



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:06 PM GMT

PDB ID : 1OVA  
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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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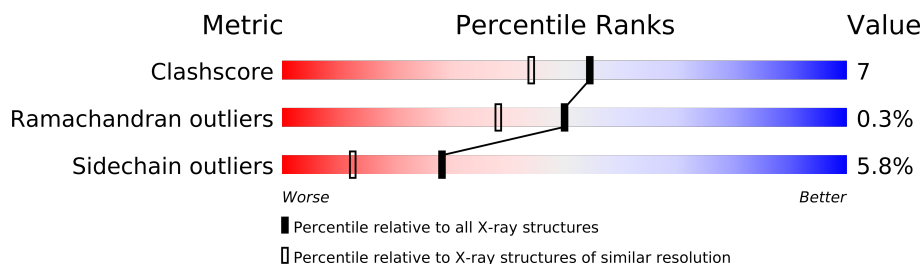
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	386	
2	B	386	
3	C	386	
3	D	386	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12269 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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 (three-letter code: 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		

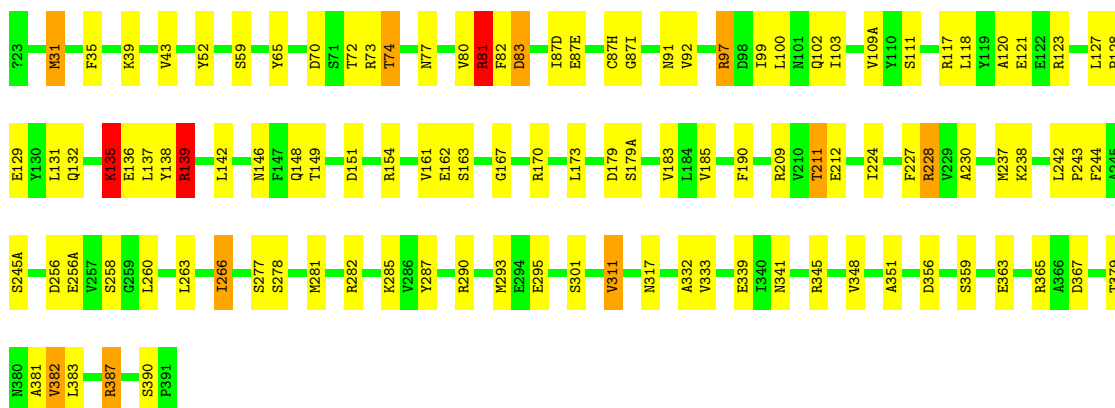
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

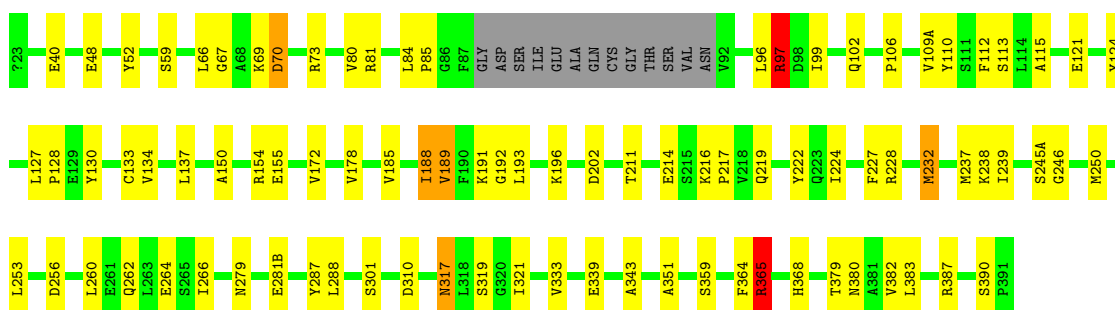
#### • Molecule 1: OVALBUMIN

Chain A: 



