



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:06 AM UTC

PDB ID : 1OVA / pdb_00001ova
Title : CRYSTAL STRUCTURE OF UNCLEAVED OVALBUMIN AT 1.95
ANGSTROMS RESOLUTION
Authors : Stein, P.E.; Leslie, A.G.W.
Deposited on : 1990-11-26
Resolution : 1.95 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)	:	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

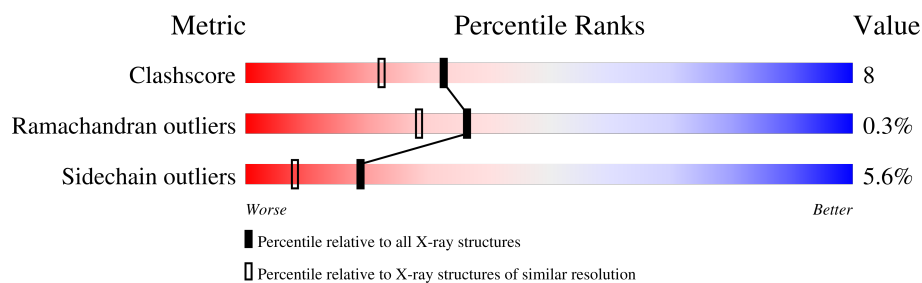
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	386	 60% 33% 6% .
2	B	386	 64% 28% 5% .
3	C	386	 60% 28% 8% . .
3	D	386	 62% 32% 5% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12269 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 OVALBUMIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	P	S	0	0	0
			2940	1876	489	551	2	22			

- Molecule 2 is a protein called OVALBUMIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	373	Total	C	N	O	P	S	0	0	0
			2816	1808	454	532	1	21			

- Molecule 3 is a protein called OVALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	374	Total	C	N	O	S	0	0	0
			2854	1832	469	531	22			
3	D	386	Total	C	N	O	S	0	0	0
			2924	1870	473	559	22			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

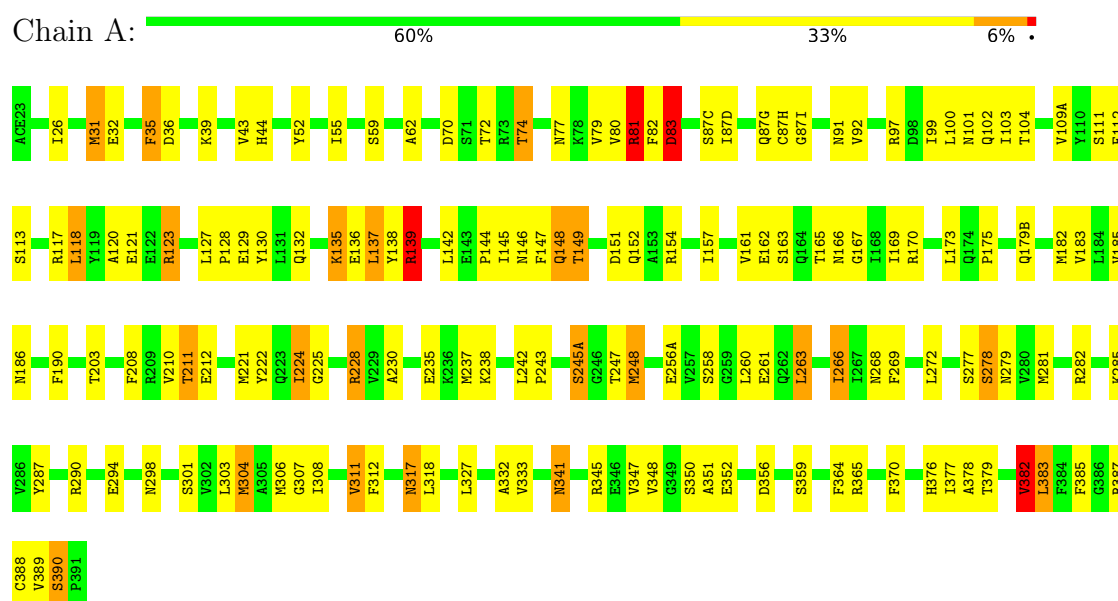
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	167	Total	O	0	0
			167	167		
6	B	156	Total	O	0	0
			156	156		
6	C	172	Total	O	0	0
			172	172		
6	D	183	Total	O	0	0
			183	183		

3 Residue-property plots

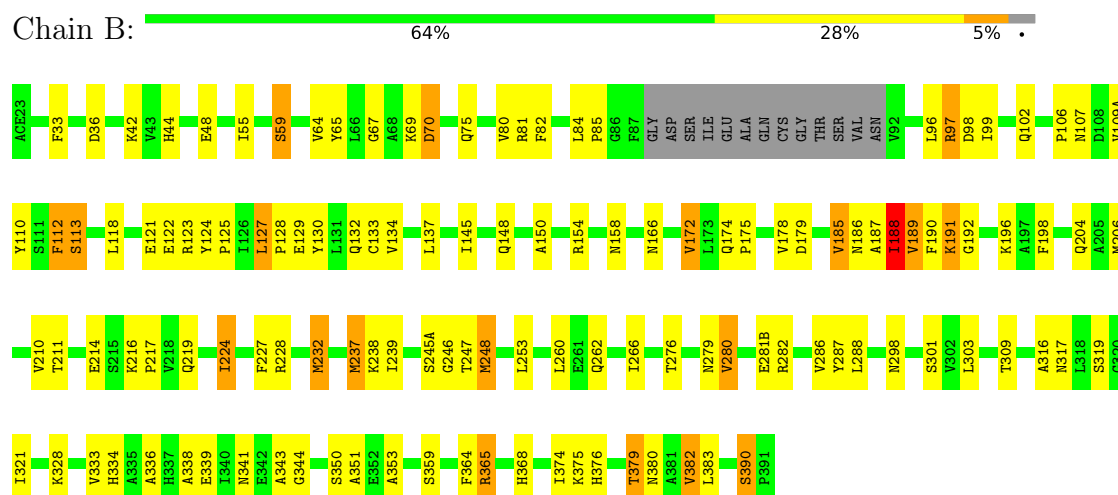
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: OVALBUMIN

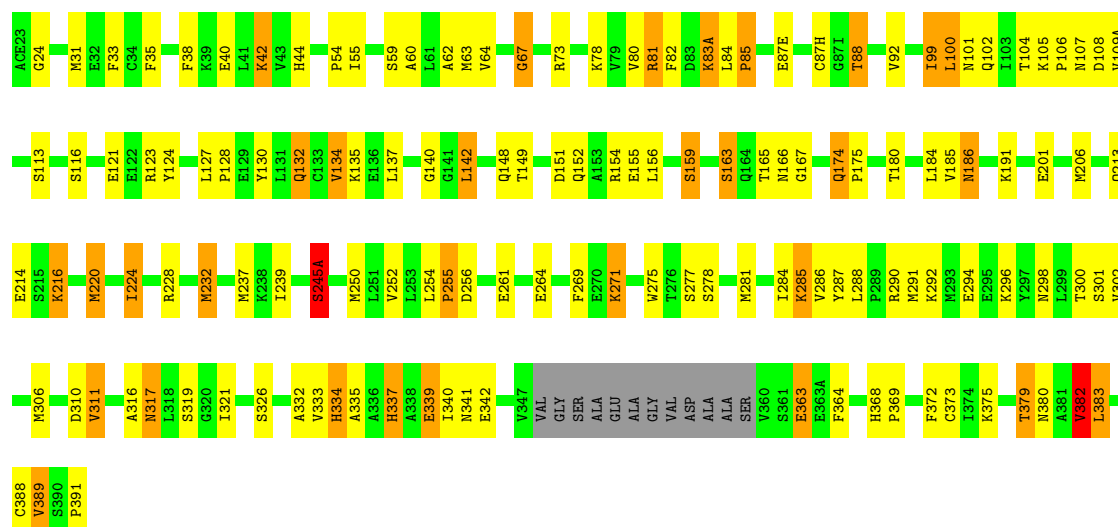


• Molecule 2: OVALBUMIN



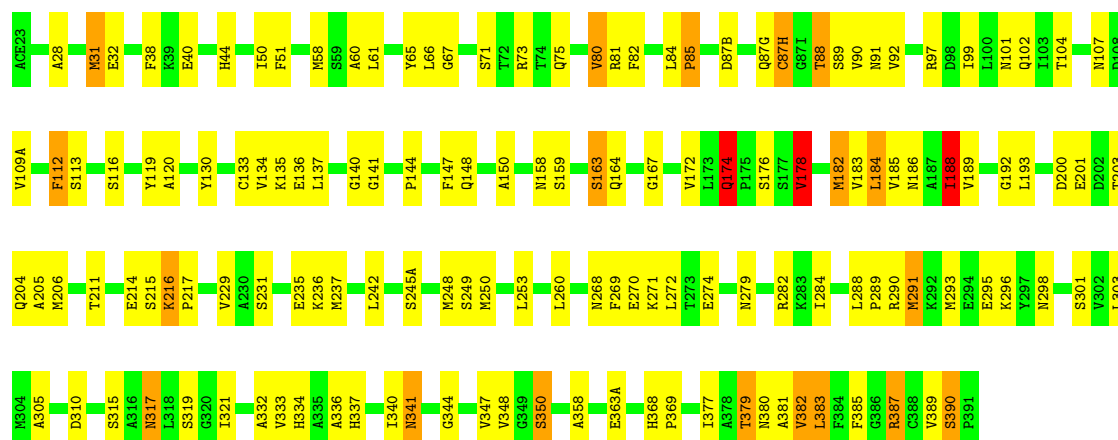
• Molecule 3: OVALBUMIN

Chain C: 



