	B	358	SER	N-CA-C	5.50	120.15	113.38
2	D	49	THR	N-CA-C	5.50	117.63	110.53
2	D	361	TRP	CG-CD2-CE3	5.50	139.40	133.90
2	D	392	HIS	CB-CG-CD2	-5.50	124.05	131.20
2	D	215	ASP	CA-CB-CG	5.50	118.10	112.60
2	D	242	ARG	NE-CZ-NH2	5.50	124.15	119.20
2	B	238	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	C	75	ILE	O-C-N	5.49	129.43	122.57
1	C	444	TRP	CB-CG-CD1	-5.49	118.67	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	498	VAL	CB-CA-C	-5.49	104.74	112.14
1	C	213	ASP	CA-CB-CG	5.48	118.08	112.60
1	C	83	HIS	CB-CG-CD2	-5.48	124.08	131.20
2	B	361	TRP	CG-CD2-CE3	5.46	139.36	133.90
1	A	253	TRP	CA-C-N	5.46	131.97	121.54
1	A	253	TRP	C-N-CA	5.46	131.97	121.54
1	C	223	VAL	N-CA-CB	-5.46	103.32	112.06
2	B	270	ARG	NE-CZ-NH1	-5.46	116.04	121.50
2	D	474	PHE	CA-CB-CG	5.46	119.26	113.80
1	A	280	ASN	CA-CB-CG	5.44	118.04	112.60
1	C	253	TRP	CA-C-N	5.44	131.93	121.54
1	C	253	TRP	C-N-CA	5.44	131.93	121.54
2	D	519	HIS	CB-CG-CD2	-5.44	124.13	131.20
2	D	397	ASN	CA-CB-CG	5.44	118.04	112.60
1	A	361	ARG	CA-CB-CG	5.43	124.97	114.10
1	C	46	ILE	N-CA-C	5.43	116.19	108.42
1	C	474	LYS	N-CA-C	5.43	118.91	112.72
1	A	93	ARG	NE-CZ-NH1	-5.42	116.08	121.50
2	D	198	ASP	CA-CB-CG	5.41	118.01	112.60
2	D	457	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	A	72	TRP	CA-C-O	-5.40	115.34	120.90
1	A	72	TRP	N-CA-C	5.39	117.01	111.03
2	D	313	VAL	CA-C-N	5.39	125.33	119.78
2	D	313	VAL	C-N-CA	5.39	125.33	119.78
2	D	12	TYR	N-CA-C	-5.38	101.82	109.62
1	C	274	HIS	CB-CG-CD2	-5.35	124.24	131.20
2	D	117	SER	N-CA-C	5.35	118.62	111.24
2	D	498	VAL	CB-CA-C	-5.35	104.92	112.14
2	B	363	HIS	CB-CG-CD2	-5.35	124.25	131.20
1	C	361	ARG	CA-CB-CG	5.34	124.79	114.10
1	A	377	THR	CA-CB-OG1	-5.34	101.59	109.60
1	C	383	HIS	CB-CG-ND1	5.34	130.70	122.70
1	A	70	VAL	N-CA-C	5.33	116.14	111.56
1	A	83	HIS	CB-CG-CD2	-5.32	124.28	131.20
1	A	431	PHE	CA-CB-CG	-5.31	108.49	113.80
1	A	444	TRP	CE2-CD2-CG	-5.30	100.83	107.20
2	D	104	ASN	CA-CB-CG	5.30	117.90	112.60
1	A	213	ASP	CA-CB-CG	5.30	117.90	112.60
1	C	416	ILE	CA-C-N	5.30	130.62	124.21
1	C	416	ILE	C-N-CA	5.30	130.62	124.21
1	A	274	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	C	444	TRP	CE2-CD2-CG	-5.29	100.85	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	ASN	CA-CB-CG	5.29	117.89	112.60
2	B	523	ARG	NE-CZ-NH1	-5.29	116.21	121.50
1	C	219	THR	CA-C-N	5.29	125.00	119.82
1	C	219	THR	C-N-CA	5.29	125.00	119.82
1	C	142	PHE	CA-C-N	5.29	125.09	119.28
1	C	142	PHE	C-N-CA	5.29	125.09	119.28
2	B	391	VAL	N-CA-CB	-5.27	103.38	110.54
2	B	520	ASP	CA-CB-CG	5.27	117.87	112.60
2	D	361	TRP	CE2-CD2-CG	-5.26	100.89	107.20
2	D	428	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	A	77	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	383	HIS	CB-CG-ND1	5.24	130.56	122.70
1	A	97	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	C	72	TRP	CA-C-O	-5.22	115.52	120.90
1	C	75	ILE	CA-C-O	5.22	127.31	120.78
1	C	472	TRP	CE2-CD2-CG	-5.22	100.93	107.20
1	C	186	PHE	CA-CB-CG	5.22	119.02	113.80
1	A	161	ASP	CA-CB-CG	5.22	117.82	112.60
2	B	361	TRP	CE2-CD2-CG	-5.21	100.95	107.20
2	B	258	GLU	N-CA-C	5.20	117.69	111.71
2	B	519	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	C	356	GLY	N-CA-C	5.20	125.49	113.18
1	C	431	PHE	CA-CB-CG	-5.20	108.61	113.80
2	D	478	HIS	CB-CG-CD2	-5.19	124.45	131.20
2	D	238	ARG	NE-CZ-NH2	5.19	123.87	119.20
2	D	407	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	31	HIS	CB-CG-CD2	-5.18	124.46	131.20
2	B	407	ASP	CA-CB-CG	5.18	117.78	112.60
1	C	97	ARG	NE-CZ-NH2	5.18	123.86	119.20
2	B	313	VAL	CA-C-N	5.17	125.11	119.78
2	B	313	VAL	C-N-CA	5.17	125.11	119.78
2	B	242	ARG	NE-CZ-NH1	-5.17	116.33	121.50
2	B	12	TYR	N-CA-C	-5.16	102.14	109.62
2	D	179	PHE	N-CA-C	-5.16	103.15	109.65
1	C	461	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	C	76	LYS	N-CA-CB	-5.14	102.00	109.82
2	D	372	ASP	CA-C-N	5.14	124.32	118.97
2	D	372	ASP	C-N-CA	5.14	124.32	118.97
1	C	104	THR	CA-CB-OG1	-5.13	101.91	109.60
2	B	49	THR	N-CA-C	5.13	117.14	110.53
1	A	199	ASN	CA-CB-CG	5.12	117.72	112.60
1	C	70	VAL	N-CA-C	5.12	115.96	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	LYS	N-CA-C	5.11	116.93	111.36
1	C	377	THR	CA-CB-CG2	5.11	119.19	110.50
2	B	242	ARG	NE-CZ-NH2	5.11	123.80	119.20
2	D	197	TRP	N-CA-C	-5.11	105.62	111.14
1	C	97	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	C	93	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	C	154	CYS	CA-C-N	5.08	125.11	119.32
1	C	154	CYS	C-N-CA	5.08	125.11	119.32
1	A	472	TRP	CE2-CD2-CG	-5.07	101.12	107.20
2	B	480	HIS	CB-CG-CD2	-5.07	124.61	131.20
2	D	270	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	C	202	VAL	CB-CA-C	-5.06	105.24	112.22
1	A	93	ARG	NE-CZ-NH2	5.06	123.75	119.20
2	B	46	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	C	81	ILE	CB-CA-C	-5.04	104.19	111.19
2	D	480	HIS	CB-CG-CD2	-5.03	124.66	131.20
2	D	56	ASN	CA-CB-CG	5.02	117.62	112.60
1	C	31	HIS	CB-CG-CD2	-5.02	124.68	131.20
1	A	444	TRP	CB-CG-CD1	-5.01	119.38	126.90
1	C	94	ALA	N-CA-C	5.01	118.52	111.90
2	B	143	LYS	O-C-N	-5.00	119.23	121.53