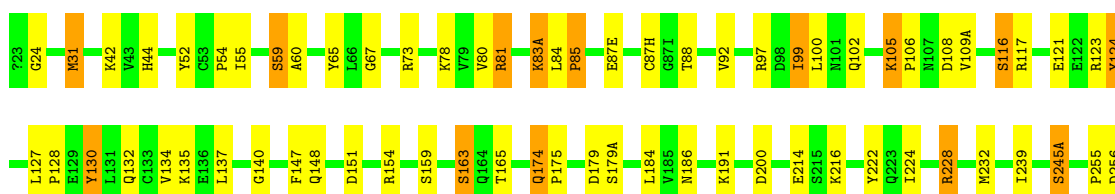
#### • Molecule 2: OVALBUMIN

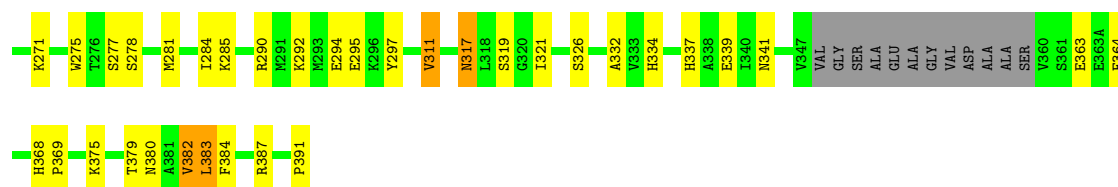
Chain B: 



#### • Molecule 3: OVALBUMIN

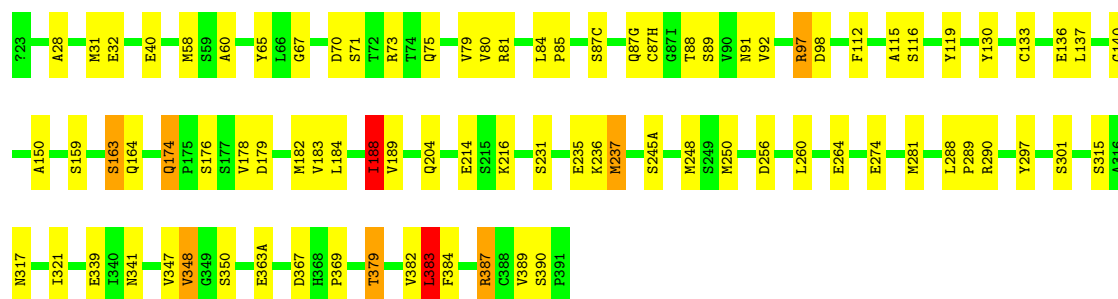
Chain C: 





- Molecule 3: OVALBUMIN

Chain D: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	27.0	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, NAG, ACE, SEP

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	1.10	2/2972 (0.1%)	1.87	58/4016 (1.4%)
2	B	1.11	2/2858 (0.1%)	1.67	34/3869 (0.9%)
3	C	1.16	2/2907 (0.1%)	1.77	47/3927 (1.2%)
3	D	1.13	2/2978 (0.1%)	1.69	40/4031 (1.0%)
All	All	1.13	8/11715 (0.1%)	1.75	179/15843 (1.1%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	264	GLU	CD-OE1	-7.08	1.17	1.25
2	B	192	GLY	N-CA	6.97	1.56	1.46
1	A	228	ARG	CD-NE	-6.20	1.35	1.46
3	D	159	SER	CA-CB	5.71	1.61	1.52
3	D	264	GLU	CD-OE1	-5.33	1.19	1.25
1	A	295	GLU	CD-OE2	-5.30	1.19	1.25
3	C	116	SER	CB-OG	5.09	1.48	1.42
3	C	59	SER	CA-CB	5.04	1.60	1.52