• Molecule 3: OVALBUMIN

Chain D: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.90Å 84.70Å 71.50Å 87.50° 104.00° 108.50°	Depositor
Resolution (Å)	(Not available) – 1.95	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.95)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12269	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, CA, NAG, ACE

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	1.44	17/2972 (0.6%)	2.17	112/4016 (2.8%)
2	B	1.43	14/2858 (0.5%)	2.07	95/3869 (2.5%)
3	C	1.51	17/2907 (0.6%)	2.13	104/3927 (2.6%)
3	D	1.50	22/2978 (0.7%)	2.12	106/4031 (2.6%)
All	All	1.47	70/11715 (0.6%)	2.12	417/15843 (2.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	C	0	1
All	All	0	2

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	192	GLY	N-CA	10.36	1.56	1.45
3	C	224	ILE	CA-CB	7.43	1.63	1.54
1	A	228	ARG	CD-NE	-7.38	1.35	1.46
3	D	192	GLY	N-CA	7.26	1.53	1.45
3	D	184	LEU	N-CA	6.68	1.54	1.46
3	D	337	HIS	CG-CD2	6.66	1.43	1.35
3	D	344	GLY	N-CA	6.66	1.52	1.45
1	A	203	THR	CA-CB	6.66	1.63	1.53
3	D	334	HIS	N-CA	6.42	1.54	1.46
3	D	368	HIS	N-CA	6.38	1.51	1.46
3	C	261	GLU	C-O	6.17	1.31	1.24
1	A	247	THR	CA-CB	6.17	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	36	ASP	N-CA	6.15	1.53	1.46
2	B	344	GLY	N-CA	6.14	1.51	1.45
3	D	206	MET	N-CA	5.99	1.51	1.45
3	C	340	ILE	N-CA	5.96	1.53	1.46
3	D	120	ALA	N-CA	5.88	1.53	1.46
1	A	32	GLU	N-CA	5.86	1.53	1.46
2	B	286	VAL	N-CA	5.84	1.53	1.46
1	A	364	PHE	N-CA	5.83	1.53	1.46
3	C	364	PHE	N-CA	5.78	1.53	1.46
2	B	186	ASN	N-CA	5.78	1.54	1.46
1	A	148	GLN	N-CA	5.76	1.53	1.46
3	C	302	VAL	CA-CB	5.70	1.61	1.54
3	C	287	TYR	CA-C	5.68	1.59	1.52
1	A	347	VAL	N-CA	5.68	1.52	1.46
3	C	286	VAL	N-CA	5.65	1.53	1.46
2	B	375	LYS	N-CA	5.64	1.52	1.45
1	A	145	ILE	CA-CB	5.61	1.61	1.55
2	B	224	ILE	CA-CB	5.59	1.60	1.54
3	C	379	THR	CA-CB	5.58	1.62	1.54
3	D	148	GLN	N-CA	5.54	1.52	1.46
3	D	245(A)	SER	N-CA	5.53	1.53	1.46
3	D	58	MET	CA-CB	5.50	1.61	1.53
3	C	214	GLU	N-CA	5.48	1.52	1.46
1	A	224	ILE	CA-CB	5.47	1.60	1.54
3	C	67	GLY	C-O	5.44	1.29	1.24
3	D	295	GLU	N-CA	5.39	1.52	1.45
2	B	336	ALA	N-CA	5.39	1.52	1.46
3	D	340	ILE	N-CA	5.38	1.53	1.46
3	D	109(A)	VAL	N-CA	5.38	1.51	1.46
2	B	334	HIS	ND1-CE1	5.37	1.38	1.32
3	D	188	ILE	N-CA	5.37	1.53	1.46
3	D	336	ALA	N-CA	5.34	1.52	1.46
3	C	149	THR	N-CA	5.28	1.52	1.46
3	C	332	ALA	N-CA	5.24	1.52	1.46
1	A	345	ARG	CD-NE	-5.24	1.39	1.46
3	D	178	VAL	N-CA	5.24	1.52	1.46
1	A	376	HIS	N-CA	5.24	1.52	1.46
3	D	249	SER	N-CA	5.23	1.52	1.45
2	B	334	HIS	N-CA	5.21	1.52	1.46
1	A	186	ASN	CA-C	5.19	1.58	1.53
3	D	159	SER	CA-CB	5.18	1.61	1.53
3	C	167	GLY	N-CA	5.18	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	113	SER	N-CA	5.18	1.52	1.46
2	B	98	ASP	N-CA	5.15	1.52	1.46
1	A	222	TYR	N-CA	5.15	1.52	1.46
3	C	373	CYS	N-CA	5.13	1.52	1.46
3	C	335	ALA	C-N	5.12	1.40	1.33
3	D	185	VAL	CA-C	5.12	1.58	1.52
1	A	385	PHE	N-CA	5.10	1.52	1.46
1	A	308	ILE	N-CA	5.09	1.52	1.46
3	C	33	PHE	CA-CB	5.09	1.61	1.53
2	B	188	ILE	N-CA	5.08	1.52	1.46
3	D	144	PRO	N-CA	5.07	1.52	1.46
2	B	276	THR	CA-CB	5.07	1.62	1.53
2	B	33	PHE	N-CA	5.06	1.52	1.46
1	A	333	VAL	N-CA	5.06	1.51	1.46
3	C	165	THR	CB-OG1	5.04	1.51	1.43
1	A	389	VAL	C-N	-5.00	1.29	1.33

