



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:19 AM GMT

PDB ID : 2WME  
Title : CRYSTALLOGRAPHIC STRUCTURE OF BETAIN ALDEHYDE DEHYDROGENASE FROM PSEUDOMONAS AERUGINOSA  
Authors : Gonzalez-Segura, L.; Rudino-Pinera, E.; Munoz-Clares, R.A.; Horjales, E.  
Deposited on : 2009-06-30  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

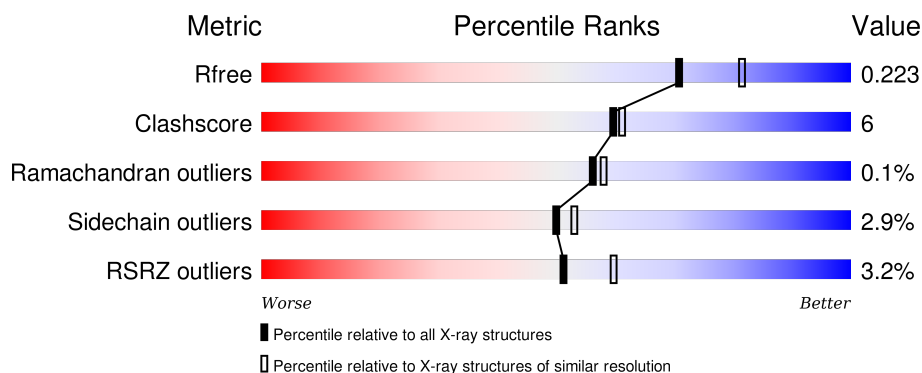
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	490	<div> <div>88%</div> <div>11% .</div> </div>
1	B	490	<div> <div>91%</div> <div>8% .</div> </div>
1	D	490	<div> <div>%</div> <div>91%</div> <div>8%</div> </div>
1	F	490	<div> <div>3%</div> <div>85%</div> <div>13% .</div> </div>
1	G	490	<div> <div>%</div> <div>88%</div> <div>10% .</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	490	
2	C	490	
2	E	490	

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
3	GOL	A	1497	-	-	-	X
3	GOL	A	1498	-	-	-	X
3	GOL	A	1501	-	-	X	-
3	GOL	B	1497	-	-	-	X
3	GOL	C	1495	-	-	-	X
3	GOL	D	1496	-	-	X	-
3	GOL	E	1496	-	-	X	-
3	GOL	G	1495	-	-	X	-
3	GOL	G	1497	-	-	-	X
4	NAP	A	1491	-	-	-	X
4	NAP	D	1491	-	-	-	X
4	NAP	F	1491	-	-	-	X
4	NAP	G	1491	-	-	-	X
4	NAP	H	1491	-	-	-	X
5	BME	D	1492[A]	-	-	-	X
5	BME	D	1492[B]	-	-	-	X
5	BME	F	1492	-	-	-	X
5	BME	G	1492[A]	-	-	-	X
5	BME	G	1492[B]	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 33548 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 BETAINE ALDEHYDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	10	0
			3824	2398	673	739	14			
1	B	489	Total	C	N	O	S	0	7	0
			3800	2386	664	736	14			
1	D	489	Total	C	N	O	S	0	0	0
			3744	2351	657	722	14			
1	F	489	Total	C	N	O	S	0	5	0
			3789	2378	666	731	14			
1	G	489	Total	C	N	O	S	0	1	0
			3753	2356	658	725	14			
1	H	489	Total	C	N	O	S	0	1	0
			3753	2356	658	725	14			

- Molecule 2 is a protein called BETAINE ALDEHYDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	489	Total	C	N	O	S	0	3	0
			3768	2364	660	729	15			
2	E	489	Total	C	N	O	S	0	3	0
			3767	2364	660	729	14			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



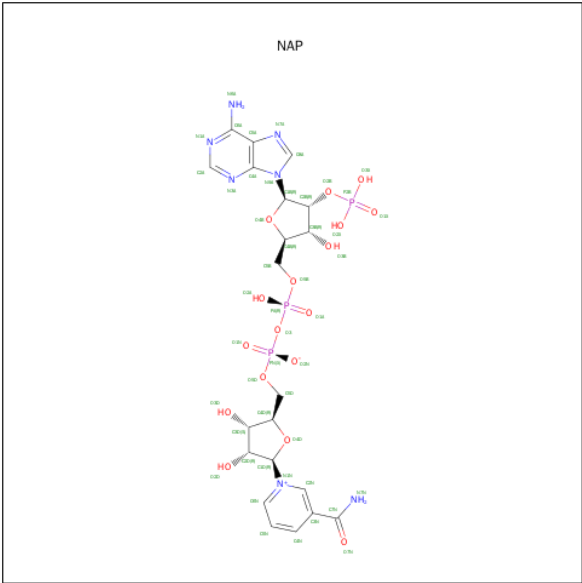
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



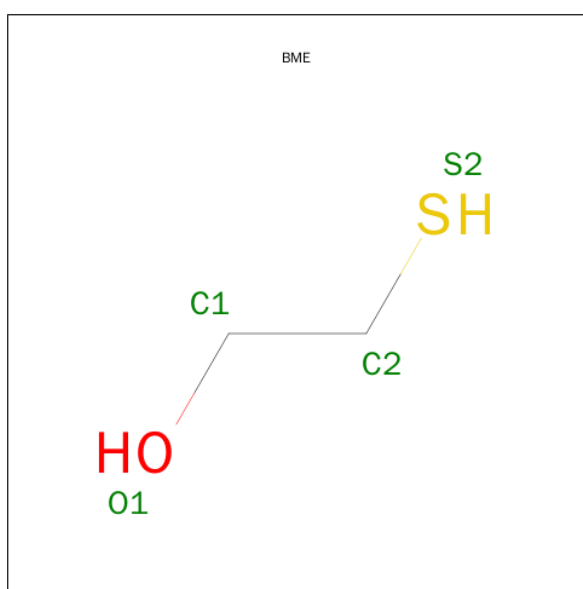
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	1
			8	4	2	2		
5	F	1	Total	C	O	S	0	0
			4	2	1	1		
5	G	1	Total	C	O	S	0	1
			8	4	2	2		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	2	Total K 2 2	0	0
6	D	2	Total K 2 2	0	0
6	E	2	Total K 2 2	0	0
6	H	2	Total K 2 2	0	0
6	B	2	Total K 2 2	0	0
6	C	2	Total K 2 2	0	0
6	A	2	Total K 2 2	0	0
6	F	2	Total K 2 2	0	0

- Molecule 7 is water.

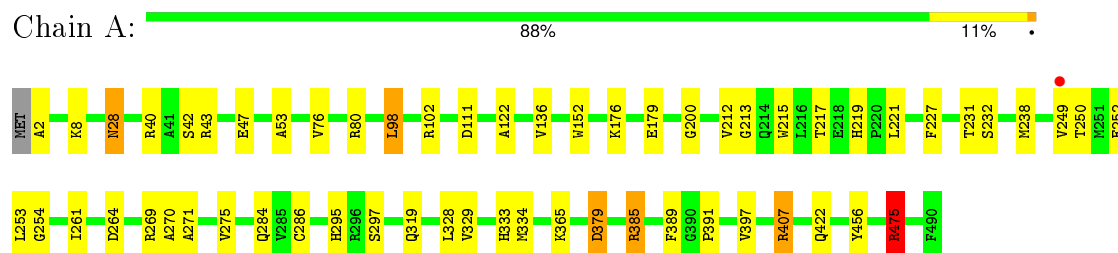
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	417	Total O 417 417	0	0
7	B	405	Total O 405 405	0	0
7	C	367	Total O 367 367	0	0
7	D	362	Total O 362 362	0	0
7	E	357	Total O 357 357	0	0
7	F	347	Total O 347 347	0	0
7	G	360	Total O 360 360	0	0
7	H	317	Total O 317 317	0	0



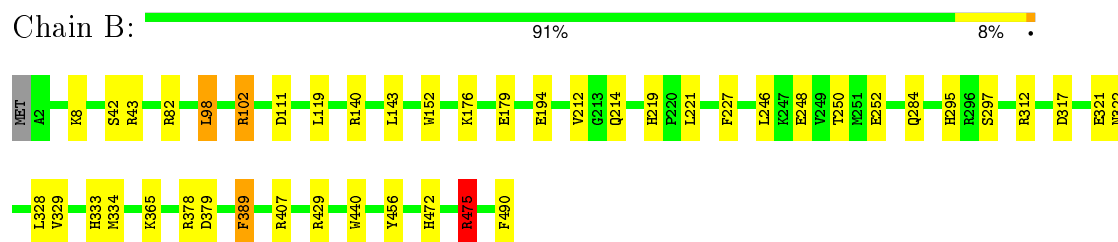
### 3 Residue-property plots

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.