There are no chirality outliers.

There are no planarity outliers.

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	3708	0	3638	72	0
1	C	3712	0	3640	63	0
2	B	4174	0	4087	70	0
2	D	4174	0	4087	62	0
3	A	14	0	6	0	0
3	C	14	0	6	0	0
4	A	17	0	0	5	0
4	C	17	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	15	0	0	3	0
5	C	15	0	0	2	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	102	0	0	7	0
7	B	114	0	0	2	0
7	C	74	0	0	2	0
7	D	143	0	0	2	0
All	All	16295	0	15464	242	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 8.

All (242) 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:146:MET:HG3	2:B:180:PRO:HB2	1.62	0.82
2:D:390:PRO:HB2	2:D:393:ILE:HD11	1.63	0.81
2:B:390:PRO:HB2	2:B:393:ILE:HD11	1.64	0.80
1:C:350:ARG:NH1	1:C:416:ILE:O	2.17	0.77
2:D:146:MET:HG3	2:D:180:PRO:HB2	1.66	0.77
2:B:499:ASN:HD21	2:D:477:HIS:H	1.32	0.76
2:B:477:HIS:H	2:D:499:ASN:HD21	1.33	0.76
1:A:49:ASN:CG	1:A:49:ASN:O	2.18	0.74
1:A:85:PRO:HB2	5:A:498:CLP:S2B	2.29	0.73
1:A:93:ARG:HG3	1:A:113:ASN:HB2	1.71	0.72
1:A:350:ARG:NH1	1:A:416:ILE:O	2.24	0.71
1:A:230:ASN:HD22	1:A:235:ALA:H	1.40	0.70
1:C:230:ASN:HD22	1:C:235:ALA:H	1.40	0.70
1:C:49:ASN:CG	1:C:49:ASN:O	2.20	0.69
1:C:93:ARG:HG3	1:C:113:ASN:HB2	1.73	0.69
2:D:180:PRO:HG2	2:D:278:GLN:NE2	2.08	0.69
2:B:180:PRO:HG2	2:B:278:GLN:NE2	2.10	0.66
1:C:85:PRO:HB2	5:C:499:CLP:S2B	2.36	0.66
2:B:431:ARG:HH21	2:B:431:ARG:HG3	1.63	0.63
1:A:93:ARG:HD3	1:A:111:THR:O	1.99	0.62
1:C:74:PRO:HG2	1:C:254:SER:HB3	1.82	0.61
1:A:74:PRO:HG2	1:A:254:SER:HB3	1.81	0.61
2:B:499:ASN:HD21	2:D:477:HIS:N	1.98	0.61
1:C:93:ARG:HD3	1:C:111:THR:O	2.02	0.59
1:A:100:TYR:CE2	1:A:110:VAL:HB	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:431:ARG:HH21	2:D:431:ARG:HG3	1.68	0.59
2:D:56:ASN:O	2:D:59:ARG:HD3	2.02	0.59
1:A:94:ALA:HB3	2:D:521:LEU:HD22	1.85	0.59
2:D:239:VAL:HG22	2:D:243:MET:HE2	1.85	0.59
2:B:239:VAL:HG22	2:B:243:MET:HE2	1.84	0.58
1:C:355:ILE:HB	1:C:360:PRO:HD3	1.85	0.58
1:C:22:GLU:O	1:C:26:LYS:HG2	2.04	0.58
1:C:100:TYR:CE2	1:C:110:VAL:HB	2.38	0.57
2:D:209:THR:HG21	2:D:309:TRP:NE1	2.19	0.57
1:A:22:GLU:O	1:A:26:LYS:HG2	2.05	0.57
2:D:100:ARG:HD2	2:D:111:VAL:O	2.05	0.57
2:B:100:ARG:HD2	2:B:111:VAL:O	2.05	0.57
1:C:367:TYR:CD2	1:C:372:MET:HE3	2.40	0.57
2:B:56:ASN:O	2:B:59:ARG:HD3	2.04	0.57