All (417) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ARG	CD-NE-CZ	21.67	154.73	124.40
1	A	139	ARG	CD-NE-CZ	14.95	145.33	124.40
2	B	365	ARG	CD-NE-CZ	14.95	145.33	124.40
3	D	274	GLU	CA-CB-CG	14.82	143.75	114.10
1	A	228	ARG	CD-NE-CZ	13.71	143.59	124.40
3	C	214	GLU	CB-CG-CD	11.48	132.12	112.60
2	B	112	PHE	CA-CB-CG	10.92	124.72	113.80
2	B	279	ASN	CA-C-N	10.62	135.01	120.46
2	B	279	ASN	C-N-CA	10.62	135.01	120.46
2	B	228	ARG	CD-NE-CZ	10.59	139.22	124.40
1	A	282	ARG	NE-CZ-NH2	10.47	128.62	119.20
1	A	170	ARG	CD-NE-CZ	10.14	138.60	124.40
3	D	107	ASN	OD1-CG-ND2	9.95	132.55	122.60
2	B	210	VAL	N-CA-C	-9.51	101.48	110.42
3	C	44	HIS	CA-CB-CG	-9.33	104.47	113.80
3	D	112	PHE	CA-CB-CG	9.13	122.93	113.80
3	C	290	ARG	CD-NE-CZ	9.08	137.11	124.40
3	D	183	VAL	O-C-N	8.89	132.86	123.26
3	D	44	HIS	CA-CB-CG	-8.65	105.15	113.80
2	B	48	GLU	CA-CB-CG	8.63	131.36	114.10
2	B	189	VAL	O-C-N	8.52	132.21	123.10
3	D	298	ASN	OD1-CG-ND2	8.45	131.05	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	205	ALA	CA-C-O	-8.10	111.81	121.05
3	C	33	PHE	CA-CB-CG	-8.06	105.74	113.80
1	A	113	SER	CA-C-O	-8.02	111.72	120.30
3	C	123	ARG	CA-CB-CG	8.01	130.12	114.10
3	C	382	VAL	CB-CA-C	7.91	120.33	111.08
3	D	87(B)	ASP	CA-CB-CG	7.88	120.48	112.60
3	C	326	SER	O-C-N	7.87	132.54	122.39
1	A	277	SER	CA-C-O	7.86	129.96	121.16
3	C	108	ASP	CA-CB-CG	-7.80	104.80	112.60
3	C	317	ASN	OD1-CG-ND2	-7.78	114.82	122.60
1	A	139	ARG	CA-CB-CG	7.76	129.62	114.10
3	C	342	GLU	CB-CG-CD	7.64	125.59	112.60
3	C	300	THR	O-C-N	7.62	129.95	122.03
3	D	174	GLN	CB-CA-C	7.61	120.44	109.26
2	B	75	GLN	O-C-N	7.55	129.84	122.07
2	B	206	MET	O-C-N	7.52	126.52	121.71
1	A	117	ARG	NE-CZ-NH2	7.50	125.95	119.20
3	D	379	THR	CA-CB-OG1	-7.48	98.38	109.60
3	C	154	ARG	CD-NE-CZ	7.44	134.82	124.40
2	B	186	ASN	OD1-CG-ND2	7.44	130.04	122.60
2	B	64	VAL	N-CA-C	7.43	117.51	110.30
1	A	118	LEU	CA-C-N	7.42	132.32	122.30
1	A	118	LEU	C-N-CA	7.42	132.32	122.30
1	A	130	TYR	CA-C-O	-7.37	112.06	120.24
3	C	298	ASN	CA-CB-CG	-7.30	105.30	112.60
1	A	341	ASN	OD1-CG-ND2	-7.29	115.31	122.60
3	C	35	PHE	CA-CB-CG	-7.29	106.52	113.80
3	D	380	ASN	CA-CB-CG	-7.22	105.38	112.60
3	C	101	ASN	OD1-CG-ND2	-7.21	115.39	122.60
3	D	158	ASN	CA-CB-CG	7.11	119.71	112.60
1	A	31	MET	CA-C-N	-7.09	111.22	120.44
1	A	31	MET	C-N-CA	-7.09	111.22	120.44
3	D	80	VAL	N-CA-C	-7.06	103.02	113.39
3	D	382	VAL	CB-CA-C	7.05	119.49	110.96
1	A	307	GLY	CA-C-N	-7.03	114.23	122.95
1	A	307	GLY	C-N-CA	-7.03	114.23	122.95
2	B	280	VAL	N-CA-C	7.02	117.78	110.62
1	A	279	ASN	CA-C-N	7.00	131.67	120.82
1	A	279	ASN	C-N-CA	7.00	131.67	120.82
2	B	127	LEU	O-C-N	6.99	127.39	121.31
2	B	198	PHE	CA-CB-CG	6.99	120.79	113.80
1	A	81	ARG	CA-CB-CG	6.97	128.05	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	188	ILE	CB-CA-C	6.97	124.19	111.30
2	B	379	THR	CA-C-O	6.95	126.69	119.05
3	C	38	PHE	CA-CB-CG	-6.92	106.88	113.80
3	C	148	GLN	OE1-CD-NE2	6.89	129.49	122.60
2	B	154	ARG	CD-NE-CZ	6.89	134.04	124.40
3	C	73	ARG	CD-NE-CZ	6.88	134.03	124.40
1	A	135	LYS	N-CA-CB	6.88	120.04	110.07
3	C	166	ASN	CA-CB-CG	-6.85	105.75	112.60
2	B	353	ALA	O-C-N	6.84	129.37	122.12
2	B	185	VAL	CB-CA-C	6.81	120.28	110.33
1	A	287	TYR	O-C-N	6.81	131.17	123.27
1	A	298	ASN	OD1-CG-ND2	6.80	129.40	122.60
3	D	290	ARG	NE-CZ-NH2	6.77	125.30	119.20
1	A	81	ARG	CD-NE-CZ	6.76	133.87	124.40
1	A	290	ARG	NE-CZ-NH2	6.75	125.28	119.20
3	D	51	PHE	CA-C-O	-6.74	111.92	120.14
3	C	383	LEU	CA-C-O	-6.73	111.79	120.00
1	A	147	PHE	CA-CB-CG	6.72	120.53	113.80
1	A	228	ARG	CG-CD-NE	6.72	126.79	112.00
2	B	107	ASN	CA-C-N	-6.72	111.91	122.65
2	B	107	ASN	C-N-CA	-6.72	111.91	122.65
3	C	335	ALA	CA-C-O	6.69	128.35	120.66
1	A	44	HIS	CA-CB-CG	-6.69	107.11	113.80
2	B	166	ASN	CA-CB-CG	-6.67	105.93	112.60
3	D	174	GLN	OE1-CD-NE2	-6.65	115.95	122.60
2	B	382	VAL	CB-CA-C	6.64	118.86	111.08
3	D	136	GLU	CA-CB-CG	6.64	127.37	114.10
1	A	138	TYR	CB-CA-C	6.60	121.45	109.37
2	B	175	PRO	CA-C-N	6.59	134.08	123.93
2	B	175	PRO	C-N-CA	6.59	134.08	123.93
2	B	82	PHE	CA-CB-CG	6.58	120.39	113.80
2	B	245(A)	SER	CA-C-N	6.57	134.29	121.41
2	B	245(A)	SER	C-N-CA	6.57	134.29	121.41
3	D	279	ASN	CA-C-N	-6.56	114.83	122.63
3	D	279	ASN	C-N-CA	-6.56	114.83	122.63
3	C	389	VAL	N-CA-CB	-6.54	103.33	112.35
1	A	304	MET	CA-C-O	-6.51	113.65	120.55
1	A	179(B)	GLN	OE1-CD-NE2	6.49	129.09	122.60
1	A	157	ILE	O-C-N	6.49	128.62	121.94
3	D	82	PHE	CA-C-N	6.48	133.92	121.54
3	D	82	PHE	C-N-CA	6.48	133.92	121.54
3	D	159	SER	CA-CB-OG	-6.48	98.14	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	97	ARG	CG-CD-NE	6.47	126.24	112.00
3	D	90	VAL	CA-C-N	-6.47	111.87	122.54
3	D	90	VAL	C-N-CA	-6.47	111.87	122.54
1	A	370	PHE	CA-CB-CG	6.47	120.27	113.80
3	C	62	ALA	N-CA-C	-6.45	104.34	111.82
2	B	69	LYS	CB-CG-CD	6.44	126.11	111.30
3	C	113	SER	CA-C-O	-6.43	113.42	120.30
1	A	166	ASN	CA-CB-CG	-6.42	106.18	112.60
3	C	214	GLU	CA-C-N	6.42	133.21	122.87
3	C	214	GLU	C-N-CA	6.42	133.21	122.87
3	C	132	GLN	CA-C-O	6.42	127.56	120.82
1	A	345	ARG	CG-CD-NE	6.42	126.12	112.00
3	C	375	LYS	CA-C-O	6.39	128.93	121.46
1	A	82	PHE	N-CA-CB	6.38	121.13	110.41
1	A	345	ARG	NE-CZ-NH1	6.38	127.88	121.50
2	B	118	LEU	CA-C-O	-6.38	113.48	120.43
3	C	306	MET	CA-C-N	-6.35	112.12	122.40
3	C	306	MET	C-N-CA	-6.35	112.12	122.40
3	C	311	VAL	CA-CB-CG1	6.35	121.19	110.40
1	A	175	PRO	CA-C-N	6.34	131.36	122.36
1	A	175	PRO	C-N-CA	6.34	131.36	122.36
2	B	125	PRO	CB-CA-C	6.31	118.49	111.11
1	A	341	ASN	CB-CG-ND2	6.29	125.83	116.40
3	D	390	SER	CA-C-O	-6.28	113.19	120.34
2	B	316	ALA	CA-C-O	-6.27	114.30	121.19
2	B	303	LEU	O-C-N	6.26	129.29	122.15
1	A	294	GLU	CB-CG-CD	6.19	123.13	112.60
2	B	191	LYS	CA-C-N	-6.17	115.60	121.46
2	B	191	LYS	C-N-CA	-6.17	115.60	121.46
3	C	104	THR	CA-CB-OG1	-6.17	100.35	109.60
3	C	81	ARG	CG-CD-NE	6.15	125.54	112.00
