



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:39 PM GMT

PDB ID : 3RIL  
Title : The acid beta-glucosidase active site exhibits plasticity in binding 3,4,5,6-tetrahydroxyazepane-based inhibitors: implications for pharmacological chaperone design for gaucher disease  
Authors : Orwig, S.D.; Lieberman, R.L.  
Deposited on : 2011-04-13  
Resolution : 2.40 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.

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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 : 1.7 (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

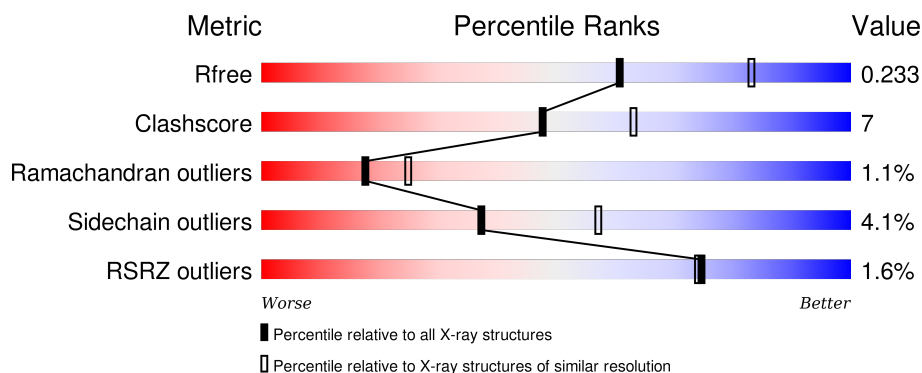
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	497	<div> <div>87%</div> <div>10% ..</div> </div>
1	B	497	<div> <div>3%</div> <div>81%</div> <div>15% ..</div> </div>
1	C	497	<div> <div>%</div> <div>83%</div> <div>13% ..</div> </div>
1	D	497	<div> <div>2%</div> <div>86%</div> <div>11% ..</div> </div>

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
2	SO4	A	506	-	-	X	-
2	SO4	C	508	-	-	-	X
2	SO4	C	511	-	-	-	X
2	SO4	D	503	-	-	-	X
4	3RK	C	513	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17164 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 Glucosylceramidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3921	2526	670	709	16			
1	B	497	Total	C	N	O	S	0	0	0
			3929	2532	671	710	16			
1	C	496	Total	C	N	O	S	0	0	0
			3921	2526	670	709	16			
1	D	497	Total	C	N	O	S	0	0	0
			3929	2532	671	710	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	495	HIS	ARG	VARIANT	UNP P04062
B	495	HIS	ARG	VARIANT	UNP P04062
C	495	HIS	ARG	VARIANT	UNP P04062
D	495	HIS	ARG	VARIANT	UNP P04062

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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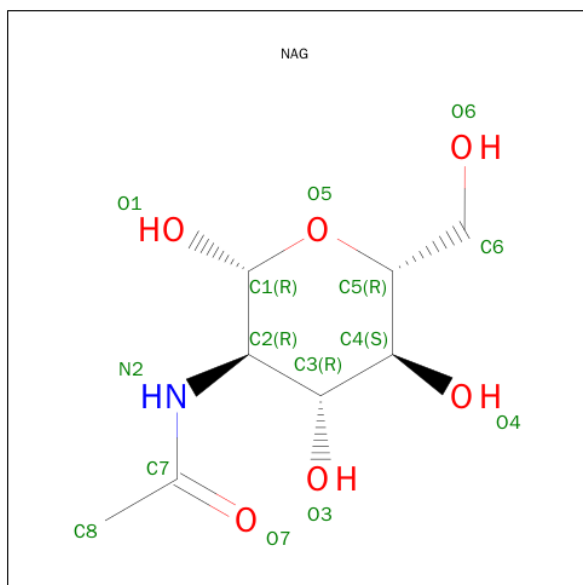
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total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