1:A:367:TYR:CD2	1:A:372:MET:HE3	2.40	0.56
2:B:209:THR:HG21	2:B:309:TRP:NE1	2.20	0.56
2:B:477:HIS:N	2:D:499:ASN:HD21	2.02	0.56
1:C:70:VAL:HG11	4:C:497:CFM:S2B	2.46	0.56
1:A:70:VAL:HG11	4:A:496:CFM:S2B	2.45	0.56
1:C:53:GLN:HB3	1:C:56:LEU:HD12	1.88	0.56
2:D:488:GLU:HA	2:D:491:MET:HE3	1.88	0.56
2:B:55:LEU:HA	2:B:58:GLN:OE1	2.07	0.55
2:B:209:THR:HG22	2:B:213:MET:SD	2.47	0.55
2:B:522:VAL:HG11	2:D:105:ARG:HD2	1.88	0.55
2:D:21:LYS:HD2	7:D:532:HOH:O	2.06	0.55
2:D:55:LEU:HA	2:D:58:GLN:OE1	2.06	0.55
2:B:322:LEU:HD23	1:C:474:LYS:HG2	1.87	0.55
2:B:488:GLU:HA	2:B:491:MET:HE3	1.89	0.55
1:A:103:THR:H	1:A:107:ASN:HD21	1.55	0.54
1:A:230:ASN:HD22	1:A:235:ALA:N	2.04	0.54
1:A:355:ILE:HB	1:A:360:PRO:HD3	1.88	0.54
2:D:209:THR:HG22	2:D:213:MET:SD	2.47	0.54
2:B:369:LEU:HD13	2:B:379:LEU:HD23	1.90	0.54
2:D:369:LEU:HD13	2:D:379:LEU:HD23	1.89	0.53
1:C:230:ASN:HD22	1:C:235:ALA:N	2.05	0.53
1:C:96:ARG:NH2	4:C:497:CFM:S5	2.82	0.53
1:C:104:THR:HA	1:C:108:ALA:O	2.09	0.53
1:C:186:PHE:HD1	2:D:120:GLU:HG2	1.73	0.53
1:C:30:LYS:HB3	1:C:47:ILE:HG12	1.91	0.53
1:A:53:GLN:HB3	1:A:56:LEU:HD12	1.91	0.53
5:A:498:CLP:S2A	2:B:92:SER:HB3	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:TYR:CZ	1:C:68:LYS:HG2	2.45	0.52
2:B:264:PRO:HG2	2:B:270:ARG:NH1	2.24	0.52
1:C:361:ARG:HB2	1:C:379:TYR:OH	2.10	0.52
1:A:104:THR:HA	1:A:108:ALA:O	2.09	0.52
1:C:473:LYS:N	1:C:473:LYS:HD2	2.25	0.52
2:B:47:THR:HG22	2:B:52:TYR:CZ	2.45	0.52
2:B:403:LYS:HE2	2:B:421:VAL:O	2.09	0.52
1:A:144:LEU:CD1	2:B:43:VAL:HG21	2.39	0.51
2:D:403:LYS:HE2	2:D:421:VAL:O	2.10	0.51
1:A:103:THR:H	1:A:107:ASN:ND2	2.09	0.51
1:C:422:GLY:HA2	1:C:439:ARG:O	2.11	0.51
1:A:361:ARG:HB2	1:A:379:TYR:OH	2.11	0.50
2:D:95:CYS:HB3	2:D:99:PHE:CZ	2.46	0.50
1:A:27:ASP:HA	1:A:30:LYS:HE3	1.94	0.50
1:A:64:TYR:CZ	1:A:68:LYS:HG2	2.46	0.50
1:C:103:THR:H	1:C:107:ASN:HD21	1.58	0.50
2:D:264:PRO:HG2	2:D:270:ARG:NH1	2.26	0.50
1:C:27:ASP:HA	1:C:30:LYS:HE3	1.93	0.50
1:C:226:ILE:HA	1:C:253:TRP:HB2	1.93	0.50
1:A:119:GLN:HA	2:B:189:PHE:O	2.11	0.50
1:A:239:ARG:HE	1:A:252:GLN:HE21	1.60	0.50
1:A:229:TYR:CE1	4:A:496:CFM:S2A	3.04	0.50
1:A:422:GLY:HA2	1:A:439:ARG:O	2.11	0.50
1:A:144:LEU:HD13	2:B:43:VAL:HG21	1.94	0.50
2:D:124:VAL:HG23	2:D:125:PHE:CD1	2.46	0.49
2:B:105:ARG:HD2	2:D:522:VAL:HG11	1.95	0.49