3	C	237	MET	CA-C-O	6.15	128.03	121.45
3	C	186	ASN	CB-CG-ND2	6.14	125.61	116.40
3	C	152	GLN	CB-CG-CD	-6.13	102.18	112.60
2	B	288	LEU	O-C-N	6.11	128.36	121.94
3	D	205	ALA	O-C-N	6.10	130.21	123.01
3	C	255	PRO	CA-C-O	-6.09	114.24	121.67
3	D	107	ASN	CA-CB-CG	-6.08	106.52	112.60
2	B	298	ASN	CA-C-O	6.08	128.01	121.02
3	C	40	GLU	N-CA-C	6.08	117.58	111.07
3	D	385	PHE	CA-CB-CG	-6.05	107.75	113.80
2	B	298	ASN	OD1-CG-ND2	6.05	128.65	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	100	LEU	O-C-N	6.04	128.53	122.12
3	C	165	THR	CA-CB-CG2	6.04	120.77	110.50
3	C	379	THR	CA-C-O	6.03	125.69	119.05
2	B	328	LYS	CA-C-N	-6.03	114.83	122.37
2	B	328	LYS	C-N-CA	-6.03	114.83	122.37
2	B	390	SER	CA-C-O	-6.03	114.19	121.00
3	C	152	GLN	OE1-CD-NE2	6.00	128.60	122.60
3	D	66	LEU	CA-C-O	-6.00	114.16	120.63
1	A	129	GLU	CA-CB-CG	5.99	126.08	114.10
1	A	208	PHE	O-C-N	5.99	130.34	123.27
1	A	145	ILE	O-C-N	-5.97	117.77	122.97
3	D	214	GLU	CA-CB-CG	5.96	126.01	114.10
3	D	31	MET	CA-CB-CG	-5.94	102.21	114.10
3	C	382	VAL	CA-C-O	5.93	127.74	120.74
2	B	148	GLN	OE1-CD-NE2	5.93	128.53	122.60
2	B	132	GLN	N-CA-C	-5.93	104.73	111.07
3	D	101	ASN	CA-CB-CG	5.92	118.52	112.60
2	B	42	LYS	CA-C-N	5.91	128.09	120.70
2	B	42	LYS	C-N-CA	5.91	128.09	120.70
2	B	228	ARG	CB-CA-C	5.90	119.33	109.89
3	D	245(A)	SER	N-CA-CB	-5.90	100.60	110.39
1	A	282	ARG	NE-CZ-NH1	-5.89	115.61	121.50
3	C	326	SER	CA-C-O	-5.88	112.31	119.43
3	D	270	GLU	CB-CG-CD	5.85	122.55	112.60
3	C	337	HIS	CA-C-O	5.85	126.82	120.32
3	D	167	GLY	N-CA-C	-5.85	107.25	115.32
1	A	332	ALA	CB-CA-C	5.83	119.13	110.14
3	D	102	GLN	OE1-CD-NE2	-5.83	116.77	122.60
2	B	55	ILE	CA-CB-CG2	5.83	120.41	110.50
2	B	341	ASN	OD1-CG-ND2	-5.83	116.78	122.60
2	B	281(B)	GLU	CA-CB-CG	5.82	125.75	114.10
1	A	26	ILE	O-C-N	5.82	128.38	121.80
1	A	235	GLU	N-CA-C	-5.79	105.54	113.30
2	B	158	ASN	CA-CB-CG	5.78	118.38	112.60
1	A	390	SER	CA-C-O	-5.77	115.46	121.06
3	C	285	LYS	CA-C-N	-5.77	116.04	123.19
3	C	285	LYS	C-N-CA	-5.77	116.04	123.19
3	D	172	VAL	CB-CA-C	5.75	119.89	112.14
2	B	192	GLY	CA-C-O	5.74	126.64	121.47
3	D	104	THR	CA-C-N	5.74	128.46	120.65
3	D	104	THR	C-N-CA	5.74	128.46	120.65
2	B	123	ARG	CA-CB-CG	-5.74	102.63	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	CYS	CA-C-N	5.74	128.67	121.85
1	A	388	CYS	C-N-CA	5.74	128.67	121.85
3	D	61	LEU	CA-C-O	-5.73	113.62	120.10
1	A	221	MET	CA-C-O	-5.73	115.05	121.81
1	A	137	LEU	N-CA-C	-5.72	105.96	113.12
2	B	374	ILE	CA-C-N	-5.72	113.19	122.81
2	B	374	ILE	C-N-CA	-5.72	113.19	122.81
3	C	201	GLU	CB-CG-CD	5.72	122.33	112.60
3	C	254	LEU	CA-C-N	5.72	125.62	119.85
3	C	254	LEU	C-N-CA	5.72	125.62	119.85
2	B	309	THR	CA-CB-OG1	-5.72	101.02	109.60
3	D	50	ILE	CA-C-N	-5.72	111.92	121.64
3	D	50	ILE	C-N-CA	-5.72	111.92	121.64
3	C	281	MET	O-C-N	5.71	131.84	122.70
3	D	377	ILE	CA-C-O	-5.69	115.14	121.17
3	C	264	GLU	CA-C-N	5.69	128.22	120.54
3	C	264	GLU	C-N-CA	5.69	128.22	120.54
1	A	112	PHE	CA-C-O	-5.68	114.69	120.71
3	D	31	MET	CA-C-N	-5.66	112.26	120.29
3	D	31	MET	C-N-CA	-5.66	112.26	120.29
3	C	180	THR	CA-C-O	-5.65	114.48	120.92
1	A	327	LEU	O-C-N	5.64	129.96	123.02
3	D	231	SER	CB-CA-C	5.64	120.03	109.71
3	C	206	MET	O-C-N	5.63	125.76	121.65
3	D	333	VAL	O-C-N	5.63	129.12	123.10
3	C	167	GLY	N-CA-C	-5.63	107.33	115.27
1	A	139	ARG	NE-CZ-NH1	5.63	127.13	121.50
1	A	268	ASN	CA-C-O	-5.63	115.29	121.31
3	D	381	ALA	CA-C-N	-5.62	115.34	122.37
3	D	381	ALA	C-N-CA	-5.62	115.34	122.37
3	D	347	VAL	O-C-N	-5.62	117.13	123.03
1	A	101	ASN	OD1-CG-ND2	-5.62	116.98	122.60
3	C	300	THR	CA-C-O	-5.61	115.11	121.00
3	D	38	PHE	CA-C-N	5.61	127.79	120.28
3	D	38	PHE	C-N-CA	5.61	127.79	120.28
3	C	296	LYS	CA-C-O	-5.61	113.88	120.60
2	B	44	HIS	CA-CB-CG	-5.60	108.20	113.80
3	D	347	VAL	CB-CA-C	5.60	119.44	110.82
1	A	377	ILE	CA-C-N	5.60	127.72	120.44
1	A	377	ILE	C-N-CA	5.60	127.72	120.44
3	C	298	ASN	OD1-CG-ND2	5.59	128.19	122.60
1	A	104	THR	CA-CB-OG1	-5.58	101.23	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	311	VAL	N-CA-CB	5.58	122.77	111.05
3	D	216	LYS	CA-CB-CG	5.58	125.26	114.10
3	C	156	LEU	O-C-N	5.57	127.88	122.09
3	C	288	LEU	CB-CA-C	5.57	117.55	109.20
1	A	365	ARG	CD-NE-CZ	5.57	132.19	124.40
1	A	245(A)	SER	N-CA-C	5.57	121.30	113.56
3	C	88	THR	CA-C-N	5.56	130.27	120.87
3	C	88	THR	C-N-CA	5.56	130.27	120.87
3	D	284	ILE	O-C-N	5.55	129.10	123.00
1	A	111	SER	N-CA-CB	-5.55	102.06	110.77
3	D	40	GLU	N-CA-C	5.54	117.40	111.36
3	D	217	PRO	O-C-N	-5.54	116.45	123.10
3	C	339	GLU	CA-C-O	-5.54	114.35	120.38
3	D	147	PHE	CA-CB-CG	5.53	119.33	113.80
3	D	303	LEU	CA-C-N	-5.52	112.45	120.29
3	D	303	LEU	C-N-CA	-5.52	112.45	120.29
3	D	268	ASN	CA-C-O	-5.52	115.41	121.31
1	A	277	SER	CA-C-N	5.51	132.07	121.54
1	A	277	SER	C-N-CA	5.51	132.07	121.54
1	A	52	TYR	O-C-N	-5.51	116.76	123.10
2	B	248	MET	CA-C-O	-5.50	114.83	120.99
3	D	350	SER	O-C-N	5.49	127.94	122.12
3	D	172	VAL	O-C-N	-5.49	116.54	121.87
2	B	172	VAL	CB-CA-C	5.49	119.55	112.14
3	D	245(A)	SER	O-C-N	-5.48	115.09	122.43
3	D	347	VAL	CA-CB-CG2	5.47	119.69	110.40
3	D	363(A)	GLU	CA-CB-CG	5.46	125.02	114.10
3	D	310	ASP	O-C-N	5.46	127.90	122.12
1	A	123	ARG	CA-C-O	-5.45	113.94	120.10
1	A	248	MET	N-CA-CB	-5.45	102.07	111.55
3	D	282	ARG	CA-C-N	-5.45	114.02	122.09
3	D	282	ARG	C-N-CA	-5.45	114.02	122.09
3	D	332	ALA	CA-C-N	-5.45	115.36	122.94
3	D	332	ALA	C-N-CA	-5.45	115.36	122.94
1	A	35	PHE	CA-CB-CG	-5.45	108.35	113.80
1	A	112	PHE	O-C-N	5.45	130.12	123.21
1	A	318	LEU	N-CA-CB	-5.44	102.74	110.79
3	D	141	GLY	CA-C-O	5.44	128.69	121.51
1	A	62	ALA	CA-C-N	5.44	127.51	120.44
1	A	62	ALA	C-N-CA	5.44	127.51	120.44
1	A	152	GLN	O-C-N	5.44	127.96	122.09
3	D	319	SER	CA-C-O	5.43	126.07	119.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	82	PHE	N-CA-C	-5.42	106.16	112.89
3	C	256	ASP	CA-C-O	5.42	126.17	120.42
3	D	178	VAL	CA-C-O	-5.42	114.60	120.67