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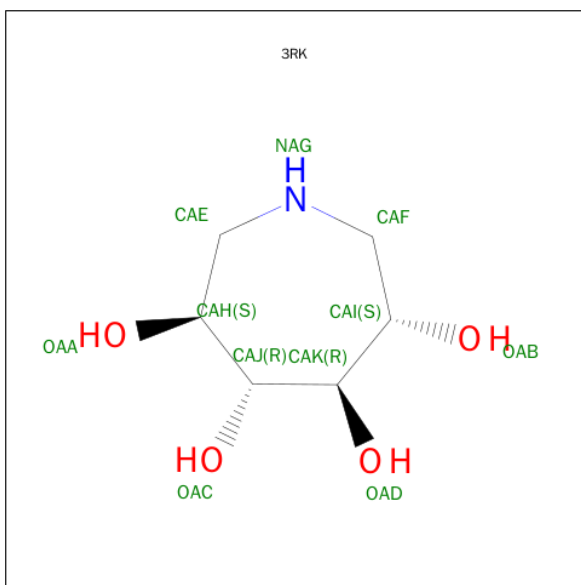
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 4 is (3S,4R,5R,6S)-AZEPANE-3,4,5,6-TETROL (three-letter code: 3RK) (formula:  $C_6H_{13}NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			11	6	1	4		
4	B	1	Total	C	N	O	0	0
			11	6	1	4		
4	C	1	Total	C	N	O	0	0
			11	6	1	4		
4	D	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 5 is water.

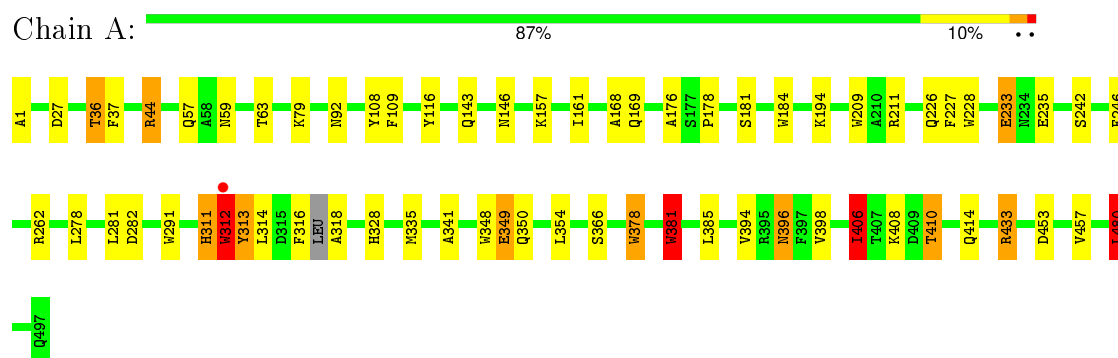
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	305	Total	O	0	0
			305	305		
5	B	293	Total	O	0	0
			293	293		
5	C	322	Total	O	0	0
			322	322		
5	D	264	Total	O	0	0
			264	264		



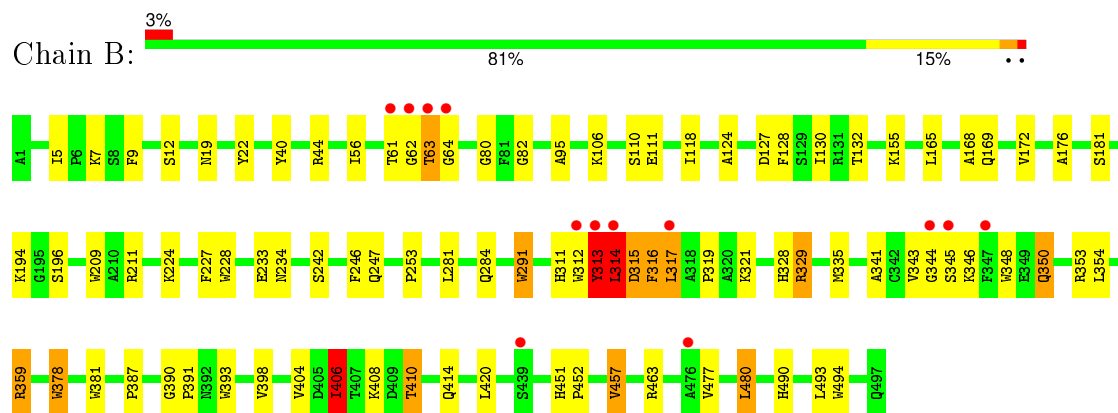
### 3 Residue-property plots

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.