2:B:124:VAL:HG23	2:B:125:PHE:CD1	2.47	0.49
1:A:68:LYS:HB2	1:A:151:GLN:HG3	1.94	0.49
2:B:247:MET:HB3	2:B:249:VAL:HG23	1.94	0.49
1:C:68:LYS:HB2	1:C:151:GLN:HG3	1.95	0.49
2:B:95:CYS:HB3	2:B:99:PHE:CZ	2.47	0.49
2:D:264:PRO:HG2	2:D:270:ARG:HH11	1.78	0.49
1:A:387:TYR:O	1:A:391:MET:HG2	2.13	0.49
2:B:352:VAL:O	2:B:356:THR:HG23	2.13	0.49
1:C:275:CYS:HA	1:C:358:LEU:HD22	1.95	0.49
2:B:264:PRO:HG2	2:B:270:ARG:HH11	1.78	0.48
1:C:387:TYR:O	1:C:391:MET:HG2	2.13	0.48
2:D:47:THR:HG22	2:D:52:TYR:CZ	2.48	0.48
1:A:226:ILE:HA	1:A:253:TRP:HB2	1.94	0.48
2:B:475:ASP:HB3	2:D:521:LEU:O	2.13	0.48
2:D:352:VAL:O	2:D:356:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:CD1	2:B:59:ARG:HD2	2.44	0.48
1:A:193:LEU:HD13	1:A:197:ILE:HD11	1.95	0.47
1:A:275:CYS:HA	1:A:358:LEU:HD22	1.97	0.47
1:A:17:LEU:O	1:A:25:ARG:HG2	2.14	0.47
1:C:17:LEU:O	1:C:25:ARG:HG2	2.14	0.47
2:D:426:ASP:O	2:D:429:HIS:HB2	2.15	0.47
1:C:417:LYS:N	1:C:418:PRO:HD3	2.30	0.47
1:A:96:ARG:NH2	4:A:496:CFM:S5	2.88	0.47
1:C:239:ARG:HE	1:C:252:GLN:HE21	1.61	0.47
1:A:63:ALA:O	1:A:194:GLY:HA3	2.15	0.47
1:C:355:ILE:HG22	1:C:356:GLY:H	1.78	0.47
2:B:521:LEU:O	2:D:475:ASP:HB3	2.15	0.47
1:C:229:TYR:CE1	4:C:497:CFM:S2A	3.08	0.47
2:B:493:ILE:O	2:B:497:LEU:HG	2.15	0.47
2:D:72:PRO:O	2:D:76:VAL:HG23	2.15	0.47
2:D:88:TYR:O	2:D:149:VAL:HA	2.15	0.47
1:C:193:LEU:HD13	1:C:197:ILE:HD11	1.96	0.46
2:B:457:HIS:CD2	2:D:512:MET:HB2	2.51	0.46
2:D:180:PRO:HG2	2:D:278:GLN:HE21	1.77	0.46
1:A:345:ARG:HB3	7:A:596:HOH:O	2.14	0.46
1:A:367:TYR:HD2	1:A:372:MET:HE3	1.81	0.46
1:C:132:ALA:O	1:C:170:LYS:HE3	2.16	0.46
2:D:305:VAL:HG23	2:D:309:TRP:CE3	2.51	0.46
1:A:62:CYS:HB3	2:B:94:GLY:HA3	1.98	0.46
1:A:30:LYS:HB3	1:A:47:ILE:HG12	1.97	0.46
2:B:499:ASN:ND2	2:D:477:HIS:H	2.06	0.46
1:C:63:ALA:O	1:C:194:GLY:HA3	2.16	0.46
2:B:213:MET:HE2	2:B:308:THR:O	2.16	0.45
2:B:494:LEU:O	2:B:498:VAL:HG23	2.16	0.45
2:D:213:MET:HE2	2:D:308:THR:O	2.16	0.45
1:C:103:THR:H	1:C:107:ASN:ND2	2.13	0.45
1:C:367:TYR:HD2	1:C:372:MET:HE3	1.80	0.45
1:A:186:PHE:HD1	2:B:120:GLU:HG2	1.80	0.45
2:D:509:THR:O	2:D:516:ASP:HA	2.16	0.45
1:A:53:GLN:HA	1:A:54:PRO:HD3	1.88	0.45
2:B:426:ASP:O	2:B:429:HIS:HB2	2.16	0.45
1:C:13:ILE:O	1:C:17:LEU:HG	2.16	0.45
1:A:355:ILE:HG22	1:A:356:GLY:H	1.82	0.45