2	B	188	ILE	N-CA-CB	-5.41	102.49	111.36
2	B	260	LEU	CB-CA-C	5.40	121.05	110.67
3	C	159	SER	CB-CA-C	-5.39	101.69	110.85
3	C	216	LYS	CB-CA-C	5.39	117.28	109.20
1	A	378	ALA	O-C-N	5.38	127.62	122.07
1	A	303	LEU	N-CA-CB	-5.38	102.21	110.12
1	A	169	ILE	CA-C-N	5.38	131.53	122.87
1	A	169	ILE	C-N-CA	5.38	131.53	122.87
3	C	154	ARG	NE-CZ-NH1	5.37	126.87	121.50
3	D	200	ASP	O-C-N	5.37	127.81	122.12
3	D	242	LEU	CA-C-O	5.37	124.66	119.62
1	A	154	ARG	N-CA-C	-5.36	105.60	111.82
3	D	135	LYS	N-CA-C	-5.35	105.53	111.36
2	B	145	ILE	CA-C-O	5.34	125.47	121.09
2	B	204	GLN	O-C-N	5.34	129.24	123.10
3	C	310	ASP	CA-C-O	-5.34	114.07	120.10
3	D	58	MET	CA-CB-CG	-5.33	103.45	114.10
3	C	245(A)	SER	N-CA-C	5.32	119.61	113.38
3	D	215	SER	CA-C-O	-5.32	114.89	121.06
2	B	82	PHE	CA-C-N	5.32	127.67	120.38
2	B	82	PHE	C-N-CA	5.32	127.67	120.38
3	D	148	GLN	N-CA-C	-5.32	105.38	111.07
1	A	79	VAL	CA-C-O	-5.32	115.42	120.95
2	B	188	ILE	CB-CA-C	5.32	121.13	111.30
2	B	247	THR	O-C-N	5.31	129.38	122.42
3	C	107	ASN	OD1-CG-ND2	5.30	127.91	122.60
3	C	316	ALA	O-C-N	-5.30	116.70	123.06
1	A	186	ASN	CA-CB-CG	5.30	117.90	112.60
3	D	99	ILE	O-C-N	5.30	127.41	121.90
1	A	31	MET	CA-CB-CG	-5.29	103.51	114.10
2	B	65	TYR	CA-C-N	5.29	131.65	121.54
2	B	65	TYR	C-N-CA	5.29	131.65	121.54
3	D	305	ALA	CA-C-O	5.29	125.89	119.49
1	A	383	LEU	N-CA-CB	-5.29	102.30	110.13
3	D	271	LYS	N-CA-CB	5.29	117.89	110.12
1	A	382	VAL	N-CA-CB	5.29	117.03	111.00
1	A	347	VAL	CB-CA-C	5.28	119.14	110.69
3	C	64	VAL	CA-C-N	5.28	127.61	120.38
3	C	64	VAL	C-N-CA	5.28	127.61	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	363	GLU	N-CA-CB	5.27	117.72	109.97
3	C	388	CYS	CA-C-O	-5.27	115.06	120.54
3	C	134	VAL	CB-CA-C	5.26	120.31	112.16
3	C	261	GLU	N-CA-C	5.26	117.42	111.11
3	D	290	ARG	CA-CB-CG	5.26	124.61	114.10
2	B	129	GLU	CA-C-N	5.26	127.59	120.65
2	B	129	GLU	C-N-CA	5.26	127.59	120.65
2	B	343	ALA	N-CA-CB	5.26	117.73	109.69
3	D	201	GLU	CB-CG-CD	5.25	121.53	112.60
1	A	278	SER	CA-C-N	5.25	128.09	120.79
1	A	278	SER	C-N-CA	5.25	128.09	120.79
3	C	101	ASN	N-CA-C	-5.25	105.55	111.28
1	A	52	TYR	CA-C-O	5.24	127.06	121.45
3	D	317	ASN	OD1-CG-ND2	-5.24	117.36	122.60
3	D	229	VAL	CA-C-N	5.24	131.01	121.89
3	D	229	VAL	C-N-CA	5.24	131.01	121.89
2	B	364	PHE	CB-CA-C	5.24	119.23	111.17
1	A	317	ASN	OD1-CG-ND2	-5.22	117.38	122.60
3	C	142	LEU	CB-CA-C	5.22	118.37	109.75
1	A	135	LYS	CA-CB-CG	5.22	124.54	114.10
1	A	101	ASN	CB-CA-C	5.21	119.71	110.85
2	B	70	ASP	CA-C-N	5.21	127.26	120.28
2	B	70	ASP	C-N-CA	5.21	127.26	120.28
3	C	155	GLU	CA-C-N	5.21	127.58	120.54
3	C	155	GLU	C-N-CA	5.21	127.58	120.54
2	B	179	ASP	CA-C-O	5.20	126.51	121.05
1	A	345	ARG	NH1-CZ-NH2	-5.20	112.55	119.30
2	B	122	GLU	CA-C-O	5.20	125.77	119.38
3	C	154	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	A	352	GLU	N-CA-C	-5.19	105.63	111.28
2	B	376	HIS	O-C-N	5.18	129.13	123.22
3	C	317	ASN	O-C-N	5.18	129.06	122.84
3	C	364	PHE	N-CA-CB	-5.18	102.47	110.65
1	A	279	ASN	O-C-N	5.17	127.62	122.08
2	B	379	THR	N-CA-C	-5.17	106.99	113.72
2	B	210	VAL	CB-CA-C	5.17	118.54	111.87
2	B	113	SER	CA-C-O	-5.16	114.84	120.36
2	B	125	PRO	N-CA-C	-5.16	102.14	110.55
3	C	296	LYS	O-C-N	5.16	129.57	123.33
3	D	200	ASP	N-CA-CB	5.16	117.70	110.12
3	D	358	ALA	N-CA-C	5.16	116.90	111.28
3	D	387	ARG	NE-CZ-NH1	5.16	126.66	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	293	MET	CA-C-O	-5.15	114.76	120.38
2	B	247	THR	CA-C-O	-5.14	113.28	119.15
3	D	87(H)	CYS	N-CA-CB	5.14	118.47	109.72
3	C	245(A)	SER	CA-CB-OG	-5.14	100.82	111.10
3	D	368	HIS	CA-C-O	-5.14	116.24	120.71
1	A	221	MET	O-C-N	5.14	128.71	122.85
3	D	88	THR	CA-C-N	5.13	128.05	120.82
3	D	88	THR	C-N-CA	5.13	128.05	120.82
3	C	113	SER	O-C-N	5.13	129.22	123.27
3	C	290	ARG	CA-C-N	-5.12	114.43	122.73
3	C	290	ARG	C-N-CA	-5.12	114.43	122.73
1	A	182	MET	CB-CA-C	5.12	118.51	109.80
1	A	210	VAL	N-CA-C	-5.12	105.72	110.53
2	B	59	SER	CA-C-O	-5.11	115.00	120.42
1	A	261	GLU	CA-C-N	-5.11	113.43	120.28
1	A	261	GLU	C-N-CA	-5.11	113.43	120.28
3	C	87(E)	GLU	CG-CD-OE2	-5.11	106.65	118.40
2	B	187	ALA	CA-C-N	-5.11	114.23	122.25
2	B	187	ALA	C-N-CA	-5.11	114.23	122.25
1	A	83	ASP	CA-CB-CG	-5.10	107.50	112.60
3	D	291	MET	CA-C-N	-5.10	115.58	122.77
3	D	291	MET	C-N-CA	-5.10	115.58	122.77
3	C	333	VAL	CA-C-N	-5.09	115.97	123.00
3	C	333	VAL	C-N-CA	-5.09	115.97	123.00
3	C	123	ARG	CB-CG-CD	5.09	123.01	111.30
3	D	211	THR	CA-CB-OG1	-5.09	101.97	109.60
3	C	185	VAL	O-C-N	5.08	128.32	123.14
3	D	203	THR	CA-CB-OG1	-5.08	101.98	109.60
1	A	144	PRO	CB-CA-C	5.08	117.89	110.63
2	B	338	ALA	CA-C-O	5.08	126.53	120.28
3	D	182	MET	CB-CA-C	5.08	119.73	109.68
3	D	85	PRO	CB-CA-C	5.08	117.60	111.46
3	D	186	ASN	OD1-CG-ND2	5.08	127.67	122.60
1	A	290	ARG	CA-CB-CG	5.07	124.25	114.10
1	A	149	THR	CB-CA-C	5.07	118.47	109.65
3	C	213	GLN	CA-C-N	-5.07	114.94	122.74
3	C	213	GLN	C-N-CA	-5.07	114.94	122.74
3	C	334	HIS	ND1-CE1-NE2	-5.07	103.33	108.40
1	A	165	THR	OG1-CB-CG2	5.06	119.42	109.30
1	A	225	GLY	CA-C-N	5.06	129.53	121.99
1	A	225	GLY	C-N-CA	5.06	129.53	121.99
1	A	263	LEU	CA-C-O	5.05	125.91	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	228	ARG	CA-C-O	5.05	126.62	120.81
3	D	205	ALA	N-CA-C	-5.05	102.22	110.20
2	B	379	THR	CA-CB-OG1	-5.05	102.03	109.60
3	C	220	MET	CB-CA-C	5.05	118.36	110.19
1	A	365	ARG	NE-CZ-NH1	5.04	126.54	121.50
2	B	282	ARG	CA-CB-CG	5.04	124.18	114.10
3	C	42	LYS	CB-CA-C	5.04	119.95	110.63
2	B	280	VAL	N-CA-CB	-5.04	103.69	110.54
2	B	343	ALA	CA-C-N	-5.04	112.51	121.93
2	B	343	ALA	C-N-CA	-5.04	112.51	121.93
2	B	282	ARG	N-CA-CB	-5.03	102.79	111.55
1	A	312	PHE	O-C-N	5.03	128.62	122.34
2	B	174	GLN	O-C-N	5.03	127.87	121.34
1	A	345	ARG	N-CA-C	5.01	117.85	111.69
3	C	35	PHE	CA-C-N	-5.01	113.56	120.28
3	C	35	PHE	C-N-CA	-5.01	113.56	120.28
1	A	208	PHE	CA-C-O	-5.01	114.81	120.32