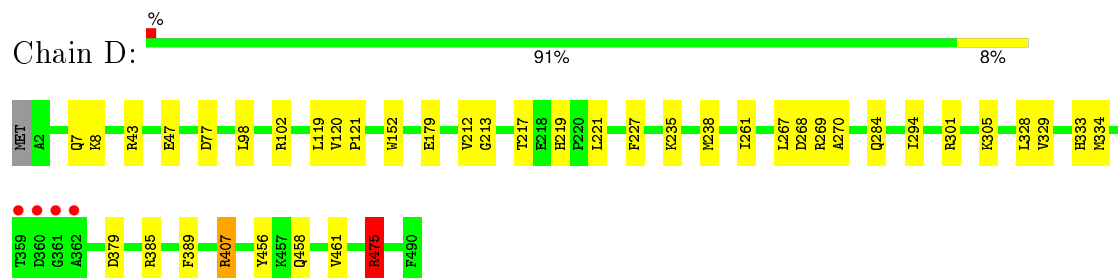
#### • Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE



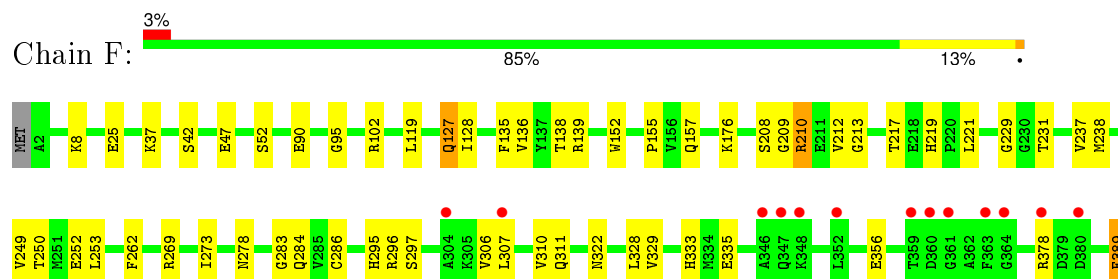
#### • Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE



#### • Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE

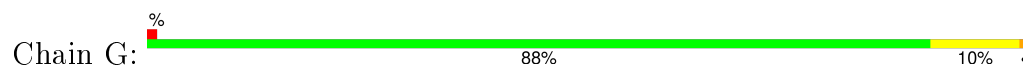


#### • Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE

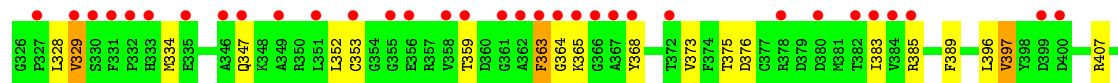
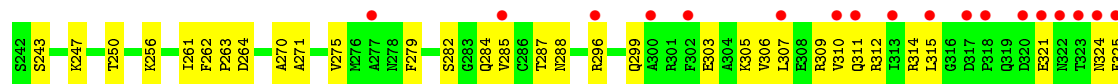
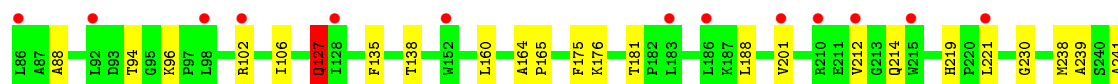
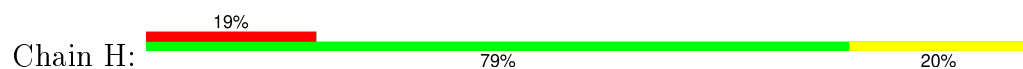




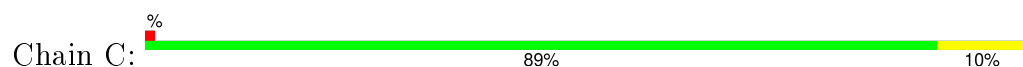
• Molecule 1: BETAINNE ALDEHYDE DEHYDROGENASE



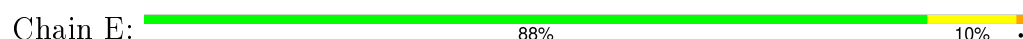
• Molecule 1: BETAINNE ALDEHYDE DEHYDROGENASE

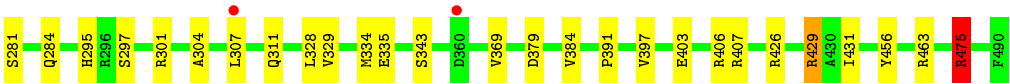


• Molecule 2: BETAINNE ALDEHYDE DEHYDROGENASE



• Molecule 2: BETAINNE ALDEHYDE DEHYDROGENASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	334.95Å 133.01Å 101.81Å 90.00° 94.94° 90.00°	Depositor
Resolution (Å)	42.68 – 2.10 42.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.2 (42.68-2.10) 95.1 (42.66-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.20 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.166 , 0.211 0.167 , 0.223	Depositor DCC
$R_{free}$ test set	12459 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 245989 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	33548	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CSO, K, NAP, BME

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	1.04	0/3892	0.91	11/5273 (0.2%)
1	B	1.00	2/3868 (0.1%)	0.87	9/5242 (0.2%)
1	D	0.98	0/3812	0.82	5/5166 (0.1%)
1	F	0.92	0/3857	0.79	4/5225 (0.1%)
1	G	0.95	3/3821 (0.1%)	0.82	3/5178 (0.1%)
1	H	0.85	1/3821 (0.0%)	0.79	2/5178 (0.0%)
2	C	0.95	1/3821 (0.0%)	0.84	8/5177 (0.2%)
2	E	0.95	1/3827 (0.0%)	0.87	12/5185 (0.2%)
All	All	0.96	8/30719 (0.0%)	0.84	54/41624 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	248	GLU	CB-CG	6.22	1.64	1.52
1	G	412	GLU	CG-CD	6.12	1.61	1.51
1	H	127	GLN	CB-CG	5.33	1.67	1.52
2	E	44	GLU	CG-CD	5.31	1.59	1.51
1	B	440	TRP	CB-CG	5.28	1.59	1.50
1	G	175	PHE	CE1-CZ	5.22	1.47	1.37
1	G	473	TYR	CD2-CE2	5.09	1.47	1.39
2	C	413	TYR	CD2-CE2	5.05	1.47	1.39

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	ARG	NE-CZ-NH1	12.35	126.47	120.30
1	B	475	ARG	NE-CZ-NH1	11.50	126.05	120.30
1	A	475	ARG	NE-CZ-NH2	-10.35	115.12	120.30
2	E	3	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	A	407	ARG	NE-CZ-NH1	10.27	125.43	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	475	ARG	NE-CZ-NH1	8.53	124.56	120.30
2	E	269	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	B	475	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	F	269	ARG	NE-CZ-NH2	-7.72	116.44	120.30
2	C	269	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	B	140	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	H	475	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	269	ARG	NE-CZ-NH2	-7.50	116.55	120.30
2	E	246	LEU	CA-CB-CG	7.44	132.42	115.30
1	A	407	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	429	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	A	385	ARG	NE-CZ-NH1	7.32	123.96	120.30
2	C	96	LYS	CD-CE-NZ	-7.19	95.16	111.70
2	C	246	LEU	CA-CB-CG	7.19	131.83	115.30
1	H	475	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	G	475	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	C	475	ARG	NE-CZ-NH1	6.93	123.77	120.30
2	E	269	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	G	407	ARG	NE-CZ-NH2	-6.79	116.91	120.30
2	C	269	ARG	NE-CZ-NH1	6.78	123.69	120.30
2	C	407	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	D	407	ARG	NE-CZ-NH1	6.43	123.52	120.30
2	E	429	ARG	NE-CZ-NH2	-6.39	117.10	120.30
2	C	475	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	385	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	G	475	ARG	NE-CZ-NH2	-6.25	117.18	120.30
2	E	475	ARG	NE-CZ-NH1	6.23	123.42	120.30
2	E	98	LEU	CA-CB-CG	6.18	129.50	115.30
1	D	407	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	269	ARG	NE-CZ-NH1	5.99	123.30	120.30
2	E	463	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	B	111	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	312	ARG	NE-CZ-NH2	-5.81	117.40	120.30
2	E	246	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	B	429	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	F	139	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	77	ASP	CB-CG-OD1	5.62	123.36	118.30
1	D	269	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	317	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	111	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	F	269	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	379	ASP	CB-CG-OD1	5.35	123.11	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	264	ASP	CB-CG-OD1	5.26	123.03	118.30
1	F	426	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	111	ASP	CB-CG-OD1	5.22	123.00	118.30
2	E	246	LEU	CB-CG-CD2	5.22	119.87	111.00
2	E	84	ASP	CB-CG-OD1	5.12	122.90	118.30
1	B	475	ARG	CD-NE-CZ	5.10	130.74	123.60
2	C	246	LEU	CB-CG-CD2	5.04	119.57	111.00

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	3824	0	3787	46	0
1	B	3800	0	3761	29	0
1	D	3744	0	3714	27	0
1	F	3789	0	3758	53	0
1	G	3753	0	3720	40	0
1	H	3753	0	3720	70	0
2	C	3768	0	3732	31	0
2	E	3767	0	3732	41	0
3	A	36	0	48	6	0
3	B	18	0	24	3	0
3	C	18	0	24	2	0
3	D	12	0	16	7	0
3	E	12	0	16	6	0
3	F	6	0	8	1	0
3	G	18	0	24	4	0
3	H	6	0	8	1	0
4	A	31	0	11	9	0
4	B	31	0	11	4	0
4	C	31	0	11	0	0
4	D	31	0	11	7	0
4	E	31	0	11	2	0
4	F	31	0	11	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	31	0	11	1	0
4	H	31	0	11	2	0
5	A	4	0	6	3	0
5	B	4	0	5	1	0
5	D	8	0	11	0	0
5	F	4	0	6	2	0
5	G	8	0	12	3	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	0	0
7	A	417	0	0	2	0
7	B	405	0	0	6	0
7	C	367	0	0	9	0
7	D	362	0	0	10	0
7	E	357	0	0	8	0
7	F	347	0	0	8	0
7	G	360	0	0	6	0
7	H	317	0	0	17	0
All	All	33548	0	30220	348	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (348) 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:C:297:SER:HB3	7:C:2223:HOH:O	1.32	1.25
1:G:73:ARG:HD2	7:G:2072:HOH:O	1.34	1.25
1:G:43:ARG:HH11	1:G:43:ARG:HG2	1.07	1.09
1:A:286:CYS:SG	5:A:1492:BME:S2	2.46	1.07
1:G:335:GLU:HG2	7:G:2256:HOH:O	1.55	1.05
2:E:3:ARG:CZ	7:E:2002:HOH:O	2.05	1.03
2:E:3:ARG:NH1	7:E:2002:HOH:O	1.96	0.98
1:H:359:THR:HG22	1:H:364:GLY:HA2	1.46	0.97
1:F:286:CYS:SG	5:F:1492:BME:S2	2.58	0.95
4:A:1491:NAP:O2X	3:A:1501:GOL:H31	1.69	0.90