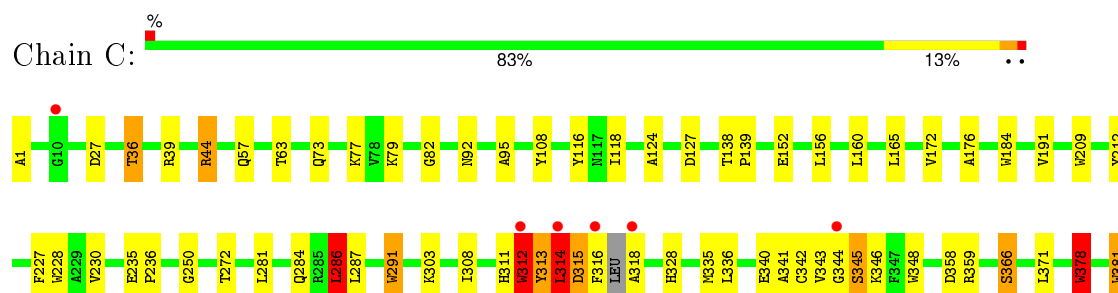
#### • Molecule 1: Glucosylceramidase

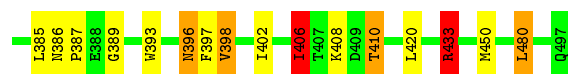


#### • Molecule 1: Glucosylceramidase

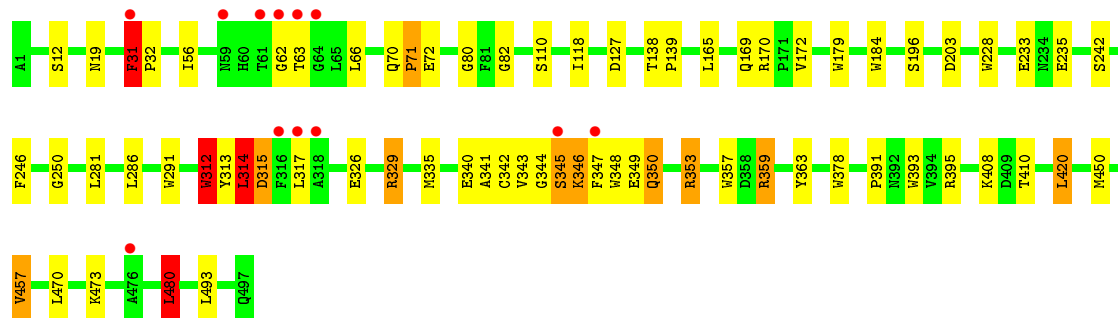
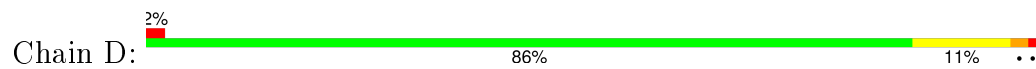


#### • Molecule 1: Glucosylceramidase





• Molecule 1: Glucosylceramidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.22Å 91.42Å 152.66Å 90.00° 110.95° 90.00°	Depositor
Resolution (Å)	44.54 – 2.40 44.54 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.3 (44.54-2.40) 96.3 (44.54-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.171 , 0.232 0.171 , 0.233	Depositor DCC
$R_{free}$ test set	5291 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.1	EDS
Estimated twinning fraction	0.457 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 105940 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17164	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: 3RK, NAG, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.90	6/4041 (0.1%)	0.89	4/5509 (0.1%)
1	B	0.87	6/4050 (0.1%)	0.86	4/5523 (0.1%)
1	C	0.88	5/4041 (0.1%)	0.88	7/5509 (0.1%)
1	D	0.88	8/4050 (0.2%)	0.88	7/5523 (0.1%)
All	All	0.88	25/16182 (0.2%)	0.88	22/22064 (0.1%)