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87(I)	GLY	Peptide
3	C	245(A)	SER	Peptide

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	2940	0	2906	57	0
2	B	2816	0	2751	40	0
3	C	2854	0	2812	51	0
3	D	2924	0	2865	37	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	12	0	0
4	D	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
6	A	167	0	0	8	0
6	B	156	0	0	6	0
6	C	172	0	0	0	0
6	D	183	0	0	4	0
All	All	12269	0	11385	182	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 (182) 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)
3:C:174:GLN:HE21	3:C:174:GLN:H	1.13	0.97
3:D:248:MET:HE3	3:D:383:LEU:HD23	1.52	0.90
1:A:139:ARG:HH11	1:A:139:ARG:HB3	1.46	0.81
1:A:31:MET:HE3	1:A:269:PHE:HD1	1.49	0.78
1:A:230:ALA:HB2	1:A:281:MET:HG2	1.67	0.76
2:B:239:ILE:HD12	2:B:253:LEU:HG	1.68	0.75
3:C:109(A):VAL:HG21	3:C:245(A):SER:HB2	1.67	0.75
1:A:77:ASN:HD21	1:A:83:ASP:HA	1.52	0.72
1:A:87(D):ILE:HD11	1:A:91:ASN:HB2	1.73	0.71
3:C:55:ILE:HG12	3:C:99:ILE:HD12	1.73	0.69
3:D:31:MET:HE3	3:D:269:PHE:HD1	1.59	0.68
3:D:87(H):CYS:HA	3:D:92:VAL:HG21	1.74	0.68
1:A:99:ILE:HD11	1:A:379:THR:HG21	1.76	0.68
1:A:31:MET:HE3	1:A:269:PHE:CD1	2.28	0.68
1:A:120:ALA:HB2	1:A:142:LEU:HD21	1.75	0.67
3:C:24:GLY:HA2	3:C:83(A):LYS:HD3	1.76	0.67
3:C:31:MET:HE3	3:C:269:PHE:HD1	1.63	0.64
1:A:80:VAL:O	1:A:81:ARG:HB2	1.98	0.64
1:A:256(A):GLU:C	1:A:258:SER:H	2.07	0.62
1:A:31:MET:HE1	1:A:272:LEU:HD23	1.83	0.61
3:C:255:PRO:O	3:C:368:HIS:HE1	1.83	0.61
1:A:162:GLU:HG3	1:A:167:GLY:HA2	1.84	0.60
3:C:271:LYS:HE2	3:C:271:LYS:HA	1.82	0.60
3:C:87(H):CYS:HA	3:C:92:VAL:HG21	1.84	0.60
3:C:132:GLN:O	3:C:135:LYS:HG3	2.02	0.59
3:C:174:GLN:HB2	3:C:175:PRO:HD2	1.84	0.58
3:C:59:SER:HB2	3:C:100:LEU:HD11	1.86	0.58
3:C:174:GLN:H	3:C:174:GLN:NE2	1.93	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:LYS:HE3	6:B:488:HOH:O	2.04	0.57
2:B:232:MET:HE1	2:B:239:ILE:HG12	1.85	0.57
1:A:224:ILE:HG21	1:A:356:ASP:HB3	1.86	0.56
1:A:139:ARG:HE	2:B:106:PRO:HB2	1.70	0.56
3:C:83(A):LYS:HD2	3:C:83(A):LYS:C	2.31	0.56
3:C:121:GLU:HB3	3:C:124:TYR:CE2	2.40	0.55
1:A:173:LEU:HD11	1:A:183:VAL:HG11	1.88	0.55
1:A:263:LEU:HA	1:A:266:ILE:HD13	1.88	0.55
1:A:70:ASP:O	1:A:74:THR:HG23	2.07	0.54
1:A:99:ILE:O	1:A:103:ILE:HG12	2.07	0.54
3:C:250:MET:HE1	3:C:291:MET:HE1	1.88	0.54
2:B:379:THR:O	2:B:380:ASN:HB2	2.07	0.53
3:C:31:MET:HG2	3:C:382:VAL:HG12	1.89	0.53
3:C:191:LYS:HD3	3:D:163:SER:HA	1.91	0.53
1:A:224:ILE:HG12	1:A:285:LYS:HG2	1.90	0.53
3:D:112:PHE:HD1	3:D:188:ILE:HD11	1.72	0.53
2:B:59:SER:HA	2:B:96:LEU:HD21	1.90	0.53
3:C:54:PRO:HG2	3:C:382:VAL:HG22	1.91	0.53
1:A:190:PHE:CE1	1:A:248:MET:HE1	2.44	0.53
2:B:219:GLN:NE2	2:B:219:GLN:HA	2.23	0.52
1:A:237:MET:HE1	1:A:263:LEU:HD13	1.92	0.52
1:A:258:SER:HA	6:A:617:HOH:O	2.10	0.52
3:D:28:ALA:O	3:D:32:GLU:HG3	2.10	0.52
2:B:317:ASN:C	2:B:317:ASN:HD22	2.18	0.51
1:A:97:ARG:HD2	1:A:137:LEU:HB3	1.93	0.51
1:A:256(A):GLU:C	1:A:258:SER:N	2.69	0.51
3:D:260:LEU:HD22	3:D:369:PRO:HB2	1.92	0.51
3:C:317:ASN:C	3:C:317:ASN:HD22	2.19	0.50
3:C:228:ARG:NH2	3:C:278:SER:HA	2.26	0.50
3:C:292:LYS:HG3	3:C:339:GLU:HG2	1.92	0.50
3:D:188:ILE:HD13	3:D:189:VAL:N	2.27	0.50
1:A:139:ARG:HB3	1:A:139:ARG:NH1	2.21	0.50
3:C:116:SER:O	3:C:140:GLY:HA3	2.12	0.50
2:B:262:GLN:O	2:B:266:ILE:HG23	2.12	0.50
1:A:72:THR:HG23	1:A:311:VAL:HG13	1.94	0.49
3:D:116:SER:O	3:D:140:GLY:HA3	2.13	0.49
3:D:288:LEU:HD12	3:D:289:PRO:HD2	1.94	0.49
1:A:59:SER:CB	1:A:100:LEU:HD11	2.42	0.49
1:A:31:MET:HG2	1:A:382:VAL:HG12	1.94	0.49
3:C:224:ILE:HG12	3:C:285:LYS:HG2	1.94	0.48
3:D:150:ALA:HB1	3:D:178:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109(A):VAL:HG21	1:A:245(A):SER:HB2	1.94	0.48
2:B:127:LEU:HA	2:B:128:PRO:HD3	1.70	0.48
2:B:237:MET:HE1	2:B:253:LEU:HD23	1.95	0.48
3:C:228:ARG:HH22	3:C:278:SER:HA	1.78	0.48
1:A:190:PHE:CZ	1:A:248:MET:HE1	2.49	0.48
1:A:139:ARG:NH2	6:A:531:HOH:O	2.46	0.48
2:B:216:LYS:HA	2:B:217:PRO:HD2	1.55	0.48
3:C:317:ASN:HD22	3:C:319:SER:H	1.61	0.47
1:A:87(H):CYS:HA	1:A:92:VAL:HG21	1.95	0.47
3:C:239:ILE:HD12	3:C:275:TRP:HB3	1.96	0.47
2:B:188:ILE:HD13	2:B:189:VAL:N	2.29	0.47
2:B:109(A):VAL:HG23	2:B:110:TYR:CD2	2.49	0.47
3:C:127:LEU:HA	3:C:128:PRO:HD3	1.75	0.47
3:D:84:LEU:HA	3:D:85:PRO:HD3	1.74	0.47
3:D:164:GLN:NE2	6:D:413:HOH:O	2.47	0.47
3:D:250:MET:HE1	3:D:291:MET:HE1	1.97	0.47
3:C:250:MET:HE2	3:C:252:VAL:HG22	1.97	0.46
3:D:71:SER:O	3:D:75:GLN:HG3	2.16	0.46
1:A:211:THR:OG1	1:A:212:GLU:N	2.47	0.46