2:D:247:MET:HB3	2:D:249:VAL:HG23	1.99	0.45
2:B:305:VAL:HG23	2:B:309:TRP:CE3	2.51	0.45
1:A:472:TRP:HB2	7:A:543:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:THR:HG21	2:B:309:TRP:HE1	1.81	0.45
2:D:438:LYS:HE3	2:D:461:GLU:O	2.17	0.45
2:B:180:PRO:HG2	2:B:278:GLN:HE21	1.80	0.45
1:C:209:LYS:HB2	1:C:209:LYS:HE3	1.83	0.45
2:D:494:LEU:O	2:D:498:VAL:HG23	2.18	0.45
2:B:438:LYS:HE3	2:B:461:GLU:O	2.17	0.44
1:A:13:ILE:O	1:A:17:LEU:HG	2.18	0.44
1:A:132:ALA:O	1:A:170:LYS:HE3	2.17	0.44
2:B:47:THR:HB	2:B:431:ARG:HH11	1.82	0.44
1:A:96:ARG:HD2	4:A:496:CFM:S3B	2.57	0.44
5:A:498:CLP:S2B	2:B:188:SER:HB3	2.57	0.44
1:C:359:ARG:HB2	4:C:497:CFM:S3A	2.57	0.44
1:A:229:TYR:CD2	1:A:254:SER:HB2	2.53	0.44
1:A:359:ARG:HB2	4:A:496:CFM:S3A	2.58	0.44
2:D:71:GLN:O	2:D:196:GLY:HA3	2.17	0.44
2:D:487:TYR:O	2:D:491:MET:HG3	2.18	0.44
2:B:231:GLU:HB3	2:B:237:PHE:CZ	2.53	0.44
1:A:218:SER:HB2	7:A:501:HOH:O	2.18	0.44
2:B:86:MET:HG3	2:B:138:CYS:SG	2.57	0.44
2:B:88:TYR:O	2:B:149:VAL:HA	2.18	0.44
1:C:163:ILE:HG12	1:C:182:ARG:NH2	2.32	0.44
1:C:186:PHE:CD1	2:D:120:GLU:HG2	2.51	0.44
2:D:86:MET:HG3	2:D:138:CYS:SG	2.57	0.44
2:D:202:GLU:O	2:D:206:ARG:HG3	2.17	0.44
2:B:72:PRO:O	2:B:76:VAL:HG23	2.18	0.44
2:B:405:ALA:O	2:B:409:ILE:HG23	2.18	0.43
2:D:47:THR:HB	2:D:431:ARG:HH11	1.83	0.43
2:D:493:ILE:O	2:D:497:LEU:HG	2.18	0.43
1:C:20:TYR:CE1	1:C:28:ARG:HG3	2.53	0.43
2:B:192:SER:OG	2:B:194:VAL:HG22	2.18	0.43
1:C:97:ARG:O	1:C:231:ILE:HA	2.19	0.43
1:C:304:LYS:HA	1:C:307:GLU:HG2	2.00	0.43
2:B:487:TYR:O	2:B:491:MET:HG3	2.18	0.43
1:A:209:LYS:HB2	1:A:209:LYS:HE3	1.79	0.43
1:C:417:LYS:HA	1:C:418:PRO:HD2	1.48	0.43
2:D:4:GLN:HG2	7:D:580:HOH:O	2.18	0.43
1:A:64:TYR:CE2	1:A:88:CYS:HB3	2.53	0.43
1:A:163:ILE:HG12	1:A:182:ARG:NH2	2.34	0.43
1:C:229:TYR:CD2	1:C:254:SER:HB2	2.54	0.43
2:D:209:THR:HG21	2:D:309:TRP:HE1	1.81	0.43
1:A:304:LYS:HA	1:A:307:GLU:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:502:LEU:HD22	2:D:523:ARG:HD3	2.01	0.42
1:A:412:PHE:O	1:A:416:ILE:HG13	2.19	0.42
1:C:96:ARG:HD2	4:C:497:CFM:S3B	2.59	0.42
1:A:479:TRP:O	1:A:480:GLU:HB2	2.19	0.42
2:B:509:THR:O	2:B:516:ASP:HA	2.18	0.42
2:D:313:VAL:HA	2:D:314:PRO:HD3	1.85	0.42
1:A:97:ARG:O	1:A:231:ILE:HA	2.19	0.42
2:B:71:GLN:O	2:B:196:GLY:HA3	2.19	0.42
2:B:502:LEU:HD22	2:B:523:ARG:HD3	2.01	0.42