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

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	378	TRP	CD2-CE2	8.58	1.51	1.41
1	C	378	TRP	CD2-CE2	7.35	1.50	1.41
1	B	378	TRP	CD2-CE2	7.30	1.50	1.41
1	D	378	TRP	CD2-CE2	7.17	1.50	1.41
1	D	312	TRP	CD2-CE2	7.11	1.49	1.41
1	B	291	TRP	CD2-CE2	7.02	1.49	1.41
1	A	312	TRP	CD2-CE2	6.84	1.49	1.41
1	B	393	TRP	CD2-CE2	6.76	1.49	1.41
1	C	291	TRP	CD2-CE2	6.75	1.49	1.41
1	A	291	TRP	CD2-CE2	6.74	1.49	1.41
1	D	291	TRP	CD2-CE2	6.68	1.49	1.41
1	D	357	TRP	CD2-CE2	6.01	1.48	1.41
1	C	312	TRP	CG-CD2	5.89	1.53	1.43
1	D	348	TRP	CD2-CE2	5.83	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	179	TRP	CD2-CE2	5.75	1.48	1.41
1	B	228	TRP	CD2-CE2	5.71	1.48	1.41
1	C	312	TRP	CD2-CE2	5.71	1.48	1.41
1	D	393	TRP	CD2-CE2	5.64	1.48	1.41
1	A	348	TRP	CD2-CE2	5.64	1.48	1.41
1	C	348	TRP	CD2-CE2	5.57	1.48	1.41
1	B	348	TRP	CD2-CE2	5.28	1.47	1.41
1	A	381	TRP	CD2-CE2	5.22	1.47	1.41
1	D	228	TRP	CD2-CE2	5.12	1.47	1.41
1	B	494	TRP	CD2-CE2	5.01	1.47	1.41
1	A	184	TRP	CD2-CE2	5.01	1.47	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	LEU	CA-CB-CG	8.64	135.18	115.30
1	B	314	LEU	CA-CB-CG	8.57	135.02	115.30
1	D	314	LEU	CA-CB-CG	8.12	133.97	115.30
1	D	312	TRP	CA-CB-CG	7.43	127.82	113.70
1	A	406	ILE	CB-CA-C	-7.34	96.92	111.60
1	C	433	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	D	480	LEU	CA-CB-CG	7.02	131.44	115.30
1	C	314	LEU	CA-CB-CG	6.98	131.36	115.30
1	D	353	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	433	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	C	406	ILE	CB-CA-C	-6.67	98.27	111.60
1	B	480	LEU	CA-CB-CG	6.42	130.07	115.30
1	C	480	LEU	CA-CB-CG	6.18	129.52	115.30
1	C	39	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	286	LEU	CA-CB-CG	5.87	128.81	115.30
1	C	314	LEU	N-CA-C	-5.71	95.58	111.00
1	D	353	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	406	ILE	CG1-CB-CG2	-5.51	99.29	111.40
1	D	359	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	313	TYR	C-N-CA	5.21	134.73	121.70
1	D	420	LEU	CB-CG-CD1	-5.14	102.25	111.00
1	B	359	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	349	GLU	Peptide

## 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	3921	0	3831	47	0
1	B	3929	0	3844	76	0
1	C	3921	0	3831	58	0
1	D	3929	0	3844	56	0
2	A	55	0	0	3	0
2	B	35	0	0	1	0
2	C	55	0	0	1	0
2	D	35	0	0	1	0
3	A	14	0	13	0	0
3	B	14	0	13	3	0
3	C	14	0	13	0	0
3	D	14	0	13	3	0
4	A	11	0	13	0	0
4	B	11	0	13	0	0
4	C	11	0	13	2	0
4	D	11	0	13	4	0
5	A	305	0	0	9	0
5	B	293	0	0	11	1
5	C	322	0	0	5	1
5	D	264	0	0	4	0
All	All	17164	0	15454	231	1

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 7.