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:286:CYS:SG	5:G:1492[B]:BME:S2	2.70	0.90
1:H:284:GLN:HE22	1:H:329:VAL:H	1.19	0.87
1:G:43:ARG:HG2	1:G:43:ARG:NH1	1.86	0.87
3:D:1496:GOL:C1	7:D:2312:HOH:O	2.25	0.85
1:A:2:ALA:HB2	7:A:2007:HOH:O	1.76	0.84
1:G:286:CYS:SG	5:G:1492[A]:BME:S2	2.56	0.83
1:H:80:ARG:O	7:H:2070:HOH:O	1.96	0.83
1:F:425:ALA:HB1	1:F:429:ARG:HH21	1.42	0.83
3:G:1495:GOL:H2	7:G:2359:HOH:O	1.79	0.82
1:F:157:GLN:OE1	3:F:1495:GOL:H11	1.79	0.82
1:D:219:HIS:HD2	1:D:221:LEU:H	1.29	0.80
1:H:446:GLU:OE2	7:H:2275:HOH:O	2.00	0.79
3:D:1496:GOL:H12	7:D:2312:HOH:O	1.83	0.79
1:B:250:THR:HG22	1:B:252[B]:GLU:OE2	1.83	0.78
1:F:176:LYS:HD2	1:F:212[B]:VAL:HG13	1.65	0.78
1:G:43:ARG:HH11	1:G:43:ARG:CG	1.93	0.78
1:H:18:ALA:HB3	7:H:2015:HOH:O	1.85	0.77
1:F:429:ARG:NH2	1:G:483:LEU:O	2.19	0.76
2:C:219:HIS:HD2	2:C:221:LEU:H	1.34	0.75
1:H:359:THR:CG2	1:H:364:GLY:HA2	2.16	0.75
3:D:1496:GOL:O3	7:D:2362:HOH:O	2.05	0.75
1:B:295:HIS:HD2	1:B:297:SER:OG	1.71	0.74
1:H:307:LEU:O	1:H:311:GLN:HG3	1.89	0.73
1:H:359:THR:HG22	1:H:364:GLY:CA	2.18	0.72
1:A:219:HIS:HD2	1:A:221:LEU:H	1.37	0.72
1:B:219:HIS:HD2	1:B:221:LEU:H	1.36	0.71
1:D:213:GLY:O	1:D:217:THR:HG23	1.89	0.71
1:A:379:ASP:OD2	1:A:407:ARG:HD2	1.91	0.71
1:G:284:GLN:HE22	1:G:329:VAL:H	1.38	0.70
1:A:152:TRP:CH2	1:A:389:PHE:CE2	2.79	0.70
1:B:250:THR:CG2	1:B:252[B]:GLU:OE2	2.40	0.70
2:E:284:GLN:HE22	2:E:329:VAL:H	1.40	0.70
2:E:304:ALA:HA	3:E:1496:GOL:H11	1.73	0.69
2:C:286[B]:CSO:OD	2:C:389:PHE:CZ	2.44	0.69
2:E:127:GLN:HE22	2:E:135:PHE:HD1	1.41	0.69
1:F:250:THR:CG2	1:F:252[B]:GLU:OE2	2.41	0.68
1:H:88:ALA:HB3	7:H:2076:HOH:O	1.94	0.68
1:H:230:GLY:N	4:H:1491:NAP:O2A	2.23	0.68
1:A:176:LYS:CD	1:A:212[A]:VAL:HG23	2.22	0.68
1:F:219:HIS:HD2	1:F:221:LEU:H	1.41	0.68
1:F:403:GLU:OE2	7:F:2279:HOH:O	2.12	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:284:GLN:HE22	2:C:329:VAL:H	1.42	0.67
1:A:98:LEU:HD22	1:A:319:GLN:HA	1.75	0.67
4:A:1491:NAP:C8A	3:A:1501:GOL:H2	2.24	0.67
1:G:333:HIS:NE2	1:G:389:PHE:O	2.24	0.67
3:D:1496:GOL:C3	7:D:2362:HOH:O	2.43	0.67
1:F:127:GLN:HG2	1:H:138:THR:O	1.94	0.67
4:A:1491:NAP:H8A	3:A:1501:GOL:H2	1.76	0.67
4:D:1491:NAP:O1X	7:D:2355:HOH:O	2.13	0.66
3:G:1495:GOL:O1	3:G:1495:GOL:O3	2.08	0.66
2:E:246:LEU:HD11	1:F:253:LEU:HD12	1.76	0.66
1:A:219:HIS:CD2	1:A:221:LEU:H	2.14	0.66
1:F:47:GLU:OE1	1:F:219:HIS:HE1	1.78	0.66
4:D:1491:NAP:H8A	4:D:1491:NAP:O1N	1.95	0.66
2:C:333:HIS:NE2	2:C:389:PHE:O	2.29	0.65
1:F:138:THR:O	1:H:127:GLN:HG2	1.96	0.65
2:E:429:ARG:NH2	1:H:483:LEU:O	2.29	0.65
1:D:284:GLN:HE22	1:D:329:VAL:H	1.43	0.65
2:C:47:GLU:OE1	2:C:219:HIS:HE1	1.78	0.65
1:F:176:LYS:NZ	4:F:1491:NAP:O3X	2.29	0.65
2:E:127:GLN:NE2	2:E:135:PHE:HD1	1.93	0.65
1:B:219:HIS:CD2	1:B:221:LEU:H	2.15	0.65
3:D:1496:GOL:H11	7:D:2312:HOH:O	1.90	0.65
1:F:295:HIS:HD2	1:F:297:SER:H	1.43	0.64
1:B:284:GLN:HE22	1:B:329:VAL:H	1.44	0.64
1:F:284:GLN:HE22	1:F:329:VAL:H	1.44	0.64
2:E:397:VAL:O	2:E:407:ARG:NH2	2.29	0.64
1:F:397:VAL:O	1:F:407:ARG:NH2	2.30	0.64
1:H:328:LEU:HD12	1:H:334:MET:HA	1.78	0.64
1:A:47:GLU:OE1	1:A:219:HIS:HE1	1.82	0.63
1:H:31:ASN:HA	1:H:365:LYS:O	1.98	0.63
1:A:176:LYS:HD2	1:A:212[A]:VAL:HG23	1.79	0.63
3:C:1496:GOL:H31	7:C:2005:HOH:O	1.98	0.63
4:D:1491:NAP:H3B	7:D:2355:HOH:O	1.98	0.62
1:A:176:LYS:HD2	1:A:212[A]:VAL:CG2	2.30	0.62
1:G:47:GLU:OE1	1:G:219:HIS:HE1	1.83	0.62
1:G:475:ARG:HD3	1:H:456:TYR:CZ	2.35	0.62
1:H:160:LEU:HG	1:H:188:LEU:HD21	1.83	0.61
3:D:1496:GOL:H31	7:D:2362:HOH:O	2.01	0.61
1:H:271:ALA:O	1:H:275:VAL:HG22	2.01	0.61
4:B:1491:NAP:O1X	7:B:2399:HOH:O	2.16	0.60
1:F:127:GLN:HE22	1:F:135:PHE:HD1	1.49	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:475:ARG:HD3	1:D:456:TYR:CZ	2.37	0.60
3:B:1495:GOL:H31	3:B:1496:GOL:H11	1.84	0.60
1:D:179:GLU:HB2	4:D:1491:NAP:O3X	2.00	0.60
1:A:176:LYS:HD2	1:A:212[B]:VAL:HG13	1.84	0.59
2:C:246:LEU:HD13	1:D:461:VAL:HG23	1.84	0.59
2:C:456:TYR:CZ	1:D:475:ARG:HD3	2.37	0.59
1:H:296:ARG:HA	1:H:397:VAL:HG12	1.84	0.59
2:E:219:HIS:HD2	2:E:221:LEU:H	1.49	0.59
1:H:54:VAL:O	1:H:58:LYS:HD2	2.01	0.59
1:A:261:ILE:HD12	1:A:270:ALA:HB1	1.84	0.59
2:C:146:VAL:HG12	2:C:224:LYS:HB3	1.84	0.58
2:E:246:LEU:HD11	1:F:253:LEU:CD1	2.32	0.58
1:G:219:HIS:HD2	1:G:221:LEU:H	1.52	0.58
1:A:28:ASN:HD22	1:A:28:ASN:C	2.07	0.58
1:D:379:ASP:OD2	1:D:407:ARG:HD3	2.04	0.58
1:F:296:ARG:HG3	7:F:2225:HOH:O	2.03	0.58
1:A:254:GLY:HA2	5:A:1492:BME:H22	1.85	0.57
1:H:250:THR:HG21	7:H:2288:HOH:O	2.05	0.57
1:H:285:VAL:HB	1:H:288:ASN:OD1	2.04	0.57
1:H:94:THR:OG1	1:H:96:LYS:HG3	2.05	0.57
1:A:152:TRP:CH2	1:A:389:PHE:HE2	2.22	0.57
2:E:157:GLN:OE1	3:E:1495:GOL:H11	2.05	0.56
1:F:238:MET:HG3	1:F:249:VAL:HG21	1.86	0.56
1:H:315:LEU:HD21	1:H:368:TYR:CD1	2.40	0.56
1:A:40:ARG:NH1	1:A:179:GLU:OE1	2.34	0.56
1:H:375:THR:OG1	1:H:376:ASP:N	2.38	0.56
1:H:239:ALA:O	1:H:243:SER:OG	2.22	0.56
1:G:412:GLU:CD	1:G:412:GLU:H	2.09	0.56
2:E:301:ARG:HD3	7:E:2232:HOH:O	2.05	0.56
3:B:1495:GOL:H2	7:B:2370:HOH:O	2.05	0.56
3:B:1495:GOL:H32	7:B:2403:HOH:O	2.06	0.55
1:H:175:PHE:HZ	7:H:2131:HOH:O	1.88	0.55
1:D:219:HIS:CD2	1:D:221:LEU:H	2.18	0.55
1:H:315:LEU:HD21	1:H:368:TYR:HD1	1.71	0.55
1:A:264:ASP:O	1:A:422:GLN:NE2	2.39	0.55
3:E:1496:GOL:O3	7:E:2357:HOH:O	1.93	0.55
2:C:213:GLY:O	2:C:217:THR:HG23	2.08	0.54
2:E:456:TYR:CZ	1:F:475:ARG:HD3	2.42	0.54
1:F:295:HIS:CD2	1:F:297:SER:H	2.22	0.54
1:H:29:PRO:HD3	7:H:2080:HOH:O	2.08	0.54
1:G:379:ASP:OD2	1:G:407:ARG:CD	2.56	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1492:BME:H11	7:B:2402:HOH:O	2.06	0.54
1:B:179:GLU:HB2	4:B:1491:NAP:O3X	2.07	0.54
1:H:314:ARG:HD3	7:H:2211:HOH:O	2.07	0.54
1:F:250:THR:HG22	1:F:252[B]:GLU:OE2	2.07	0.53
1:H:6:GLU:HG3	1:H:37:LYS:HB3	1.89	0.53
2:E:406:ARG:HH11	2:E:406:ARG:HG2	1.73	0.53
1:F:102:ARG:HD3	7:F:2095:HOH:O	2.07	0.53
1:D:152:TRP:CH2	1:D:389:PHE:HE2	2.26	0.53
4:E:1491:NAP:H52A	7:E:2350:HOH:O	2.09	0.53
2:E:176:LYS:HD2	2:E:212[B]:VAL:HG13	1.90	0.53
2:E:475:ARG:HD3	1:F:456:TYR:CZ	2.44	0.53
1:F:128:ILE:HD12	1:F:136:VAL:HG22	1.91	0.53
1:G:128:ILE:HD12	1:G:136:VAL:HG22	1.88	0.53
1:H:282:SER:HA	1:H:325:PHE:CE1	2.44	0.53
1:B:379:ASP:OD2	1:B:407:ARG:HD3	2.09	0.53
1:H:219:HIS:HD2	1:H:221:LEU:H	1.57	0.53
1:A:231:THR:HA	1:A:253:LEU:HD13	1.89	0.53
2:C:297:SER:CB	7:C:2223:HOH:O	2.14	0.53
3:C:1497:GOL:H12	7:C:2146:HOH:O	2.08	0.53
1:B:379:ASP:OD2	1:B:407:ARG:CD	2.57	0.53
2:C:246:LEU:HD22	1:D:238:MET:SD	2.49	0.53
1:G:250:THR:HG22	1:G:252[B]:GLU:OE2	2.08	0.53
3:E:1496:GOL:H12	7:E:2230:HOH:O	2.09	0.52
1:H:31:ASN:ND2	7:H:2024:HOH:O	2.41	0.52
1:A:379:ASP:OD2	1:A:407:ARG:CD	2.58	0.52
2:E:334:MET:HG3	2:E:369:VAL:HG23	1.91	0.52
1:F:229:GLY:O	1:F:253:LEU:HA	2.09	0.52
1:D:379:ASP:OD2	1:D:407:ARG:CD	2.58	0.52
1:A:250:THR:CG2	1:A:252[B]:GLU:OE2	2.58	0.52
1:H:262:PHE:HB3	1:H:263:PRO:HD2	1.92	0.52
1:A:227:PHE:HE1	4:A:1491:NAP:O4B	1.93	0.51
1:F:210:ARG:HH12	4:F:1491:NAP:H61A	1.59	0.51
1:H:31:ASN:HB2	1:H:365:LYS:HE2	1.91	0.51
1:H:315:LEU:N	7:H:2214:HOH:O	2.43	0.51
1:D:102:ARG:HD3	7:D:2084:HOH:O	2.08	0.51
1:H:261:ILE:HD12	1:H:270:ALA:HB1	1.92	0.51
1:B:333:HIS:NE2	1:B:389:PHE:O	2.40	0.51
1:F:176:LYS:HD2	1:F:212[A]:VAL:HG22	1.93	0.51
2:E:307:LEU:CD2	3:E:1496:GOL:H2	2.41	0.51
1:H:127:GLN:HE22	1:H:135:PHE:HD1	1.58	0.51
2:E:379:ASP:OD2	2:E:407:ARG:HD2	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:HIS:HD2	1:A:297:SER:OG	1.93	0.51
1:G:229:GLY:HA2	5:G:1492[B]:BME:H11	1.93	0.51
1:H:307:LEU:CD1	1:H:353:CYS:HB3	2.41	0.51
1:D:47:GLU:OE1	1:D:219:HIS:HE1	1.94	0.51
1:A:475:ARG:HD3	1:B:456:TYR:CZ	2.46	0.51
1:B:143:LEU:HD23	1:B:475:ARG:CG	2.41	0.51
2:E:138:THR:O	1:G:127:GLN:HG2	2.11	0.51
2:C:262:PHE:HE1	2:C:401:GLU:HG3	1.76	0.51
4:A:1491:NAP:O2A	3:A:1501:GOL:O1	2.25	0.50
2:E:47:GLU:OE1	2:E:219:HIS:HE1	1.95	0.50
1:F:90:GLU:OE2	1:F:155:PRO:HD2	2.12	0.50
2:C:28:ASN:HB2	2:C:35:LEU:HD21	1.93	0.50
1:H:256:LYS:NZ	1:H:383:ILE:O	2.29	0.50
1:A:456:TYR:CZ	1:B:475:ARG:HD3	2.47	0.49
1:G:472:HIS:NE2	1:H:472:HIS:NE2	2.54	0.49
1:G:217:THR:HG21	1:G:237:VAL:HG13	1.93	0.49
1:A:284:GLN:HE22	1:A:329:VAL:H	1.60	0.49