2:B:505:LEU:HD13	2:B:523:ARG:CZ	2.50	0.42
1:A:475:LEU:O	2:B:266:ASP:HA	2.19	0.41
2:B:202:GLU:O	2:B:206:ARG:HG3	2.20	0.41
1:C:23:LYS:HG3	7:C:552:HOH:O	2.20	0.41
1:C:227:GLY:CA	1:C:279:MET:HG3	2.51	0.41
1:A:415:ARG:HG3	7:A:508:HOH:O	2.21	0.41
2:B:96:VAL:O	2:B:100:ARG:HG3	2.20	0.41
2:B:368:ALA:O	2:B:442:MET:HA	2.20	0.41
7:B:581:HOH:O	1:C:474:LYS:HA	2.20	0.41
2:D:192:SER:OG	2:D:194:VAL:HG22	2.21	0.41
1:A:20:TYR:CE1	1:A:28:ARG:HG3	2.55	0.41
1:C:154:CYS:HB2	1:C:155:PRO:HD3	2.03	0.41
1:C:277:ARG:NH1	1:C:383:HIS:HB2	2.35	0.41
1:C:355:ILE:O	1:C:380:GLU:HG3	2.20	0.41
2:D:221:ASN:OD1	2:D:287:ALA:HA	2.21	0.41
1:A:277:ARG:NH1	1:A:383:HIS:HB2	2.36	0.41
1:A:140:THR:HG22	7:A:525:HOH:O	2.20	0.41
1:A:141:LEU:HD13	2:B:59:ARG:HD2	2.03	0.41
2:B:431:ARG:HG3	2:B:431:ARG:NH2	2.33	0.41
5:C:499:CLP:S2A	2:D:92:SER:HB3	2.61	0.41
2:D:362:LEU:O	2:D:365:LYS:HB2	2.21	0.41
1:C:302:PRO:HD2	1:C:369:ASP:OD2	2.21	0.41
1:C:381:PHE:CZ	4:C:497:CFM:S2B	3.14	0.41
1:A:94:ALA:HB3	2:D:521:LEU:CD2	2.49	0.41
1:A:136:ASP:O	1:A:140:THR:HG23	2.20	0.41
2:D:368:ALA:O	2:D:442:MET:HA	2.21	0.41
2:D:405:ALA:O	2:D:409:ILE:HG23	2.21	0.41
2:D:505:LEU:HD13	2:D:523:ARG:CZ	2.50	0.41
1:C:64:TYR:CE2	1:C:88:CYS:HB3	2.56	0.41
2:D:231:GLU:HB3	2:D:237:PHE:CZ	2.56	0.41
1:A:227:GLY:CA	1:A:279:MET:HG3	2.50	0.40
1:C:20:TYR:HB2	1:C:25:ARG:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:PRO:HG3	7:C:509:HOH:O	2.20	0.40
2:B:272:TYR:HB2	7:B:530:HOH:O	2.20	0.40
1:A:96:ARG:HA	7:A:512:HOH:O	2.21	0.40
1:A:302:PRO:HD2	1:A:369:ASP:OD2	2.21	0.40
1:A:332:LYS:HE2	7:A:575:HOH:O	2.21	0.40
2:B:74:GLY:HA3	2:B:193:HIS:O	2.21	0.40
1:C:226:ILE:HG22	1:C:279:MET:HB3	2.04	0.40
1:A:20:TYR:HB2	1:A:25:ARG:HG3	2.04	0.40
1:A:186:PHE:CD1	2:B:120:GLU:HG2	2.56	0.40
1:A:426:LYS:HA	2:B:104:ASN:ND2	2.37	0.40
2:B:209:THR:CG2	2:B:213:MET:SD	3.10	0.40
1:C:136:ASP:O	1:C:140:THR:HG23	2.21	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	463/492 (94%)	433 (94%)	28 (6%)	2 (0%)	30	49
1	C	464/492 (94%)	437 (94%)	26 (6%)	1 (0%)	43	63
2	B	520/523 (99%)	508 (98%)	11 (2%)	1 (0%)	43	63
2	D	520/523 (99%)	507 (98%)	12 (2%)	1 (0%)	43	63
All	All	1967/2030 (97%)	1885 (96%)	77 (4%)	5 (0%)	36	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
2	B	255	SER
2	D	255	SER