All (179) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ARG	CD-NE-CZ	22.24	154.73	123.60
1	A	282	ARG	NE-CZ-NH2	16.65	128.62	120.30
1	A	139	ARG	CD-NE-CZ	15.52	145.33	123.60
2	B	365	ARG	CD-NE-CZ	15.52	145.33	123.60
1	A	345	ARG	NE-CZ-NH1	15.16	127.88	120.30
1	A	228	ARG	CD-NE-CZ	14.28	143.59	123.60
3	D	274	GLU	CA-CB-CG	13.80	143.75	113.40
1	A	139	ARG	NE-CZ-NH1	13.65	127.13	120.30
3	C	154	ARG	NE-CZ-NH1	13.15	126.87	120.30
3	D	387	ARG	NE-CZ-NH1	12.71	126.66	120.30
1	A	365	ARG	NE-CZ-NH1	12.48	126.54	120.30
2	B	228	ARG	NE-CZ-NH1	12.03	126.31	120.30
3	C	154	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	A	117	ARG	NE-CZ-NH2	11.31	125.95	120.30
2	B	228	ARG	CD-NE-CZ	11.16	139.22	123.60
3	C	97	ARG	NE-CZ-NH2	-11.15	114.72	120.30
1	A	170	ARG	NE-CZ-NH1	10.77	125.69	120.30
1	A	170	ARG	CD-NE-CZ	10.72	138.60	123.60
1	A	97	ARG	NE-CZ-NH1	10.49	125.54	120.30
1	A	170	ARG	NE-CZ-NH2	-10.43	115.08	120.30
3	D	290	ARG	NE-CZ-NH2	9.99	125.30	120.30
1	A	290	ARG	NE-CZ-NH2	9.96	125.28	120.30
3	C	117	ARG	NE-CZ-NH1	9.93	125.27	120.30
2	B	154	ARG	NE-CZ-NH1	9.93	125.26	120.30
3	C	117	ARG	NE-CZ-NH2	-9.73	115.44	120.30
3	C	290	ARG	CD-NE-CZ	9.65	137.11	123.60
3	C	364	PHE	CB-CG-CD2	-9.60	114.08	120.80
1	A	256	ASP	CB-CG-OD1	9.51	126.86	118.30
1	A	282	ARG	NE-CZ-NH1	-9.38	115.61	120.30
1	A	365	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	A	97	ARG	NE-CZ-NH2	-9.09	115.76	120.30
2	B	365	ARG	NE-CZ-NH1	9.09	124.84	120.30
3	C	256	ASP	CB-CG-OD1	9.03	126.42	118.30
3	D	256	ASP	CB-CG-OD1	8.94	126.35	118.30
3	C	65	TYR	CB-CG-CD1	-8.88	115.67	121.00
3	D	387	ARG	NE-CZ-NH2	-8.66	115.97	120.30
2	B	202	ASP	CB-CG-OD2	-8.37	110.77	118.30
3	C	228	ARG	NE-CZ-NH1	8.33	124.47	120.30
3	C	124	TYR	CB-CG-CD2	8.23	125.94	121.00
2	B	48	GLU	CA-CB-CG	8.16	131.36	113.40
3	C	179	ASP	CB-CG-OD1	8.08	125.57	118.30
3	C	154	ARG	CD-NE-CZ	8.02	134.82	123.60
1	A	227	PHE	CB-CG-CD1	-7.95	115.24	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	290	ARG	NE-CZ-NH1	7.87	124.23	120.30
3	D	367	ASP	CB-CG-OD1	7.65	125.18	118.30
3	C	123	ARG	CA-CB-CG	7.60	130.12	113.40
3	C	290	ARG	NE-CZ-NH2	-7.47	116.57	120.30
3	C	52	TYR	CB-CG-CD1	-7.46	116.52	121.00
2	B	154	ARG	CD-NE-CZ	7.46	134.04	123.60
3	C	73	ARG	CD-NE-CZ	7.45	134.03	123.60
1	A	139	ARG	CA-CB-CG	7.38	129.62	113.40
1	A	81	ARG	CD-NE-CZ	7.33	133.87	123.60
3	C	200	ASP	CB-CG-OD2	7.21	124.79	118.30
1	A	228	ARG	CG-CD-NE	7.14	126.79	111.80
2	B	154	ARG	NE-CZ-NH2	-6.95	116.82	120.30
2	B	97	ARG	CG-CD-NE	6.88	126.24	111.80
3	C	311	VAL	CA-CB-CG1	6.86	121.19	110.90
3	D	70	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	345	ARG	CG-CD-NE	6.82	126.12	111.80