1:F:219:HIS:CD2	1:F:221:LEU:H	2.26	0.49
1:H:164:ALA:HB3	1:H:165:PRO:CD	2.42	0.49
1:G:40:ARG:NH1	1:G:179:GLU:OE1	2.39	0.49
1:G:295:HIS:HE1	1:G:399:ASP:O	1.95	0.49
1:H:359:THR:HA	1:H:363:PHE:HB2	1.95	0.49
1:H:397:VAL:O	1:H:407:ARG:NH2	2.45	0.49
1:D:261:ILE:HD12	1:D:270:ALA:HB1	1.95	0.49
1:B:328:LEU:HD12	1:B:334:MET:HA	1.93	0.49
2:C:429:ARG:NH2	7:C:2308:HOH:O	2.46	0.49
1:F:208:SER:O	1:F:212[B]:VAL:HG12	2.12	0.49
1:B:295:HIS:CD2	1:B:297:SER:OG	2.60	0.49
2:C:262:PHE:CE1	2:C:401:GLU:HG3	2.48	0.49
1:H:160:LEU:HD21	1:H:188:LEU:HD11	1.95	0.48
2:C:264:ASP:O	2:C:422:GLN:NE2	2.45	0.48
2:E:127:GLN:NE2	2:E:135:PHE:CD1	2.78	0.48
1:D:267:LEU:HB3	1:D:305:LYS:HE3	1.94	0.48
1:G:152:TRP:CH2	1:G:389:PHE:CE2	3.01	0.48
1:G:379:ASP:OD2	1:G:407:ARG:HD2	2.13	0.48
1:G:379:ASP:OD2	1:G:407:ARG:HD3	2.13	0.48
1:A:43:ARG:HG3	1:A:215:TRP:CE2	2.49	0.48
1:A:238:MET:HG3	1:A:249:VAL:HG21	1.94	0.48
1:F:306:VAL:O	1:F:310:VAL:HG23	2.14	0.48
1:F:262:PHE:CG	1:F:426:ARG:HD3	2.48	0.48
2:E:295:HIS:CD2	2:E:297:SER:H	2.32	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:GLU:HG2	1:F:37[B]:LYS:HD3	1.96	0.48
1:F:231:THR:HA	1:F:253:LEU:HD13	1.96	0.48
1:G:345:LYS:HE2	1:G:351:LEU:HD22	1.94	0.47
1:H:285:VAL:HG21	7:H:2196:HOH:O	2.13	0.47
1:A:152:TRP:NE1	4:A:1491:NAP:O2N	2.46	0.47
2:E:307:LEU:O	2:E:311:GLN:HG3	2.14	0.47
2:C:331:PHE:HD2	7:C:2249:HOH:O	1.96	0.47
1:D:301:ARG:HG3	7:D:2229:HOH:O	2.13	0.47
1:D:152:TRP:CH2	1:D:389:PHE:CE2	3.02	0.47
2:C:2:ALA:N	7:C:2001:HOH:O	2.48	0.47
1:H:176:LYS:NZ	4:H:1491:NAP:O3X	2.47	0.47
1:B:102:ARG:NH2	1:B:321:GLU:OE1	2.47	0.47
1:H:94:THR:HG22	1:H:181:THR:HG21	1.96	0.47
2:C:53:ALA:HB2	7:C:2173:HOH:O	2.13	0.47
2:E:256:LYS:HE2	2:E:384:VAL:O	2.15	0.47
4:G:1491:NAP:O1X	7:G:2356:HOH:O	2.20	0.47
2:C:176:LYS:HD2	2:C:212[B]:VAL:HG13	1.97	0.47
1:A:152:TRP:CE3	1:A:329:VAL:HG11	2.50	0.47
4:A:1491:NAP:H3B	7:A:2410:HOH:O	2.14	0.46
1:D:261:ILE:HB	1:D:294:ILE:HD12	1.96	0.46
1:G:376:ASP:OD2	7:G:2274:HOH:O	2.21	0.46
2:E:456:TYR:CE2	1:F:475:ARG:HD3	2.51	0.46
1:G:222:ILE:O	1:G:247:LYS:HE3	2.15	0.46
5:F:1492:BME:H11	7:F:2344:HOH:O	2.15	0.46
1:G:284:GLN:HE22	1:G:329:VAL:N	2.12	0.46
1:A:76:VAL:O	1:A:80:ARG:HG2	2.16	0.46
2:E:128:ILE:HD12	2:E:136:VAL:HG22	1.97	0.46
1:A:275[B]:VAL:HG12	1:B:490:PHE:CD2	2.51	0.46
1:B:82:ARG:NH2	1:B:194:GLU:OE1	2.45	0.46
3:H:1495:GOL:H32	7:H:2129:HOH:O	2.15	0.46
1:H:60:TRP:HB2	1:H:201:VAL:HG21	1.97	0.46
1:H:305:LYS:HB3	1:H:309:ARG:NH1	2.30	0.46
2:E:307:LEU:HD23	3:E:1496:GOL:H2	1.97	0.45
1:B:98:LEU:O	1:B:102:ARG:HB2	2.15	0.45
1:H:23:THR:HG22	1:H:39:GLN:HA	1.99	0.45
2:E:76:VAL:O	2:E:80:ARG:HG2	2.16	0.45
1:H:7:GLN:HB2	1:H:38:VAL:HG13	1.98	0.45
1:F:95:GLY:HA2	7:F:2102:HOH:O	2.16	0.45
1:A:271:ALA:O	1:A:275[A]:VAL:HG22	2.17	0.45
3:G:1495:GOL:H12	3:G:1496:GOL:O2	2.17	0.45
1:F:310:VAL:HG12	7:F:2261:HOH:O	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:242:SER:HB3	1:H:238:MET:HB3	1.98	0.45
1:G:250:THR:CG2	1:G:252[B]:GLU:OE2	2.65	0.45
1:H:24:PHE:HA	7:H:2019:HOH:O	2.17	0.45
1:D:120:VAL:HB	1:D:121:PRO:HD3	1.99	0.45
2:E:3:ARG:HG3	2:E:3:ARG:O	2.13	0.44
1:B:176:LYS:HG3	1:B:212[A]:VAL:HG23	1.98	0.44
2:C:328:LEU:HD21	2:C:391:PRO:HD3	2.00	0.44
1:A:254:GLY:CA	5:A:1492:BME:H22	2.47	0.44
2:E:3:ARG:NH2	7:E:2002:HOH:O	2.35	0.44
1:H:352:LEU:HB3	1:H:373:VAL:HG12	1.99	0.44
1:D:7:GLN:HA	3:D:1495:GOL:H12	1.98	0.44
2:C:152:TRP:CE3	2:C:329:VAL:HG11	2.53	0.44
1:A:397:VAL:O	1:A:407:ARG:NH2	2.50	0.44
1:F:152:TRP:CH2	1:F:389:PHE:CE2	3.06	0.44
1:F:209:GLY:HA3	4:F:1491:NAP:C4A	2.46	0.44
1:B:176:LYS:HG3	1:B:212[A]:VAL:CG2	2.47	0.44
1:A:328:LEU:HD12	1:A:334:MET:HA	1.99	0.44
1:G:161:TRP:HZ3	3:G:1495:GOL:H11	1.82	0.44
1:B:143:LEU:HD23	1:B:475:ARG:HG2	1.99	0.44
2:E:214:GLN:HG3	2:E:214:GLN:O	2.17	0.44
1:D:333:HIS:NE2	1:D:389:PHE:O	2.42	0.44
1:G:120:VAL:HB	1:G:121:PRO:HD3	1.99	0.44
1:H:307:LEU:HB2	1:H:352:LEU:HD21	2.00	0.43
4:B:1491:NAP:H3B	7:B:2399:HOH:O	2.18	0.43
2:C:379:ASP:OD2	2:C:407:ARG:HD2	2.18	0.43
4:A:1491:NAP:H8A	3:A:1501:GOL:C2	2.47	0.43
2:E:429:ARG:HG2	7:E:2301:HOH:O	2.18	0.43
2:E:403:GLU:O	2:E:407:ARG:HG3	2.19	0.43
1:H:312:ARG:HG2	7:H:2208:HOH:O	2.17	0.43
2:C:127:GLN:NE2	7:C:2124:HOH:O	2.50	0.43
4:D:1491:NAP:H8A	4:D:1491:NAP:PN	2.59	0.43
1:A:122:ALA:HB2	1:D:119:LEU:HD21	2.00	0.43
1:B:143:LEU:HD23	1:B:475:ARG:HG3	2.00	0.43
1:F:213:GLY:O	1:F:217:THR:HG23	2.18	0.43
1:F:119:LEU:HD21	1:G:122:ALA:HB2	1.99	0.43
1:A:152:TRP:CZ2	1:A:389:PHE:CE2	3.07	0.43
1:G:231:THR:HA	1:G:253:LEU:HD13	2.00	0.43
1:H:324:ASN:ND2	7:H:2219:HOH:O	2.24	0.42
1:F:278:ASN:O	1:F:283:GLY:HA2	2.19	0.42
1:H:102:ARG:NH2	1:H:321:GLU:HG3	2.33	0.42
1:D:284:GLN:HE22	1:D:329:VAL:N	2.15	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:217:THR:HG21	1:F:237:VAL:HG13	2.01	0.42
2:C:416:ALA:HA	2:C:438:ILE:O	2.19	0.42
2:E:50:VAL:O	2:E:54:VAL:HG23	2.18	0.42
1:B:152:TRP:CE3	1:B:329:VAL:HG11	2.54	0.42
1:A:152:TRP:CZ2	1:A:389:PHE:HE2	2.37	0.42
1:F:398:TYR:HA	7:F:2279:HOH:O	2.19	0.42
1:A:176:LYS:HD3	1:A:212[A]:VAL:HG23	1.98	0.42
1:D:227:PHE:HE1	4:D:1491:NAP:O4B	2.02	0.42
1:F:475:ARG:HD2	7:F:2328:HOH:O	2.19	0.42
2:E:8:LYS:NZ	2:E:17:GLU:OE2	2.45	0.42
1:B:227:PHE:HE1	4:B:1491:NAP:O4B	2.03	0.42
1:G:285:VAL:HB	1:G:288:ASN:OD1	2.20	0.42
1:A:333:HIS:NE2	1:A:389:PHE:O	2.41	0.42
1:G:431:ILE:HD12	1:G:434:LEU:HD12	2.02	0.41
1:F:250:THR:HG21	1:F:252[B]:GLU:OE2	2.19	0.41
1:A:53:ALA:HA	1:A:200:GLY:O	2.20	0.41
1:H:417:ALA:HB1	1:H:434:LEU:HD13	2.01	0.41
2:C:120:VAL:HB	2:C:121:PRO:HD3	2.02	0.41
1:D:235:LYS:HE2	1:D:458:GLN:OE1	2.20	0.41
1:G:140:ARG:NH2	7:G:2141:HOH:O	2.38	0.41
1:B:119:LEU:HD21	2:C:122:ALA:HB2	2.02	0.41
1:F:328:LEU:HD21	1:F:391:PRO:HD3	2.02	0.41
1:H:299:GLN:NE2	1:H:303:GLU:OE2	2.48	0.41
1:H:127:GLN:HE21	1:H:127:GLN:HB2	1.38	0.41
2:C:250:THR:HG22	2:C:252[B]:GLU:OE2	2.21	0.41
2:C:219:HIS:CD2	2:C:221:LEU:H	2.25	0.41
1:F:378:ARG:HH21	1:F:378:ARG:HG2	1.85	0.41
2:E:219:HIS:CD2	2:E:221:LEU:H	2.35	0.41
1:B:379:ASP:OD2	1:B:407:ARG:HD2	2.20	0.41
1:A:328:LEU:HD21	1:A:391:PRO:HD3	2.03	0.41
1:H:264:ASP:OD2	7:H:2184:HOH:O	2.22	0.41
2:E:262:PHE:CG	2:E:426:ARG:HD3	2.56	0.41
1:G:152:TRP:CH2	1:G:389:PHE:CD2	3.09	0.41
4:D:1491:NAP:H2B	4:D:1491:NAP:O1N	2.20	0.41
1:A:253:LEU:HD12	1:B:246[B]:LEU:HD22	2.02	0.41
1:A:213:GLY:O	1:A:217:THR:HG23	2.21	0.41
1:H:279:PHE:CE2	1:H:310:VAL:HG22	2.56	0.41
1:D:328:LEU:HD12	1:D:334:MET:HA	2.02	0.41
2:E:328:LEU:HD21	2:E:391:PRO:HD3	2.02	0.41
1:H:241:ALA:HB1	1:H:247:LYS:HB2	2.02	0.41
1:F:307:LEU:O	1:F:311:GLN:HG3	2.21	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:176:LYS:HD2	1:H:212:VAL:HG23	2.03	0.40
1:F:333:HIS:NE2	1:F:389:PHE:O	2.45	0.40
1:H:79:LEU:HD22	1:H:106:ILE:HG23	2.02	0.40
4:A:1491:NAP:H2B	3:A:1501:GOL:H11	2.04	0.40
1:A:98:LEU:O	1:A:102:ARG:HG3	2.21	0.40
1:H:96:LYS:NZ	7:H:2090:HOH:O	2.39	0.40
1:B:472:HIS:HB2	7:B:2375:HOH:O	2.20	0.40
1:F:273:ILE:HG23	1:F:444:TRP:HB2	2.03	0.40
2:E:227:PHE:HE1	4:E:1491:NAP:O4B	2.04	0.40
1:H:306:VAL:O	1:H:310:VAL:HG23	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	497/490 (101%)	480 (97%)	17 (3%)	0	100	100
1	B	494/490 (101%)	480 (97%)	14 (3%)	0	100	100
1	D	487/490 (99%)	470 (96%)	17 (4%)	0	100	100
1	F	492/490 (100%)	481 (98%)	11 (2%)	0	100	100
1	G	488/490 (100%)	474 (97%)	13 (3%)	1 (0%)	52	53
1	H	488/490 (100%)	462 (95%)	25 (5%)	1 (0%)	52	53
2	C	488/490 (100%)	473 (97%)	14 (3%)	1 (0%)	52	53
2	E	489/490 (100%)	468 (96%)	21 (4%)	0	100	100
All	All	3923/3920 (100%)	3788 (97%)	132 (3%)	3 (0%)	56	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	363	PHE
2	C	414	GLY
1	G	414	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	400/391 (102%)	390 (98%)	10 (2%)	55	59
1	B	397/391 (102%)	385 (97%)	12 (3%)	48	51
1	D	390/391 (100%)	383 (98%)	7 (2%)	66	72
1	F	395/391 (101%)	382 (97%)	13 (3%)	45	47
1	G	391/391 (100%)	381 (97%)	10 (3%)	54	58
1	H	391/391 (100%)	375 (96%)	16 (4%)	37	36
2	C	391/390 (100%)	380 (97%)	11 (3%)	51	55
2	E	392/390 (100%)	379 (97%)	13 (3%)	45	47
All	All	3147/3126 (101%)	3055 (97%)	92 (3%)	50	53