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Mol	Chain	Res	Type
1	A	355	ILE
1	C	355	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	397/415 (96%)	373 (94%)	24 (6%)	17	36
1	C	396/415 (95%)	373 (94%)	23 (6%)	18	38
2	B	454/455 (100%)	425 (94%)	29 (6%)	16	33
2	D	454/455 (100%)	425 (94%)	29 (6%)	16	33
All	All	1701/1740 (98%)	1596 (94%)	105 (6%)	16	34

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	14	GLN
1	A	49	ASN
1	A	51	LYS
1	A	70	VAL
1	A	93	ARG
1	A	98	ASN
1	A	107	ASN
1	A	150	VAL
1	A	193	LEU
1	A	202	VAL
1	A	223	VAL
1	A	264	LEU
1	A	359	ARG
1	A	362	HIS
1	A	372	MET
1	A	385	ASP
1	A	396	ASP
1	A	404	VAL

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Mol	Chain	Res	Type
1	A	414	LYS
1	A	420	LEU
1	A	445	ASP
1	A	467	LEU
1	A	480	GLU
2	B	7	LYS
2	B	13	PRO
2	B	34	LYS
2	B	38	ASP
2	B	47	THR
2	B	86	MET
2	B	88	TYR
2	B	153	CYS
2	B	154	MET
2	B	171	LYS
2	B	172	GLU
2	B	178	GLU
2	B	188	SER
2	B	244	LEU
2	B	258	GLU
2	B	260	VAL
2	B	279	GLU
2	B	315	LYS
2	B	334	GLU
2	B	338	GLN
2	B	346	LYS
2	B	348	ARG
2	B	350	ARG
2	B	369	LEU
2	B	394	LEU
2	B	431	ARG
2	B	453	ARG
2	B	505	LEU
2	B	512	MET
1	C	12	LEU
1	C	14	GLN
1	C	49	ASN
1	C	51	LYS
1	C	70	VAL
1	C	93	ARG
1	C	98	ASN
1	C	107	ASN