All (231) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:ASN:HD21	3:D:508:NAG:C1	1.12	1.59
1:B:19:ASN:HD21	3:B:508:NAG:C1	0.93	1.54
1:C:312:TRP:HA	1:C:313:TYR:O	1.24	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ARG:HG2	1:B:329:ARG:HH11	0.94	1.04
1:C:312:TRP:CA	1:C:313:TYR:O	2.06	1.04
1:D:329:ARG:HH11	1:D:329:ARG:HG2	1.12	1.03
1:B:329:ARG:NH1	1:B:329:ARG:HG2	1.74	1.00
1:B:62:GLY:H	1:B:63:THR:HB	1.29	0.97
1:C:340:GLU:OE2	4:C:513:3RK:HAI	1.65	0.96
1:B:344:GLY:HA3	1:B:345:SER:HB2	1.49	0.92
1:B:329:ARG:HH11	1:B:329:ARG:CG	1.84	0.88
1:D:312:TRP:HE3	1:D:313:TYR:HA	1.39	0.88
1:B:63:THR:HG23	1:B:64:GLY:H	1.37	0.88
1:D:329:ARG:NH1	1:D:329:ARG:HG2	1.85	0.86
1:D:313:TYR:HE2	1:D:342:CYS:HG	0.88	0.85
1:D:350:GLN:H	1:D:350:GLN:CD	1.79	0.85
1:D:346:LYS:HD2	1:D:349:GLU:OE1	1.77	0.85
1:B:408:LYS:HB2	1:B:410:THR:HG22	1.57	0.84
1:D:313:TYR:HE2	1:D:342:CYS:SG	2.00	0.84
1:B:408:LYS:HB2	1:B:410:THR:CG2	2.09	0.82
1:A:313:TYR:HB3	1:A:314:LEU:HB2	1.59	0.81
1:D:344:GLY:HA3	1:D:345:SER:HB2	1.62	0.81
1:D:71:PRO:N	1:D:72:GLU:HB2	1.96	0.80
1:B:62:GLY:N	1:B:63:THR:HB	1.96	0.80
1:C:1:ALA:HB2	1:C:27:ASP:OD1	1.82	0.79
1:B:312:TRP:O	1:B:315:ASP:CB	2.30	0.78
1:A:1:ALA:HB2	1:A:27:ASP:OD1	1.83	0.78
1:A:341:ALA:HB2	5:A:885:HOH:O	1.83	0.77
1:C:73:GLN:HG3	5:C:868:HOH:O	1.85	0.76
1:D:312:TRP:O	1:D:315:ASP:CB	2.35	0.75
1:C:36:THR:HG22	5:C:610:HOH:O	1.87	0.75
1:D:344:GLY:CA	1:D:345:SER:HB2	2.15	0.74
1:D:312:TRP:O	1:D:315:ASP:HB2	1.86	0.74
1:D:56:ILE:HG12	1:D:480:LEU:HD22	1.70	0.73
1:A:44:ARG:HD3	2:A:506:SO4:O2	1.88	0.73
1:D:343:VAL:HG11	1:D:359:ARG:HG2	1.71	0.72
1:B:344:GLY:HA3	1:B:345:SER:CB	2.20	0.72
1:A:349:GLU:HA	1:A:350:GLN:HB2	1.70	0.72
1:B:165:LEU:HD22	1:B:172:VAL:HB	1.70	0.71
1:D:340:GLU:OE2	4:D:509:3RK:HAFA	1.91	0.71
1:B:19:ASN:HD21	3:B:508:NAG:C2	1.96	0.71
1:B:314:LEU:HB3	1:B:316:PHE:CE2	2.26	0.70
1:B:312:TRP:O	1:B:315:ASP:HB2	1.92	0.70
1:B:406:ILE:HG22	5:B:659:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:LYS:CB	1:B:410:THR:HG22	2.21	0.70