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	28	ASN
1	A	42[A]	SER
1	A	42[B]	SER
1	A	98	LEU
1	A	136	VAL
1	A	232	SER
1	A	365	LYS
1	A	385	ARG
1	A	475	ARG
1	B	8	LYS
1	B	42[A]	SER
1	B	42[B]	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	43	ARG
1	B	98	LEU
1	B	102	ARG
1	B	214	GLN
1	B	322	ASN
1	B	365	LYS
1	B	378	ARG
1	B	389	PHE
1	B	475	ARG
2	C	5	GLU
2	C	8	LYS
2	C	43	ARG
2	C	103	SER
2	C	210	ARG
2	C	246	LEU
2	C	301	ARG
2	C	378	ARG
2	C	389	PHE
2	C	412	GLU
2	C	475	ARG
1	D	8	LYS
1	D	43	ARG
1	D	98	LEU
1	D	212	VAL
1	D	268	ASP
1	D	385	ARG
1	D	475	ARG
2	E	3	ARG
2	E	8	LYS
2	E	37	LYS
2	E	42[A]	SER
2	E	42[B]	SER
2	E	127	GLN
2	E	176	LYS
2	E	214	GLN
2	E	281	SER
2	E	335	GLU
2	E	343	SER
2	E	431	ILE
2	E	475	ARG
1	F	8	LYS
1	F	42	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	52	SER
1	F	127	GLN
1	F	210	ARG
1	F	322	ASN
1	F	335	GLU
1	F	356	GLU
1	F	389	PHE
1	F	400	ASP
1	F	412	GLU
1	F	429	ARG
1	F	475	ARG
1	G	8	LYS
1	G	43	ARG
1	G	127	GLN
1	G	212	VAL
1	G	214	GLN
1	G	322	ASN
1	G	365	LYS
1	G	378	ARG
1	G	389	PHE
1	G	475	ARG
1	H	8	LYS
1	H	42	SER
1	H	58	LYS
1	H	82	ARG
1	H	127	GLN
1	H	214	GLN
1	H	287	THR
1	H	329	VAL
1	H	347	GLN
1	H	385	ARG
1	H	389	PHE
1	H	396	LEU
1	H	397	VAL
1	H	412	GLU
1	H	464	GLU
1	H	475	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	28	ASN
1	A	83	ASN
1	A	219	HIS
1	A	284	GLN
1	A	295	HIS
1	B	7	GLN
1	B	83	ASN
1	B	127	GLN
1	B	219	HIS
1	B	284	GLN
1	B	295	HIS
2	C	7	GLN
2	C	83	ASN
2	C	127	GLN
2	C	219	HIS
2	C	284	GLN
2	C	295	HIS
2	C	319	GLN
1	D	7	GLN
1	D	83	ASN
1	D	219	HIS
1	D	284	GLN
1	D	295	HIS
2	E	7	GLN
2	E	83	ASN
2	E	127	GLN
2	E	219	HIS
2	E	284	GLN
2	E	295	HIS
1	F	7	GLN
1	F	83	ASN
1	F	219	HIS
1	F	284	GLN
1	F	295	HIS
1	F	465	ASN
1	G	7	GLN
1	G	83	ASN
1	G	219	HIS
1	G	284	GLN
1	G	295	HIS
1	H	31	ASN
1	H	83	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	127	GLN
1	H	219	HIS
1	H	284	GLN
1	H	295	HIS