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Mol	Chain	Res	Type
1	C	150	VAL
1	C	193	LEU
1	C	202	VAL
1	C	223	VAL
1	C	264	LEU
1	C	359	ARG
1	C	362	HIS
1	C	372	MET
1	C	385	ASP
1	C	396	ASP
1	C	404	VAL
1	C	414	LYS
1	C	420	LEU
1	C	445	ASP
1	C	475	LEU
2	D	7	LYS
2	D	13	PRO
2	D	34	LYS
2	D	38	ASP
2	D	47	THR
2	D	86	MET
2	D	88	TYR
2	D	153	CYS
2	D	154	MET
2	D	171	LYS
2	D	172	GLU
2	D	178	GLU
2	D	188	SER
2	D	244	LEU
2	D	258	GLU
2	D	260	VAL
2	D	279	GLU
2	D	315	LYS
2	D	334	GLU
2	D	338	GLN
2	D	346	LYS
2	D	348	ARG
2	D	350	ARG
2	D	369	LEU
2	D	394	LEU
2	D	431	ARG
2	D	453	ARG

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Mol	Chain	Res	Type
2	D	505	LEU
2	D	512	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	230	ASN
1	A	252	GLN
1	A	271	ASN
1	A	285	HIS
1	A	321	GLN
1	A	383	HIS
1	A	468	ASN
2	B	104	ASN
2	B	136	GLN
2	B	163	ASN
2	B	167	ASN
2	B	278	GLN
2	B	294	GLN
2	B	457	HIS
2	B	499	ASN
1	C	49	ASN
1	C	53	GLN
1	C	107	ASN
1	C	230	ASN
1	C	252	GLN
1	C	285	HIS
1	C	383	HIS
2	D	104	ASN
2	D	136	GLN
2	D	163	ASN
2	D	167	ASN
2	D	278	GLN
2	D	457	HIS
2	D	499	ASN
2	D	519	HIS

5.3.3 RNA ⓘ

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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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$
5	CLP	C	499	1,2	0,21,25	-	-	-		
4	CFM	C	497	1	0,24,24	-	-	-		
3	HCA	C	495	-	13,13,13	2.34	4 (30%)	15,18,18	2.00	5 (33%)
4	CFM	A	496	1	0,24,24	-	-	-		
5	CLP	A	498	1,2	0,21,25	-	-	-		
3	HCA	A	494	-	13,13,13	2.33	4 (30%)	15,18,18	2.05	6 (40%)

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
5	CLP	A	498	1,2	-	-	0/10/9/10
3	HCA	A	494	-	-	5/17/17/17	-
3	HCA	C	495	-	-	5/17/17/17	-
5	CLP	C	499	1,2	-	-	0/10/9/10

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	495	HCA	O5-C7	6.80	1.43	1.22
3	A	494	HCA	O5-C7	6.65	1.42	1.22
3	C	495	HCA	O1-C1	2.90	1.31	1.22
3	A	494	HCA	O1-C1	2.81	1.31	1.22
3	C	495	HCA	O6-C7	-2.57	1.21	1.30
3	A	494	HCA	O6-C7	-2.56	1.21	1.30
3	A	494	HCA	O3-C6	2.52	1.30	1.22
3	C	495	HCA	O3-C6	2.40	1.30	1.22

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	495	HCA	O6-C7-C3	4.65	122.07	113.14
3	A	494	HCA	O6-C7-C3	4.62	121.99	113.14
3	A	494	HCA	O2-C1-O1	-2.50	116.90	123.33
3	A	494	HCA	O4-C6-C5	2.48	121.82	114.00
3	C	495	HCA	O2-C1-O1	-2.43	117.09	123.33
3	C	495	HCA	O4-C6-C5	2.42	121.65	114.00
3	C	495	HCA	O4-C6-O3	-2.41	117.14	123.33
3	A	494	HCA	O4-C6-O3	-2.30	117.42	123.33
3	C	495	HCA	O5-C7-C3	-2.18	117.86	122.09
3	A	494	HCA	O5-C7-C3	-2.15	117.92	122.09
3	A	494	HCA	O7-C3-C2	-2.07	104.65	109.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	494	HCA	C2-C3-C4-C5
3	A	494	HCA	C7-C3-C4-C5
3	A	494	HCA	O7-C3-C4-C5
3	C	495	HCA	C2-C3-C4-C5
3	C	495	HCA	C7-C3-C4-C5
3	C	495	HCA	O7-C3-C4-C5
3	A	494	HCA	C3-C4-C5-C6
3	C	495	HCA	C3-C4-C5-C6
3	C	495	HCA	C4-C5-C6-O4
3	A	494	HCA	C4-C5-C6-O4

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	499	CLP	2	0
4	C	497	CFM	6	0
4	A	496	CFM	5	0
5	A	498	CLP	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.