3:C:294:GLU:HG3	3:C:337:HIS:HB2	1.97	0.46
2:B:80:VAL:O	2:B:81:ARG:HB2	2.14	0.46
3:C:220:MET:HE2	3:C:220:MET:HB2	1.82	0.46
3:D:236:LYS:HD2	6:D:572:HOH:O	2.15	0.46
2:B:317:ASN:ND2	2:B:319:SER:OG	2.47	0.46
3:D:112:PHE:CD1	3:D:188:ILE:HD11	2.49	0.46
1:A:348:VAL:HG21	6:A:555:HOH:O	2.15	0.46
3:D:97:ARG:HD2	3:D:137:LEU:HB3	1.98	0.46
1:A:36:ASP:HB3	1:A:306:MET:HE3	1.97	0.46
2:B:150:ALA:HB1	2:B:178:VAL:HG12	1.97	0.46
3:C:81:ARG:C	3:C:83(A):LYS:HZ3	2.23	0.46
1:A:132:GLN:HA	1:A:135:LYS:HE3	1.98	0.45
2:B:121:GLU:HB3	2:B:124:TYR:CE2	2.51	0.45
2:B:112:PHE:HD2	2:B:188:ILE:HD11	1.81	0.45
3:C:83(A):LYS:HZ2	3:C:83(A):LYS:HG3	1.51	0.45
3:D:87(G):GLN:O	3:D:87(H):CYS:C	2.60	0.45
2:B:84:LEU:HA	2:B:85:PRO:HD3	1.85	0.45
3:C:239:ILE:CD1	3:C:275:TRP:HB3	2.47	0.45
3:D:130:TYR:O	3:D:133:CYS:HB3	2.15	0.45
3:D:89:SER:C	3:D:91:ASN:H	2.23	0.45
3:C:130:TYR:CZ	3:C:134:VAL:HG11	2.52	0.45
1:A:35:PHE:O	1:A:39:LYS:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256(A):GLU:O	1:A:258:SER:N	2.51	0.44
2:B:191:LYS:HD3	2:B:339:GLU:HB3	1.99	0.44
3:C:232:MET:HE3	3:C:232:MET:HB2	1.87	0.44
2:B:190:PHE:CE1	2:B:248:MET:HE1	2.52	0.44
3:C:105:LYS:HA	3:C:106:PRO:HD3	1.89	0.44
3:D:317:ASN:C	3:D:317:ASN:HD22	2.25	0.44
2:B:351:ALA:HB2	6:B:532:HOH:O	2.17	0.44
3:D:174:GLN:CD	3:D:174:GLN:H	2.26	0.44
1:A:127:LEU:HA	1:A:128:PRO:HD2	1.64	0.44
1:A:135:LYS:HD2	1:A:136:GLU:N	2.33	0.43
1:A:242:LEU:HA	1:A:243:PRO:HD3	1.85	0.43
2:B:81:ARG:HD3	6:B:521:HOH:O	2.16	0.43
2:B:287:TYR:HB2	2:B:365:ARG:HA	2.00	0.43
3:C:67:GLY:HA3	3:C:321:ILE:HG13	2.00	0.43
1:A:161:VAL:HG21	1:A:185:VAL:HG11	1.99	0.43
1:A:238:LYS:HD3	6:A:624:HOH:O	2.19	0.43
1:A:121:GLU:OE2	1:A:148:GLN:N	2.46	0.43
3:C:109(A):VAL:CG2	3:C:245(A):SER:HB2	2.44	0.43
3:D:235:GLU:HB2	3:D:237:MET:HG2	1.99	0.43
1:A:351:ALA:HA	6:A:641:HOH:O	2.18	0.43
3:C:379:THR:O	3:C:380:ASN:HB2	2.18	0.43
3:D:119:TYR:O	3:D:182:MET:HA	2.18	0.43
1:A:146:ASN:ND2	1:A:149:THR:OG1	2.52	0.43
3:D:341:ASN:C	3:D:341:ASN:HD22	2.27	0.43
3:D:387:ARG:HD3	3:D:389:VAL:CG2	2.48	0.43
1:A:317:ASN:HD22	1:A:317:ASN:C	2.26	0.42
2:B:219:GLN:HA	2:B:219:GLN:HE21	1.84	0.42
3:C:80:VAL:O	3:C:81:ARG:HB2	2.19	0.42
2:B:196:LYS:HD2	2:B:227:PHE:CE1	2.54	0.42
3:C:102:GLN:HA	3:C:105:LYS:CE	2.49	0.42
1:A:59:SER:HB3	1:A:100:LEU:HD11	2.01	0.42
3:D:237:MET:HE1	3:D:253:LEU:HD23	2.01	0.42
3:D:348:VAL:HG21	6:D:455:HOH:O	2.19	0.42
2:B:214:GLU:HG3	3:D:379:THR:HA	2.00	0.42
3:D:237:MET:HE3	3:D:237:MET:HB2	1.93	0.42
3:D:80:VAL:O	3:D:81:ARG:HB2	2.18	0.42
3:C:60:ALA:HB1	3:C:184:LEU:HD11	2.01	0.42
3:D:31:MET:HE1	3:D:272:LEU:HD23	2.02	0.42
3:C:159:SER:O	3:C:163:SER:HB2	2.20	0.42
3:D:204:GLN:HG2	6:D:424:HOH:O	2.18	0.42
1:A:77:ASN:HD21	1:A:83:ASP:CA	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:ARG:HD2	2:B:137:LEU:HB3	2.00	0.42
3:D:65:TYR:CE1	3:D:73:ARG:HG3	2.55	0.42
3:C:271:LYS:HD3	3:C:275:TRP:CZ2	2.54	0.42
3:C:284:ILE:HG13	3:C:363:GLU:HB2	2.02	0.42
3:D:67:GLY:HA3	3:D:321:ILE:HG13	2.02	0.42
2:B:224:ILE:HB	6:B:454:HOH:O	2.19	0.42
1:A:87(G):GLN:O	1:A:87(H):CYS:C	2.63	0.41
3:C:84:LEU:HA	3:C:85:PRO:HD3	1.95	0.41
1:A:81:ARG:HH11	1:A:81:ARG:HG3	1.86	0.41
1:A:121:GLU:OE1	1:A:123:ARG:HG3	2.21	0.41
2:B:368:HIS:HD2	6:B:444:HOH:O	2.04	0.41
2:B:130:TYR:CE2	2:B:134:VAL:HG21	2.56	0.41
1:A:118:LEU:O	1:A:142:LEU:HA	2.21	0.41
2:B:113:SER:O	2:B:188:ILE:HA	2.21	0.41
3:C:78:LYS:HD3	3:C:78:LYS:HA	1.93	0.41
2:B:67:GLY:HA3	2:B:321:ILE:HG13	2.03	0.41
2:B:232:MET:HE2	2:B:232:MET:HB2	1.83	0.41
3:C:142:LEU:C	3:C:142:LEU:HD23	2.46	0.41
1:A:139:ARG:HG2	6:A:637:HOH:O	2.21	0.40
1:A:260:LEU:HD21	1:A:387:ARG:HG3	2.03	0.40
1:A:278:SER:HB3	6:A:642:HOH:O	2.21	0.40
2:B:102:GLN:NE2	6:B:469:HOH:O	2.53	0.40
2:B:219:GLN:HE21	2:B:219:GLN:CA	2.34	0.40
3:D:60:ALA:HB1	3:D:184:LEU:HD11	2.04	0.40
1:A:102:GLN:NE2	6:A:573:HOH:O	2.53	0.40
2:B:130:TYR:O	2:B:134:VAL:HG23	2.22	0.40
2:B:219:GLN:NE2	2:B:219:GLN:CA	2.85	0.40
3:C:60:ALA:HA	3:C:63:MET:HE2	2.02	0.40
3:C:186:ASN:O	3:C:334:HIS:HA	2.21	0.40
3:C:250:MET:HE3	3:C:372:PHE:HB2	2.03	0.40
2:B:133:CYS:O	2:B:137:LEU:HG	2.21	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	382/386 (99%)	358 (94%)	22 (6%)	2 (0%)	24	16
2	B	368/386 (95%)	349 (95%)	18 (5%)	1 (0%)	36	28
3	C	370/386 (96%)	356 (96%)	12 (3%)	2 (0%)	24	16
3	D	384/386 (100%)	369 (96%)	15 (4%)	0	100	100
All	All	1504/1544 (97%)	1432 (95%)	67 (4%)	5 (0%)	36	28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	ASP
2	B	246	GLY
3	C	88	THR
1	A	43	VAL
3	C	85	PRO