### 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$
2	CSO	C	286[A]	2	3,6,7	0.75	0	1,6,8	2.32	1 (100%)
2	CSO	C	286[B]	2	3,6,7	0.67	0	1,6,8	1.74	0
2	CSO	E	286	2	3,6,7	0.82	0	1,6,8	1.74	0

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
2	CSO	C	286[A]	2	-	0/1/5/7	0/0/0/0
2	CSO	C	286[B]	2	-	0/1/5/7	0/0/0/0
2	CSO	E	286	2	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	286[A]	CSO	O-C-CA	-2.32	119.43	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	286[B]	CSO	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 16 are monoatomic - leaving 36 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	NAP	A	1491	-	27,33,52	0.97	1 (3%)	34,52,80	2.39	6 (17%)
5	BME	A	1492	-	3,3,3	0.30	0	2,2,2	0.70	0
3	GOL	A	1496	-	5,5,5	0.70	0	5,5,5	0.95	0
3	GOL	A	1497	-	5,5,5	0.43	0	5,5,5	0.38	0
3	GOL	A	1498	-	5,5,5	0.50	0	5,5,5	0.56	0
3	GOL	A	1499	-	5,5,5	0.22	0	5,5,5	0.81	0
3	GOL	A	1500	-	5,5,5	0.87	0	5,5,5	1.37	1 (20%)
3	GOL	A	1501	-	5,5,5	0.52	0	5,5,5	0.65	0
4	NAP	B	1491	-	27,33,52	1.04	1 (3%)	34,52,80	1.92	4 (11%)
5	BME	B	1492	-	3,3,3	0.54	0	2,2,2	0.44	0
3	GOL	B	1495	-	5,5,5	0.59	0	5,5,5	0.60	0
3	GOL	B	1496	-	5,5,5	1.04	0	5,5,5	1.41	1 (20%)
3	GOL	B	1497	-	5,5,5	0.38	0	5,5,5	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAP	C	1491	-	27,33,52	1.13	2 (7%)	34,52,80	2.32	7 (20%)
3	GOL	C	1495	-	5,5,5	0.59	0	5,5,5	0.58	0
3	GOL	C	1496	-	5,5,5	0.73	0	5,5,5	0.56	0
3	GOL	C	1497	-	5,5,5	0.45	0	5,5,5	0.73	0
4	NAP	D	1491	-	27,33,52	0.93	1 (3%)	34,52,80	2.27	5 (14%)
5	BME	D	1492[A]	-	3,3,3	0.22	0	2,2,2	0.80	0
5	BME	D	1492[B]	-	3,3,3	0.63	0	2,2,2	0.27	0
3	GOL	D	1495	-	5,5,5	0.26	0	5,5,5	0.20	0
3	GOL	D	1496	-	5,5,5	0.66	0	5,5,5	0.48	0
4	NAP	E	1491	-	27,33,52	1.22	2 (7%)	34,52,80	2.23	5 (14%)
3	GOL	E	1495	-	5,5,5	0.31	0	5,5,5	0.41	0
3	GOL	E	1496	-	5,5,5	0.40	0	5,5,5	0.76	0
4	NAP	F	1491	-	27,33,52	1.04	2 (7%)	34,52,80	2.38	8 (23%)
5	BME	F	1492	-	3,3,3	0.79	0	2,2,2	0.43	0
3	GOL	F	1495	-	5,5,5	0.35	0	5,5,5	0.56	0
4	NAP	G	1491	-	27,33,52	0.93	1 (3%)	34,52,80	2.27	5 (14%)
5	BME	G	1492[A]	-	3,3,3	0.51	0	2,2,2	0.39	0
5	BME	G	1492[B]	-	3,3,3	0.51	0	2,2,2	0.33	0
3	GOL	G	1495	-	5,5,5	0.45	0	5,5,5	0.78	0
3	GOL	G	1496	-	5,5,5	0.39	0	5,5,5	0.70	0
3	GOL	G	1497	-	5,5,5	0.52	0	5,5,5	0.42	0
4	NAP	H	1491	-	27,33,52	0.81	0	34,52,80	2.06	2 (5%)
3	GOL	H	1495	-	5,5,5	0.56	0	5,5,5	0.64	0