3	C	383	LEU	CB-CG-CD1	6.81	122.58	111.00
3	D	179	ASP	CB-CG-OD1	6.80	124.42	118.30
2	B	40	GLU	OE1-CD-OE2	6.79	131.45	123.30
1	A	339	GLU	OE1-CD-OE2	6.78	131.44	123.30
3	D	297	TYR	CB-CG-CD2	-6.75	116.95	121.00
1	A	73	ARG	NE-CZ-NH1	6.73	123.66	120.30
3	C	52	TYR	CB-CG-CD2	6.71	125.03	121.00
2	B	281(B)	GLU	OE1-CD-OE2	6.68	131.32	123.30
3	D	179	ASP	CB-CG-OD2	-6.66	112.30	118.30
1	A	81	ARG	CA-CB-CG	6.66	128.05	113.40
3	C	214	GLU	CB-CG-CD	6.64	132.12	114.20
3	D	97	ARG	NE-CZ-NH1	6.64	123.62	120.30
3	D	250	MET	CG-SD-CE	6.61	110.77	100.20
3	D	245(A)	SER	N-CA-CB	-6.60	100.60	110.50
2	B	222	TYR	CB-CG-CD1	-6.56	117.07	121.00
3	C	81	ARG	CG-CD-NE	6.54	125.54	111.80
2	B	73	ARG	NE-CZ-NH1	6.54	123.57	120.30
3	D	31	MET	CA-CB-CG	-6.52	102.21	113.30
1	A	387	ARG	NE-CZ-NH1	-6.48	117.06	120.30
3	D	383	LEU	CB-CG-CD1	6.44	121.95	111.00
3	D	136	GLU	CA-CB-CG	6.35	127.37	113.40
3	D	183	VAL	O-C-N	6.35	132.86	122.70
3	D	188	ILE	CB-CA-C	6.30	124.19	111.60
3	D	98	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	345	ARG	NH1-CZ-NH2	-6.23	112.55	119.40
3	C	326	SER	O-C-N	6.15	132.54	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	98	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	365	ARG	CD-NE-CZ	6.14	132.19	123.60
3	C	387	ARG	NE-CZ-NH1	6.11	123.36	120.30
2	B	256	ASP	CB-CG-OD2	-6.10	112.81	118.30
2	B	52	TYR	CB-CG-CD1	-6.04	117.37	121.00
1	A	332	ALA	CB-CA-C	6.02	119.13	110.10
3	C	165	THR	CA-CB-CG2	5.98	120.77	112.40
3	C	124	TYR	CG-CD1-CE1	5.96	126.07	121.30
3	D	363(A)	GLU	OE1-CD-OE2	5.96	130.45	123.30
3	C	295	GLU	OE1-CD-OE2	-5.95	116.16	123.30
2	B	189	VAL	O-C-N	5.95	132.21	122.70
2	B	310	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	52	TYR	CB-CG-CD1	-5.87	117.48	121.00
3	C	87(E)	GLU	OE1-CD-OE2	5.87	130.35	123.30
3	D	347	VAL	CA-CB-CG2	5.86	119.69	110.90
1	A	82	PHE	N-CA-CB	5.85	121.13	110.60
3	C	87(E)	GLU	CG-CD-OE2	-5.83	106.65	118.30
3	D	58	MET	CA-CB-CG	-5.80	103.45	113.30
2	B	228	ARG	NE-CZ-NH2	-5.77	117.42	120.30
2	B	66	LEU	CA-CB-CG	5.77	128.57	115.30
3	C	130	TYR	CB-CG-CD1	-5.77	117.54	121.00
1	A	129	GLU	CA-CB-CG	5.76	126.08	113.40
1	A	31	MET	CA-CB-CG	-5.76	103.51	113.30
1	A	367	ASP	CB-CG-OD1	5.75	123.47	118.30
2	B	73	ARG	NE-CZ-NH2	-5.74	117.43	120.30
3	D	214	GLU	CA-CB-CG	5.73	126.01	113.40
1	A	256	ASP	CB-CG-OD2	-5.72	113.15	118.30
2	B	245(A)	SER	C-N-CA	5.71	134.29	122.30
3	C	281	MET	O-C-N	5.71	131.84	122.70
2	B	260	LEU	CB-CA-C	5.71	121.05	110.20
3	D	367	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	367	ASP	CB-CG-OD2	-5.68	113.19	118.30
3	C	332	ALA	N-CA-CB	5.63	117.98	110.10
1	A	111	SER	N-CA-CB	-5.62	102.06	110.50