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	308/329 (94%)	291 (94%)	17 (6%)	19	8
2	B	293/330 (89%)	278 (95%)	15 (5%)	21	10
3	C	300/331 (91%)	281 (94%)	19 (6%)	16	6
3	D	310/331 (94%)	293 (94%)	17 (6%)	19	8
All	All	1211/1321 (92%)	1143 (94%)	68 (6%)	19	8

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ILE
1	A	74	THR
1	A	81	ARG

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Mol	Chain	Res	Type
1	A	139	ARG
1	A	151	ASP
1	A	163	SER
1	A	211	THR
1	A	228	ARG
1	A	266	ILE
1	A	301	SER
1	A	304	MET
1	A	311	VAL
1	A	341	ASN
1	A	359	SER
1	A	382	VAL
1	A	383	LEU
1	A	390	SER
2	B	70	ASP
2	B	99	ILE
2	B	172	VAL
2	B	185	VAL
2	B	188	ILE
2	B	211	THR
2	B	232	MET
2	B	237	MET
2	B	280	VAL
2	B	301	SER
2	B	333	VAL
2	B	359	SER
2	B	382	VAL
2	B	383	LEU
2	B	390	SER
3	C	42	LYS
3	C	83(A)	LYS
3	C	99	ILE
3	C	137	LEU
3	C	151	ASP
3	C	163	SER
3	C	174	GLN
3	C	216	LYS
3	C	232	MET
3	C	271	LYS
3	C	277	SER
3	C	301	SER
3	C	311	VAL

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Mol	Chain	Res	Type
3	C	341	ASN
3	C	369	PRO
3	C	382	VAL
3	C	383	LEU
3	C	389	VAL
3	C	391	PRO
3	D	88	THR
3	D	134	VAL
3	D	163	SER
3	D	174	GLN
3	D	176	SER
3	D	178	VAL
3	D	188	ILE
3	D	193	LEU
3	D	216	LYS
3	D	296	LYS
3	D	301	SER
3	D	315	SER
3	D	341	ASN
3	D	350	SER
3	D	382	VAL
3	D	383	LEU
3	D	390	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	101	ASN
1	A	317	ASN
1	A	341	ASN
2	B	102	GLN
2	B	171	ASN
2	B	317	ASN
3	C	101	ASN
3	C	132	GLN
3	C	164	GLN
3	C	166	ASN
3	C	171	ASN
3	C	174	GLN
3	C	317	ASN
3	C	341	ASN

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Mol	Chain	Res	Type
3	C	368	HIS
3	C	380	ASN
3	D	47	ASN
3	D	174	GLN
3	D	219	GLN
3	D	223	GLN
3	D	317	ASN
3	D	341	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	SEP	A	350	1	8,9,10	1.19	1 (12%)	7,12,14	2.36	3 (42%)
1	SEP	A	87(C)	1	8,9,10	1.29	1 (12%)	7,12,14	2.22	3 (42%)
2	SEP	B	350	2	8,9,10	1.28	1 (12%)	7,12,14	2.50	3 (42%)

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	SEP	A	350	1	-	1/6/8/10	-
1	SEP	A	87(C)	1	-	1/6/8/10	-
2	SEP	B	350	2	-	0/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	SEP	P-OG	-2.30	1.53	1.60
1	A	87(C)	SEP	P-OG	-2.14	1.53	1.60
2	B	350	SEP	P-O2P	-2.03	1.47	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87(C)	SEP	O3P-P-OG	4.48	118.34	106.67
1	A	350	SEP	O3P-P-OG	4.40	118.14	106.67
2	B	350	SEP	O2P-P-OG	4.08	117.30	106.67
2	B	350	SEP	O3P-P-OG	3.74	116.41	106.67
2	B	350	SEP	OG-P-O1P	-3.20	97.80	106.44
1	A	350	SEP	OG-P-O1P	-3.08	98.11	106.44
1	A	350	SEP	O2P-P-OG	2.54	113.28	106.67
1	A	87(C)	SEP	OG-CB-CA	2.43	110.51	108.14
1	A	87(C)	SEP	OG-P-O1P	-2.14	100.65	106.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	87(C)	SEP	CA-CB-OG-P
1	A	350	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	393	2	14,14,15	1.60	3 (21%)	17,19,21	2.22	6 (35%)
4	NAG	C	393	3	14,14,15	1.49	3 (21%)	17,19,21	1.88	4 (23%)
4	NAG	A	393	1	14,14,15	1.84	4 (28%)	17,19,21	1.93	4 (23%)
4	NAG	D	393	3	14,14,15	1.35	1 (7%)	17,19,21	1.67	6 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	393	2	-	0/6/23/26	0/1/1/1
4	NAG	C	393	3	-	1/6/23/26	0/1/1/1
4	NAG	A	393	1	-	2/6/23/26	0/1/1/1
4	NAG	D	393	3	-	1/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	393	NAG	O7-C7	-4.34	1.13	1.23
4	B	393	NAG	O7-C7	-4.11	1.14	1.23
4	D	393	NAG	O7-C7	-3.52	1.15	1.23
4	C	393	NAG	O7-C7	-2.95	1.16	1.23
4	A	393	NAG	O5-C5	-2.75	1.38	1.43
4	A	393	NAG	C2-N2	2.62	1.50	1.46
4	C	393	NAG	C2-N2	2.54	1.50	1.46
4	A	393	NAG	C1-C2	-2.48	1.49	1.52
4	C	393	NAG	O3-C3	-2.24	1.37	1.43
4	B	393	NAG	C2-N2	2.21	1.49	1.46
4	B	393	NAG	C1-C2	-2.05	1.49	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	393	NAG	C1-O5-C5	-5.26	105.14	112.19
4	A	393	NAG	C2-N2-C7	-4.84	116.42	122.90
4	A	393	NAG	C1-O5-C5	4.34	118.00	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	393	NAG	O5-C5-C4	-4.00	101.10	110.83
4	C	393	NAG	C8-C7-N2	-3.33	110.60	116.12
4	C	393	NAG	C1-C2-N2	-3.30	105.23	110.43
4	B	393	NAG	O3-C3-C2	-3.25	102.64	109.40
4	B	393	NAG	C4-C3-C2	-3.21	106.32	111.02
4	C	393	NAG	C3-C4-C5	-2.95	104.88	110.23
4	B	393	NAG	O5-C5-C4	-2.95	103.66	110.83
4	B	393	NAG	C2-N2-C7	-2.76	119.20	122.90
4	D	393	NAG	C8-C7-N2	-2.74	111.58	116.12
4	D	393	NAG	O7-C7-N2	-2.68	117.24	121.98
4	D	393	NAG	C1-O5-C5	-2.62	108.67	112.19
4	D	393	NAG	O5-C5-C4	-2.31	105.20	110.83
4	A	393	NAG	O4-C4-C5	-2.13	104.08	109.32
4	B	393	NAG	C1-C2-N2	-2.09	107.14	110.43
4	A	393	NAG	O3-C3-C2	-2.06	105.11	109.40
4	D	393	NAG	O3-C3-C2	-2.01	105.22	109.40
4	D	393	NAG	C1-C2-N2	-2.00	107.28	110.43

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	393	NAG	C4-C5-C6-O6
4	D	393	NAG	O7-C7-N2-C2
4	A	393	NAG	O5-C5-C6-O6
4	C	393	NAG	O7-C7-N2-C2

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

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.