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	NAP	A	1491	-	-	0/17/37/67	0/3/3/5
5	BME	A	1492	-	-	0/1/1/1	0/0/0/0
3	GOL	A	1496	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1497	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1498	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1499	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1500	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1501	-	-	0/4/4/4	0/0/0/0
4	NAP	B	1491	-	-	0/17/37/67	0/3/3/5
5	BME	B	1492	-	-	0/1/1/1	0/0/0/0
3	GOL	B	1495	-	-	0/4/4/4	0/0/0/0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	1496	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1497	-	-	0/4/4/4	0/0/0/0
4	NAP	C	1491	-	-	0/17/37/67	0/3/3/5
3	GOL	C	1495	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1496	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1497	-	-	0/4/4/4	0/0/0/0
4	NAP	D	1491	-	-	0/17/37/67	0/3/3/5
5	BME	D	1492[A]	-	-	0/1/1/1	0/0/0/0
5	BME	D	1492[B]	-	-	0/1/1/1	0/0/0/0
3	GOL	D	1495	-	-	0/4/4/4	0/0/0/0
3	GOL	D	1496	-	-	0/4/4/4	0/0/0/0
4	NAP	E	1491	-	-	0/17/37/67	0/3/3/5
3	GOL	E	1495	-	-	0/4/4/4	0/0/0/0
3	GOL	E	1496	-	-	0/4/4/4	0/0/0/0
4	NAP	F	1491	-	-	0/17/37/67	0/3/3/5
5	BME	F	1492	-	-	0/1/1/1	0/0/0/0
3	GOL	F	1495	-	-	0/4/4/4	0/0/0/0
4	NAP	G	1491	-	-	0/17/37/67	0/3/3/5
5	BME	G	1492[A]	-	-	0/1/1/1	0/0/0/0
5	BME	G	1492[B]	-	-	0/1/1/1	0/0/0/0
3	GOL	G	1495	-	-	0/4/4/4	0/0/0/0
3	GOL	G	1496	-	-	0/4/4/4	0/0/0/0
3	GOL	G	1497	-	-	0/4/4/4	0/0/0/0
4	NAP	H	1491	-	-	0/17/37/67	0/3/3/5
3	GOL	H	1495	-	-	0/4/4/4	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1491	NAP	C2A-N3A	2.03	1.35	1.32
4	C	1491	NAP	C2A-N3A	2.22	1.36	1.32
4	B	1491	NAP	O4B-C1B	2.40	1.44	1.41
4	F	1491	NAP	C4A-N3A	2.50	1.39	1.35
4	F	1491	NAP	O4B-C1B	2.50	1.44	1.41
4	D	1491	NAP	O4B-C1B	2.67	1.44	1.41
4	G	1491	NAP	O4B-C1B	2.95	1.44	1.41
4	E	1491	NAP	PN-O3	3.09	1.68	1.61
4	C	1491	NAP	O4B-C1B	3.23	1.45	1.41
4	E	1491	NAP	O4B-C1B	3.55	1.45	1.41

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1491	NAP	N3A-C2A-N1A	-11.72	119.92	128.89
4	D	1491	NAP	N3A-C2A-N1A	-11.57	120.03	128.89
4	F	1491	NAP	N3A-C2A-N1A	-11.03	120.45	128.89
4	G	1491	NAP	N3A-C2A-N1A	-10.82	120.61	128.89
4	C	1491	NAP	N3A-C2A-N1A	-10.36	120.96	128.89
4	E	1491	NAP	N3A-C2A-N1A	-10.32	121.00	128.89
4	H	1491	NAP	N3A-C2A-N1A	-10.15	121.12	128.89
4	B	1491	NAP	N3A-C2A-N1A	-9.26	121.80	128.89
4	C	1491	NAP	C1B-N9A-C4A	-3.99	120.92	126.94
4	C	1491	NAP	C4A-C5A-N7A	-3.76	106.02	109.48
4	F	1491	NAP	O4B-C1B-C2B	-3.76	99.81	106.60
4	A	1491	NAP	C1B-N9A-C4A	-3.35	121.89	126.94
4	E	1491	NAP	O4B-C1B-C2B	-3.20	100.82	106.60
4	B	1491	NAP	O4B-C1B-C2B	-3.11	100.97	106.60
4	E	1491	NAP	C4A-C5A-N7A	-2.67	107.02	109.48
4	D	1491	NAP	C1B-N9A-C4A	-2.55	123.10	126.94
4	G	1491	NAP	O3-PN-O1N	-2.54	99.76	107.70
4	B	1491	NAP	C4A-C5A-N7A	-2.44	107.23	109.48
4	H	1491	NAP	O2B-P2B-O1X	-2.40	101.11	107.11
4	G	1491	NAP	C1B-N9A-C4A	-2.31	123.45	126.94
4	G	1491	NAP	O4B-C1B-C2B	-2.28	102.48	106.60
4	F	1491	NAP	C4A-C5A-N7A	-2.12	107.53	109.48
4	A	1491	NAP	C4A-C5A-N7A	-2.09	107.55	109.48
4	A	1491	NAP	O4B-C1B-C2B	-2.04	102.90	106.60
4	D	1491	NAP	O4B-C1B-C2B	-2.04	102.91	106.60
4	C	1491	NAP	P2B-O2B-C2B	2.03	126.43	121.56
4	F	1491	NAP	O3X-P2B-O2X	2.09	115.33	107.38
4	E	1491	NAP	O3-PA-O5B	2.09	108.48	102.94
4	B	1491	NAP	O2X-P2B-O1X	2.09	117.32	110.58
3	B	1496	GOL	O1-C1-C2	2.13	120.53	110.18
4	C	1491	NAP	O3-PA-O5B	2.16	108.66	102.94
4	D	1491	NAP	C2A-N1A-C6A	2.19	122.67	118.77
4	A	1491	NAP	O3X-P2B-O2X	2.23	115.86	107.38
4	A	1491	NAP	C4B-O4B-C1B	2.26	112.20	109.72
4	D	1491	NAP	O3X-P2B-O1X	2.30	117.98	110.58
4	F	1491	NAP	C4B-O4B-C1B	2.36	112.31	109.72
3	A	1500	GOL	O1-C1-C2	2.41	121.89	110.18
4	F	1491	NAP	O2B-C2B-C3B	2.48	121.16	111.51
4	C	1491	NAP	O3X-P2B-O2X	2.53	117.03	107.38
4	G	1491	NAP	O3X-P2B-O2X	2.68	117.58	107.38
4	F	1491	NAP	O2X-P2B-O1X	2.80	119.58	110.58
4	F	1491	NAP	O4B-C1B-N9A	3.19	114.78	108.10
4	C	1491	NAP	O4B-C1B-N9A	3.59	115.62	108.10

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1491	NAP	C4B-O4B-C1B	3.84	113.94	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

25 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1491	NAP	9	0
5	A	1492	BME	3	0
3	A	1501	GOL	6	0
4	B	1491	NAP	4	0
5	B	1492	BME	1	0
3	B	1495	GOL	3	0
3	B	1496	GOL	1	0
3	C	1496	GOL	1	0
3	C	1497	GOL	1	0
4	D	1491	NAP	7	0
3	D	1495	GOL	1	0
3	D	1496	GOL	6	0
4	E	1491	NAP	2	0
3	E	1495	GOL	1	0
3	E	1496	GOL	5	0
4	F	1491	NAP	3	0
5	F	1492	BME	2	0
3	F	1495	GOL	1	0
4	G	1491	NAP	1	0
5	G	1492[A]	BME	1	0
5	G	1492[B]	BME	2	0
3	G	1495	GOL	4	0
3	G	1496	GOL	1	0
4	H	1491	NAP	2	0
3	H	1495	GOL	1	0