1:B:350:GLN:H	1:B:350:GLN:CD	1.95	0.68
1:A:36:THR:HG22	5:A:752:HOH:O	1.93	0.68
1:D:313:TYR:CZ	4:D:509:3RK:HAE	2.29	0.68
1:D:165:LEU:HD22	1:D:172:VAL:HB	1.77	0.67
1:C:344:GLY:HA2	1:C:345:SER:HB3	1.77	0.67
1:D:312:TRP:CE3	1:D:313:TYR:HA	2.25	0.67
1:D:313:TYR:CE2	1:D:342:CYS:SG	2.80	0.66
1:A:349:GLU:CA	1:A:350:GLN:HB2	2.26	0.66
1:C:44:ARG:HD3	2:C:506:SO4:O1	1.96	0.66
1:B:343:VAL:HG21	1:B:359:ARG:HG2	1.78	0.65
1:B:63:THR:HG23	1:B:64:GLY:N	2.11	0.64
1:B:111:GLU:HG3	1:B:169:GLN:OE1	1.98	0.63
1:C:344:GLY:N	1:C:345:SER:HB2	2.13	0.63
1:C:313:TYR:HB3	1:C:314:LEU:HB2	1.79	0.63
1:C:344:GLY:H	1:C:345:SER:HB2	1.63	0.62
1:B:19:ASN:ND2	3:B:508:NAG:C2	2.58	0.62
1:B:63:THR:CG2	1:B:64:GLY:H	2.10	0.62
1:A:312:TRP:HD1	1:A:341:ALA:HB1	1.64	0.62
1:A:282:ASP:OD1	1:A:311:HIS:HE1	1.83	0.61
1:C:343:VAL:HG11	1:C:359:ARG:HG2	1.83	0.60
1:C:344:GLY:CA	1:C:345:SER:CB	2.79	0.60
1:B:321:LYS:HB3	5:B:832:HOH:O	2.02	0.60
1:C:344:GLY:HA2	1:C:345:SER:CB	2.32	0.59
1:A:235:GLU:OE2	1:A:311:HIS:HD2	1.85	0.59
1:B:319:PRO:HA	5:B:837:HOH:O	2.03	0.58
1:C:315:ASP:HB2	1:C:318:ALA:HB1	1.85	0.58
1:D:312:TRP:O	1:D:315:ASP:CG	2.42	0.58
1:D:19:ASN:HD21	3:D:508:NAG:C2	2.04	0.57
1:B:312:TRP:CE3	1:B:341:ALA:HB1	2.39	0.57
1:A:312:TRP:HD1	1:A:341:ALA:CB	2.17	0.57
1:B:56:ILE:HG12	1:B:480:LEU:CD2	2.34	0.57
1:D:169:GLN:HG2	1:D:170:ARG:HG3	1.86	0.56
1:D:329:ARG:CG	1:D:329:ARG:HH11	1.98	0.56
1:A:59:ASN:HB3	5:A:789:HOH:O	2.05	0.56
1:C:312:TRP:HA	1:C:313:TYR:C	2.16	0.56
1:D:344:GLY:HA3	1:D:345:SER:CB	2.27	0.56
1:B:56:ILE:HG12	1:B:480:LEU:HD22	1.88	0.56
1:A:396:ASN:HA	5:A:889:HOH:O	2.05	0.56
1:A:312:TRP:CD1	1:A:341:ALA:HB1	2.41	0.55
1:B:168:ALA:O	5:B:824:HOH:O	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:GLN:NE2	1:B:353:ARG:HG2	2.21	0.55
1:B:350:GLN:HE22	1:B:353:ARG:HE	1.53	0.55
1:A:44:ARG:CD	2:A:506:SO4:O2	2.55	0.55
1:A:143:GLN:HA	1:A:211:ARG:NH1	2.21	0.55
1:B:127:ASP:HB3	1:B:246:PHE:CG	2.42	0.55
1:D:408:LYS:O	1:D:410:THR:HG23	2.07	0.55
1:D:286:LEU:HD23	1:D:314:LEU:O	2.07	0.54