2	B	281(B)	GLU	CA-CB-CG	5.61	125.75	113.40
2	B	70	ASP	CB-CG-OD1	-5.61	113.25	118.30
2	B	69	LYS	CB-CG-CD	5.58	126.11	111.60
2	B	222	TYR	CB-CG-CD2	5.53	124.32	121.00
1	A	138	TYR	CB-CA-C	5.52	121.45	110.40
3	C	228	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	A	131	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	117	ARG	NH1-CZ-NH2	-5.47	113.38	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	GLU	OE1-CD-OE2	5.47	129.86	123.30
2	B	343	ALA	N-CA-CB	5.45	117.73	110.10
3	C	147	PHE	CD1-CE1-CZ	-5.45	113.56	120.10
3	C	311	VAL	CB-CA-C	-5.45	101.05	111.40
2	B	364	PHE	CB-CG-CD1	-5.43	117.00	120.80
1	A	179	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	293	MET	CA-CB-CG	5.40	122.48	113.30
3	D	216	LYS	CA-CB-CG	5.39	125.26	113.40
1	A	333	VAL	CG1-CB-CG2	-5.39	102.28	110.90
3	C	105	LYS	N-CA-CB	-5.38	100.91	110.60
3	C	44	HIS	CA-CB-CG	-5.37	104.47	113.60
1	A	87(E)	GLU	CG-CD-OE2	-5.37	107.56	118.30
2	B	115	ALA	N-CA-CB	-5.37	102.59	110.10
3	D	384	PHE	CB-CG-CD2	-5.36	117.05	120.80
1	A	154	ARG	NE-CZ-NH1	5.35	122.97	120.30
3	D	79	VAL	CA-CB-CG1	5.33	118.89	110.90
2	B	279	ASN	C-N-CA	5.32	135.01	121.70
1	A	81	ARG	CG-CD-NE	5.30	122.92	111.80
1	A	287	TYR	O-C-N	5.29	131.17	122.70
2	B	193	LEU	CA-CB-CG	5.29	127.47	115.30
3	D	363(A)	GLU	CA-CB-CG	5.28	125.02	113.40
3	C	222	TYR	CB-CG-CD2	-5.26	117.85	121.00
1	A	135	LYS	N-CA-CB	5.24	120.04	110.60
3	D	281	MET	CA-CB-CG	-5.24	104.40	113.30
2	B	387	ARG	NE-CZ-NH2	5.23	122.92	120.30
3	D	231	SER	CB-CA-C	5.23	120.03	110.10
3	C	97	ARG	CD-NE-CZ	5.20	130.89	123.60
3	D	40	GLU	OE1-CD-OE2	5.20	129.54	123.30
3	D	339	GLU	OE1-CD-OE2	5.19	129.53	123.30
1	A	73	ARG	NE-CZ-NH2	-5.18	117.71	120.30
3	C	108	ASP	CB-CG-OD1	5.17	122.95	118.30
3	C	297	TYR	CG-CD1-CE1	-5.14	117.19	121.30
3	C	311	VAL	N-CA-CB	5.12	122.77	111.50
3	D	115	ALA	N-CA-CB	-5.12	102.94	110.10
1	A	244	PHE	CG-CD2-CE2	5.11	126.42	120.80
2	B	155	GLU	OE1-CD-OE2	5.11	129.43	123.30
3	D	237	MET	CA-CB-CG	-5.11	104.61	113.30
3	C	31	MET	CG-SD-CE	-5.10	92.04	100.20
3	D	290	ARG	CA-CB-CG	5.10	124.61	113.40
3	D	31	MET	CG-SD-CE	-5.07	92.09	100.20
1	A	135	LYS	CA-CB-CG	5.07	124.54	113.40
1	A	339	GLU	CG-CD-OE2	-5.06	108.18	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	ALA	CB-CA-C	5.06	117.68	110.10
3	D	379	THR	CA-CB-OG1	-5.06	98.38	109.00
1	A	139	ARG	NH1-CZ-NH2	-5.05	113.84	119.40
1	A	209	ARG	CD-NE-CZ	5.05	130.67	123.60
3	D	348	VAL	CG1-CB-CG2	-5.04	102.83	110.90
3	C	387	ARG	NE-CZ-NH2	-5.03	117.78	120.30
3	D	174	GLN	CB-CA-C	5.02	120.44	110.40
3	C	384	PHE	N-CA-CB	5.01	119.62	110.60
1	A	65	TYR	CZ-CE2-CD2	-5.00	115.30	119.80
1	A	190	PHE	CB-CG-CD2	-5.00	117.30	120.80