## 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	489/490 (99%)	-0.16	1 (0%) 95 96	9, 20, 25, 36	0
1	B	489/490 (99%)	-0.12	0 100 100	10, 20, 26, 36	0
1	D	489/490 (99%)	-0.06	4 (0%) 87 90	10, 20, 27, 33	0
1	F	489/490 (99%)	0.13	13 (2%) 58 65	12, 21, 28, 34	0
1	G	489/490 (99%)	-0.09	4 (0%) 87 90	12, 20, 27, 35	0
1	H	489/490 (99%)	1.04	93 (19%) 2 2	15, 23, 31, 37	0
2	C	488/490 (99%)	-0.03	7 (1%) 78 82	11, 20, 27, 36	0
2	E	488/490 (99%)	-0.13	2 (0%) 93 94	10, 20, 26, 33	0
All	All	3910/3920 (99%)	0.07	124 (3%) 51 60	9, 20, 28, 37	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	362	ALA	6.1
1	H	363	PHE	5.8
1	H	359	THR	5.8
1	H	98	LEU	4.8
1	H	382	THR	4.7
1	H	212	VAL	4.5
1	H	318	PRO	4.4
1	H	307	LEU	4.2
1	H	380	ASP	4.2
1	H	310	VAL	4.0
1	H	12	GLY	4.0
1	H	335	GLU	4.0
1	H	331	PHE	4.0
1	H	366	GLY	3.9
1	F	359	THR	3.7
1	H	18	ALA	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	360	ASP	3.7
1	H	44	GLU	3.6
1	H	215	TRP	3.6
1	H	2	ALA	3.6
1	G	467	LEU	3.5
1	H	323	THR	3.5
2	C	360	ASP	3.5
1	H	365	LYS	3.4
1	H	378	ARG	3.4
1	D	362	ALA	3.4
1	H	21	GLY	3.4
1	H	321	GLU	3.3
1	H	9	LEU	3.2
1	H	186	LEU	3.2
1	H	325	PHE	3.2
1	H	3	ARG	3.2
1	H	358	VAL	3.2
1	F	346	ALA	3.1
1	H	330	SER	3.1
1	H	54	VAL	3.1
1	H	355	GLY	3.1
2	E	307	LEU	3.1
1	H	201	VAL	3.0
1	H	367	ALA	2.9
1	F	363	PHE	2.9
2	C	359	THR	2.9
1	H	92	LEU	2.8
1	H	183	LEU	2.8
1	H	329	VAL	2.8
1	H	43	ARG	2.8
1	D	361	GLY	2.8
1	H	28	ASN	2.8
1	F	380	ASP	2.8
1	H	372	THR	2.7
1	G	468	THR	2.7
1	H	152	TRP	2.7
1	H	26	THR	2.7
1	H	34	VAL	2.7
1	F	348	LYS	2.6
1	H	19	SER	2.6
1	H	327	PRO	2.6
1	H	368	TYR	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	351	LEU	2.6
1	H	128	ILE	2.6
1	H	102	ARG	2.6
1	H	349	ALA	2.6
1	H	6	GLU	2.5
1	D	360	ASP	2.5
1	H	48	ARG	2.5
1	H	364	GLY	2.5
1	H	385	ARG	2.5
1	H	39	GLN	2.5
1	H	86	LEU	2.5
1	H	399	ASP	2.5
1	H	347	GLN	2.5
1	H	10	TYR	2.4
1	H	16	VAL	2.4
1	H	30	ALA	2.4
1	H	300	ALA	2.4
2	C	348	LYS	2.4
1	F	352	LEU	2.4
1	H	361	GLY	2.4
1	H	32	GLY	2.4
1	H	313	ILE	2.4
1	H	383	ILE	2.4
1	F	361	GLY	2.4
1	H	346	ALA	2.3
1	H	14	ARG	2.3
1	H	315	LEU	2.3
1	F	304	ALA	2.3
1	H	59	VAL	2.3
1	H	332	PRO	2.3
1	H	277	ALA	2.3
1	H	333	HIS	2.3
1	H	384	VAL	2.3
1	H	11	ILE	2.3
1	H	400	ASP	2.2
1	H	311	GLN	2.2
1	A	249	VAL	2.2
2	C	361	GLY	2.2
2	C	438	ILE	2.2
1	H	55	GLU	2.2
1	H	356	GLU	2.2
1	F	378	ARG	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	322	ASN	2.2
1	H	324	ASN	2.2
1	F	307	LEU	2.2
1	H	221	LEU	2.2
1	H	210	ARG	2.2
1	H	438	ILE	2.2
1	H	353	CYS	2.1
1	F	347	GLN	2.1
1	H	296	ARG	2.1
1	H	320	ASP	2.1
1	H	317	ASP	2.1
1	H	35	LEU	2.1
1	H	62	ALA	2.1
1	D	359	THR	2.1
1	H	476	ILE	2.1
2	E	360	ASP	2.1
1	H	285	VAL	2.1
2	C	365	LYS	2.1
1	F	364	GLY	2.0
1	G	348	LYS	2.0
1	G	360	ASP	2.0
2	C	14	ARG	2.0
1	H	302	PHE	2.0
1	H	85	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CSO	C	286[B]	7/8	0.91	0.21	-	22,23,25,26	7
2	CSO	E	286	7/8	0.93	0.12	-	19,22,26,30	0
2	CSO	C	286[A]	7/8	0.91	0.21	-	15,22,23,25	7

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.



## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	1498	6/6	0.92	0.24	9.75	35,36,37,37	0
3	GOL	B	1497	6/6	0.89	0.22	6.21	27,38,42,44	0
5	BME	D	1492[B]	4/4	0.84	0.25	5.69	18,19,20,21	4
5	BME	D	1492[A]	4/4	0.84	0.25	5.68	28,29,30,34	4
4	NAP	F	1491	31/48	0.90	0.29	4.94	26,37,48,51	0
5	BME	G	1492[B]	4/4	0.85	0.27	4.68	37,38,39,41	4
3	GOL	A	1497	6/6	0.92	0.18	4.22	23,28,32,32	0
5	BME	F	1492	4/4	0.89	0.18	4.19	39,42,44,48	0
4	NAP	G	1491	31/48	0.90	0.21	3.83	26,31,44,48	31
5	BME	G	1492[A]	4/4	0.85	0.27	3.65	21,23,23,24	4
3	GOL	C	1495	6/6	0.86	0.19	3.55	42,47,48,50	0
4	NAP	A	1491	31/48	0.89	0.20	3.02	21,28,45,46	31
3	GOL	G	1497	6/6	0.82	0.21	2.96	33,34,35,36	0
4	NAP	D	1491	31/48	0.90	0.19	2.72	24,28,44,46	31
4	NAP	H	1491	31/48	0.79	0.28	2.20	24,33,43,44	31
3	GOL	E	1495	6/6	0.91	0.15	1.89	45,46,46,47	0
3	GOL	A	1500	6/6	0.82	0.17	1.85	25,29,30,33	0
3	GOL	D	1495	6/6	0.93	0.18	1.85	36,42,43,45	0
3	GOL	H	1495	6/6	0.79	0.22	1.55	41,46,46,47	0
3	GOL	C	1497	6/6	0.79	0.18	1.52	31,34,35,41	0
3	GOL	A	1496	6/6	0.89	0.17	1.36	21,27,28,30	0
3	GOL	D	1496	6/6	0.85	0.16	1.28	27,30,30,33	0
4	NAP	E	1491	31/48	0.93	0.14	1.09	13,19,42,44	31
3	GOL	B	1496	6/6	0.86	0.15	1.02	30,31,32,33	0
5	BME	A	1492	4/4	0.94	0.16	0.68	26,26,28,33	0
4	NAP	B	1491	31/48	0.93	0.15	0.58	19,23,39,41	31
3	GOL	G	1496	6/6	0.92	0.13	0.41	35,36,38,39	0
4	NAP	C	1491	31/48	0.93	0.14	0.38	19,25,46,50	0
3	GOL	B	1495	6/6	0.90	0.14	0.08	37,38,40,42	0
3	GOL	G	1495	6/6	0.92	0.13	0.03	35,39,39,40	0
5	BME	B	1492	4/4	0.94	0.14	-0.01	31,35,35,36	0
3	GOL	F	1495	6/6	0.94	0.11	-0.12	26,27,31,33	0
6	K	F	1494	1/1	0.99	0.10	-0.26	21,21,21,21	0
6	K	H	1494	1/1	0.95	0.13	-0.51	32,32,32,32	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	K	G	1494	1/1	0.99	0.10	-0.52	23,23,23,23	0
6	K	H	1493	1/1	0.97	0.17	-0.68	32,32,32,32	0
6	K	E	1494	1/1	0.99	0.07	-1.16	21,21,21,21	0
6	K	C	1494	1/1	0.99	0.05	-1.74	20,20,20,20	0
6	K	F	1493	1/1	0.99	0.09	-1.82	26,26,26,26	0
6	K	B	1494	1/1	0.99	0.03	-1.91	16,16,16,16	0
6	K	D	1493	1/1	0.99	0.08	-2.03	23,23,23,23	0
6	K	A	1494	1/1	0.99	0.03	-2.45	17,17,17,17	0
6	K	G	1493	1/1	0.99	0.08	-2.79	17,17,17,17	0
6	K	D	1494	1/1	0.98	0.04	-2.99	18,18,18,18	0
6	K	B	1493	1/1	0.99	0.07	-3.47	17,17,17,17	0
6	K	A	1493	1/1	0.99	0.06	-3.88	20,20,20,20	0
6	K	C	1493	1/1	0.99	0.06	-5.10	22,22,22,22	0
6	K	E	1493	1/1	0.99	0.05	-5.61	19,19,19,19	0
3	GOL	E	1496	6/6	0.79	0.46	-	41,45,46,47	0
3	GOL	A	1501	6/6	0.89	0.19	-	34,41,43,43	0
3	GOL	A	1499	6/6	0.84	0.19	-	33,35,38,41	0
3	GOL	C	1496	6/6	0.77	0.20	-	37,38,40,42	0

## 6.5 Other polymers

There are no such residues in this entry.