1:D:457:VAL:HB	1:D:493:LEU:HD23	1.89	0.54
1:B:312:TRP:O	1:B:315:ASP:HB3	2.08	0.54
1:D:395:ARG:NH1	5:D:749:HOH:O	2.41	0.53
1:A:235:GLU:OE2	1:A:311:HIS:CD2	2.61	0.53
1:B:5:ILE:HG12	1:B:22:TYR:CE2	2.44	0.53
1:C:284:GLN:HB2	1:C:286:LEU:HD13	1.90	0.52
1:D:80:GLY:C	1:D:118:ILE:HD12	2.30	0.52
1:C:366:SER:HG	1:C:378:TRP:HZ2	1.58	0.52
1:D:350:GLN:HE21	1:D:353:ARG:HE	1.56	0.52
1:C:371:LEU:O	1:C:433:ARG:HD2	2.10	0.51
1:A:92:ASN:ND2	1:A:385:LEU:HA	2.24	0.51
1:C:287:LEU:HB3	1:C:291:TRP:CD1	2.46	0.51
1:B:62:GLY:CA	1:B:63:THR:HB	2.40	0.51
1:D:82:GLY:HA3	1:D:118:ILE:O	2.11	0.51
1:D:127:ASP:HB3	1:D:246:PHE:CG	2.46	0.51
1:B:106:LYS:O	1:B:110:SER:HB3	2.11	0.51
1:B:329:ARG:NH1	1:B:329:ARG:CG	2.53	0.50
1:A:328:HIS:HD2	5:A:622:HOH:O	1.94	0.50
1:B:211:ARG:HD2	5:B:722:HOH:O	2.10	0.50
1:C:82:GLY:HA3	1:C:118:ILE:O	2.12	0.50
1:C:312:TRP:O	1:C:341:ALA:HA	2.12	0.50
1:D:12:SER:OG	2:D:501:SO4:O2	2.20	0.50
1:B:132:THR:HG22	1:B:247:GLN:NE2	2.28	0.49
1:B:95:ALA:HB1	1:B:406:ILE:HD13	1.94	0.49
1:D:56:ILE:HG12	1:D:480:LEU:CD2	2.40	0.49
1:D:70:GLN:C	1:D:72:GLU:HB2	2.31	0.49
1:D:235:GLU:OE2	4:D:509:3RK:HAF	2.13	0.49
1:B:406:ILE:HD11	1:C:191:VAL:HG22	1.93	0.49
1:D:66:LEU:HD11	1:D:473:LYS:HB2	1.94	0.49
1:D:196:SER:HB2	1:D:250:GLY:O	2.13	0.48
1:C:176:ALA:HB3	1:C:230:VAL:HG12	1.96	0.48
1:B:234:ASN:OD1	1:B:311:HIS:HE1	1.96	0.48
1:C:408:LYS:O	1:C:410:THR:HG23	2.14	0.48
1:C:79:LYS:HE2	1:C:228:TRP:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LYS:O	1:A:410:THR:HG23	2.13	0.47
1:B:194:LYS:HB2	1:B:242:SER:HA	1.96	0.47
1:A:181:SER:HA	1:A:209:TRP:CZ3	2.49	0.47
1:D:31:PHE:HB3	1:D:32:PRO:C	2.35	0.47
1:B:408:LYS:CB	1:B:410:THR:CG2	2.84	0.47
1:D:31:PHE:HB3	1:D:32:PRO:CA	2.45	0.47
1:D:19:ASN:ND2	3:D:508:NAG:C2	2.70	0.47
1:B:463:ARG:HB2	5:B:703:HOH:O	2.15	0.47
1:D:450:MET:HE2	5:D:674:HOH:O	2.14	0.47
1:B:328:HIS:HD2	5:B:765:HOH:O	1.96	0.47
1:D:235:GLU:CD	4:D:509:3RK:HAF	2.36	0.46
1:A:246:PHE:HB3	1:A:394:VAL:HG21	1.98	0.46
1:D:343:VAL:HG23	1:D:363:TYR:HE1	1.81	0.46
1:A:109:PHE:O	1:A:168:ALA:HA	2.16	0.46