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2940	0	2906	49	0
2	B	2816	0	2751	38	0
3	C	2854	0	2812	43	0
3	D	2924	0	2865	30	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12269	0	11385	157	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (157) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:174:GLN:HE21	3:C:174:GLN:H	1.13	0.97
1:A:139:ARG:HB3	1:A:139:ARG:HH11	1.46	0.81
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: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: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
1:A:80:VAL:O	1:A:81:ARG:HB2	1.98	0.64
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
1:A:256(A):GLU:C	1:A:258:SER:H	2.07	0.58
3:C:174:GLN:NE2	3:C:174:GLN:H	1.93	0.58
2:B:238:LYS:HE3	6:B:488:HOH:O	2.04	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: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
2:B:379:THR:O	2:B:380:ASN:HB2	2.07	0.53
3:D:248:MET:HE2	3:D:383:LEU:HD23	1.89	0.53
2:B:219:GLN:NE2	2:B:219:GLN:HA	2.23	0.53
3:C:191:LYS:HD3	3:D:163:SER:HA	1.91	0.53
3:C:31:MET:HG2	3:C:382:VAL:HG12	1.89	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:C:54:PRO:HG2	3:C:382:VAL:HG22	1.91	0.53
2:B:59:SER:HA	2:B:96:LEU:HD21	1.90	0.53
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
3:C:83(A):LYS:HD2	3:C:83(A):LYS:C	2.31	0.51
1:A:97:ARG:HD2	1:A:137:LEU:HB3	1.93	0.51
3:D:260:LEU:HD22	3:D:369:PRO:HB2	1.92	0.51
3:D:188:ILE:HD13	3:D:189:VAL:N	2.27	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
1:A:139:ARG:NH1	1:A:139:ARG:HB3	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
2:B:232:MET:HE1	2:B:239:ILE:HG12	1.95	0.49
3:C:271:LYS:HZ3	3:C:275:TRP:HE1	1.58	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
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
3:C:228:ARG:HH22	3:C:278:SER:HA	1.78	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:237:MET:HE1	1:A:263:LEU:HD13	1.96	0.47
3:C:239:ILE:HD12	3:C:275:TRP:HB3	1.96	0.47
1:A:87(H):CYS:HA	1:A:92:VAL:HG21	1.95	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:D:164:GLN:NE2	6:D:413:HOH:O	2.47	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:248:MET:CE	3:D:383:LEU:HD23	2.45	0.47
2:B:317:ASN:C	2:B:317:ASN:HD22	2.18	0.47
3:D:71:SER:O	3:D:75:GLN:HG3	2.16	0.46
3:C:294:GLU:HG3	3:C:337:HIS:HB2	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:211:THR:OG1	1:A:212:GLU:N	2.47	0.46
2:B:80:VAL:O	2:B:81:ARG:HB2	2.14	0.46
3:D:236:LYS:HD2	6:D:572:HOH:O	2.15	0.46
3:C:317:ASN:C	3:C:317:ASN:HD22	2.19	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
2:B:150:ALA:HB1	2:B:178:VAL:HG12	1.97	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
1:A:256(A):GLU:C	1:A:258:SER:N	2.69	0.45
3:C:239:ILE:CD1	3:C:275:TRP:HB3	2.47	0.45
2:B:84:LEU:HA	2:B:85:PRO:HD3	1.85	0.45
3:D:130:TYR:O	3:D:133:CYS:HB3	2.15	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
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:105:LYS:HA	3:C:106:PRO:HD3	1.89	0.44
2:B:351:ALA:HB2	6:B:532:HOH:O	2.17	0.44
1:A:127:LEU:HA	1:A:128:PRO:HD2	1.64	0.44
2:B:81:ARG:HD3	6:B:521:HOH:O	2.16	0.43
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: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
3:C:109(A):VAL:CG2	3:C:245(A):SER:HB2	2.44	0.43
1:A:121:GLU:OE2	1:A:148:GLN:N	2.46	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:387:ARG:HD3	3:D:389:VAL:CG2	2.48	0.43
3:C:80:VAL:O	3:C:81:ARG:HB2	2.19	0.42
2:B:219:GLN:HE21	2:B:219:GLN:HA	1.84	0.42
3:C:102:GLN:HA	3:C:105:LYS:CE	2.49	0.42
2:B:196:LYS:HD2	2:B:227:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:59:SER:HB3	1:A:100:LEU:HD11	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: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:204:GLN:HG2	6:D:424:HOH:O	2.18	0.42
3:C:159:SER:O	3:C:163:SER:HB2	2.20	0.42
1:A:77:ASN:HD21	1:A:83:ASP:CA	2.28	0.42
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
3:C:84:LEU:HA	3:C:85:PRO:HD3	1.95	0.41
1:A:81:ARG:HG3	1:A:81:ARG:HH11	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
3:D:87(G):GLN:O	3:D:87(H):CYS:C	2.60	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
2:B:250:MET:HE1	2:B:288:LEU:HD21	2.02	0.41
3:C:78:LYS:HD3	3:C:78:LYS:HA	1.93	0.41
3:C:81:ARG:C	3:C:83(A):LYS:HZ1	2.23	0.41
2:B:67:GLY:HA3	2:B:321:ILE:HG13	2.03	0.41
1:A:139:ARG:HG2	6:A:637:HOH:O	2.21	0.40
2:B:219:GLN:CA	2:B:219:GLN:HE21	2.34	0.40
3:D:60:ALA:HB1	3:D:184:LEU:HD11	2.04	0.40
2:B:102:GLN:NE2	6:B:469:HOH:O	2.53	0.40
1:A:278:SER:HB3	6:A:642:HOH:O	2.21	0.40
1:A:260:LEU:HD21	1:A:387:ARG:HG3	2.03	0.40
2:B:219:GLN:CA	2:B:219:GLN:NE2	2.85	0.40
2:B:130:TYR:O	2:B:134:VAL:HG23	2.22	0.40
3:C:186:ASN:O	3:C:334:HIS:HA	2.21	0.40
1:A:102:GLN:NE2	6:A:573:HOH:O	2.53	0.40
2:B:133:CYS:O	2:B:137:LEU:HG	2.21	0.40
3:D:89:SER:C	3:D:91:ASN:H	2.23	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	382/386 (99%)	358 (94%)	22 (6%)	2 (0%)	38	23
2	B	368/386 (95%)	349 (95%)	18 (5%)	1 (0%)	50	38
3	C	370/386 (96%)	356 (96%)	12 (3%)	2 (0%)	38	23
3	D	384/386 (100%)	369 (96%)	15 (4%)	0	100	100
All	All	1504/1544 (97%)	1432 (95%)	67 (4%)	5 (0%)	50	38

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%)	289 (94%)	19 (6%)	26	10
2	B	293/330 (89%)	276 (94%)	17 (6%)	28	12
3	C	300/331 (91%)	280 (93%)	20 (7%)	23	8
3	D	310/331 (94%)	296 (96%)	14 (4%)	38	21
All	All	1211/1321 (92%)	1141 (94%)	70 (6%)	28	12

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	THR
1	A	81	ARG
1	A	135	LYS
1	A	139	ARG
1	A	151	ASP
1	A	163	SER
1	A	179(A)	SER
1	A	211	THR
1	A	228	ARG
1	A	266	ILE
1	A	277	SER
1	A	301	SER
1	A	311	VAL
1	A	317	ASN
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	97	ARG
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	301	SER
2	B	317	ASN
2	B	333	VAL
2	B	359	SER
2	B	365	ARG
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	148	GLN
3	C	151	ASP
3	C	163	SER

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Mol	Chain	Res	Type
3	C	174	GLN
3	C	179(A)	SER
3	C	216	LYS
3	C	232	MET
3	C	277	SER
3	C	311	VAL
3	C	317	ASN
3	C	341	ASN
3	C	369	PRO
3	C	375	LYS
3	C	382	VAL
3	C	383	LEU
3	C	391	PRO
3	D	87(C)	SER
3	D	88	THR
3	D	163	SER
3	D	174	GLN
3	D	176	SER
3	D	188	ILE
3	D	301	SER
3	D	315	SER
3	D	317	ASN
3	D	341	ASN
3	D	350	SER
3	D	382	VAL
3	D	383	LEU
3	D	390	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) 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	164	GLN
2	B	171	ASN
2	B	219	GLN
2	B	317	ASN
2	B	337	HIS
3	C	132	GLN

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Mol	Chain	Res	Type
3	C	164	GLN
3	C	174	GLN
3	C	317	ASN
3	C	341	ASN
3	C	368	HIS
3	C	380	ASN
3	D	47	ASN
3	D	132	GLN
3	D	174	GLN
3	D	219	GLN
3	D	223	GLN
3	D	279	ASN
3	D	317	ASN
3	D	341	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	9,9,10	5.70	3 (33%)	10,12,14	2.46	5 (50%)
1	SEP	A	87(C)	1	9,9,10	6.61	2 (22%)	10,12,14	3.29	4 (40%)
2	SEP	B	350	2	9,9,10	6.71	3 (33%)	10,12,14	2.56	5 (50%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	350	SEP	O-C	19.63	1.24	1.11
1	A	87(C)	SEP	O-C	19.33	1.24	1.11
1	A	350	SEP	O-C	16.57	1.22	1.11
1	A	87(C)	SEP	CA-C	3.22	1.54	1.48
2	B	350	SEP	CA-C	3.20	1.54	1.48
1	A	350	SEP	CA-C	2.87	1.53	1.48
1	A	350	SEP	P-OG	-2.03	1.53	1.60
2	B	350	SEP	P-O2P	-2.03	1.47	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87(C)	SEP	C-CA-N	-6.40	107.44	113.83
1	A	87(C)	SEP	P-OG-CB	6.18	136.07	118.19
1	A	87(C)	SEP	O3P-P-OG	4.24	118.34	106.65
1	A	350	SEP	O3P-P-OG	4.16	118.14	106.65
1	A	350	SEP	P-OG-CB	4.02	129.83	118.19
2	B	350	SEP	O2P-P-OG	3.86	117.30	106.65
2	B	350	SEP	C-CA-N	-3.72	110.12	113.83
2	B	350	SEP	O3P-P-OG	3.54	116.41	106.65
2	B	350	SEP	P-OG-CB	3.51	128.34	118.19
1	A	350	SEP	C-CA-N	-3.19	110.64	113.83
2	B	350	SEP	OG-P-O1P	-3.04	97.80	106.71
1	A	350	SEP	OG-P-O1P	-2.93	98.11	106.71
1	A	350	SEP	O2P-P-OG	2.40	113.28	106.65
1	A	87(C)	SEP	OG-P-O1P	-2.07	100.65	106.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	A	393	1	12,14,15	2.10	3 (25%)	15,19,21	1.61	2 (13%)
4	NAG	B	393	2	12,14,15	1.69	2 (16%)	15,19,21	2.20	5 (33%)
4	NAG	C	393	3	12,14,15	1.71	3 (25%)	15,19,21	2.40	4 (26%)
4	NAG	D	393	3	12,14,15	1.33	1 (8%)	15,19,21	2.03	5 (33%)

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	A	393	1	-	0/6/23/26	0/1/1/1
4	NAG	B	393	2	-	0/6/23/26	0/1/1/1
4	NAG	C	393	3	-	0/6/23/26	0/1/1/1
4	NAG	D	393	3	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	393	NAG	O7-C7	-4.37	1.13	1.23
4	B	393	NAG	O7-C7	-4.14	1.14	1.23
4	A	393	NAG	O5-C5	-3.95	1.38	1.45
4	A	393	NAG	C2-N2	3.63	1.50	1.46
4	D	393	NAG	O7-C7	-3.54	1.15	1.23
4	C	393	NAG	C2-N2	3.53	1.50	1.46
4	B	393	NAG	C2-N2	3.05	1.49	1.46
4	C	393	NAG	O7-C7	-2.96	1.16	1.23
4	C	393	NAG	O3-C3	-2.30	1.37	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	393	NAG	O5-C5-C4	-7.52	101.10	110.65
4	B	393	NAG	O5-C5-C4	-5.51	103.66	110.65
4	D	393	NAG	O5-C5-C4	-4.30	105.20	110.65
4	A	393	NAG	C2-N2-C7	-3.97	116.42	123.09
4	D	393	NAG	C3-C2-N2	-3.90	105.82	111.76
4	B	393	NAG	C3-C2-N2	-3.20	106.89	111.76
4	B	393	NAG	O3-C3-C2	-3.07	102.64	109.09
4	C	393	NAG	C3-C4-C5	-2.98	104.88	110.20
4	C	393	NAG	C8-C7-N2	-2.82	110.60	116.11
4	D	393	NAG	O5-C5-C6	-2.69	104.16	106.98
4	D	393	NAG	C8-C7-N2	-2.32	111.58	116.11
4	B	393	NAG	C2-N2-C7	-2.32	119.20	123.09
4	D	393	NAG	O7-C7-N2	-2.23	117.24	121.90
4	A	393	NAG	C3-C2-N2	-2.07	108.61	111.76
4	B	393	NAG	C4-C3-C2	-2.04	106.32	111.32
4	C	393	NAG	C6-C5-C4	2.02	117.88	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.