1:D:350:GLN:NE2	1:D:353:ARG:HE	2.14	0.46
1:D:343:VAL:HA	1:D:344:GLY:HA2	1.43	0.46
1:A:44:ARG:NH1	2:A:506:SO4:O3	2.44	0.46
1:B:343:VAL:HG23	1:B:345:SER:HB2	1.98	0.45
1:D:344:GLY:CA	1:D:345:SER:CB	2.83	0.45
1:D:391:PRO:HA	5:D:652:HOH:O	2.16	0.45
1:A:37:PHE:CE2	1:A:480:LEU:HD13	2.52	0.45
1:B:128:PHE:CZ	1:B:398:VAL:HG22	2.52	0.45
1:A:176:ALA:HB2	1:A:227:PHE:CE2	2.52	0.45
1:C:344:GLY:CA	1:C:345:SER:HB2	2.47	0.45
1:B:457:VAL:HB	1:B:493:LEU:HD23	1.98	0.45
1:C:236:PRO:O	1:C:250:GLY:HA2	2.17	0.45
1:D:139:PRO:HA	1:D:184:TRP:CD1	2.52	0.45
1:C:381:TRP:CE3	1:C:381:TRP:HA	2.52	0.44
1:A:316:PHE:CE1	1:B:317:LEU:HD21	2.53	0.44
1:D:203:ASP:C	1:D:203:ASP:OD1	2.56	0.44
1:C:313:TYR:HB3	1:C:314:LEU:CB	2.47	0.44
1:C:342:CYS:SG	1:C:398:VAL:HG21	2.58	0.44
1:C:313:TYR:HD1	1:C:314:LEU:HD23	1.83	0.44
1:B:284:GLN:OE1	1:B:313:TYR:O	2.35	0.44
1:A:262:ARG:NH1	5:A:733:HOH:O	2.50	0.44
1:A:318:ALA:N	1:B:317:LEU:O	2.51	0.44
1:A:408:LYS:O	1:A:410:THR:CG2	2.66	0.44
1:B:12:SER:OG	2:B:501:SO4:O1	2.31	0.44
1:C:152:GLU:O	1:C:156:LEU:HB2	2.18	0.44
1:C:328:HIS:HD2	5:C:922:HOH:O	2.01	0.44
1:C:389:GLY:O	1:C:396:ASN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLN:NE2	5:A:775:HOH:O	2.41	0.43
1:B:354:LEU:HA	1:B:414:GLN:OE1	2.19	0.43
1:B:40:TYR:O	1:B:490:HIS:HA	2.19	0.43
1:C:406:ILE:HG13	1:C:406:ILE:H	1.70	0.43
1:A:406:ILE:HG22	1:A:406:ILE:O	2.19	0.43
1:C:139:PRO:HA	1:C:184:TRP:CD1	2.52	0.43
1:A:178:PRO:HG2	1:A:233:GLU:HA	2.01	0.43
1:A:108:TYR:CD2	1:A:116:TYR:CE1	3.06	0.43
1:C:127:ASP:OD2	4:C:513:3RK:OAC	2.35	0.43
1:B:314:LEU:HA	1:B:316:PHE:H	1.84	0.43
1:C:358:ASP:HB2	5:C:784:HOH:O	2.18	0.43
1:B:80:GLY:C	1:B:118:ILE:HD12	2.39	0.43
1:B:130:ILE:HD13	1:C:393:TRP:HA	2.01	0.42
1:B:406:ILE:HD12	5:B:707:HOH:O	2.19	0.42
1:A:79:LYS:HE2	1:A:228:TRP:CE2	2.53	0.42
1:C:381:TRP:HA	1:C:381:TRP:HE3	1.85	0.42
1:A:453:ASP:OD1	1:A:453:ASP:C	2.58	0.42
1:C:108:TYR:CE1	1:C:402:ILE:HD12	2.54	0.42
1:B:63:THR:CG2	1:B:64:GLY:N	2.78	0.42
1:C:160:LEU:HA	1:C:160:LEU:HD23	1.85	0.42
1:B:165:LEU:HD22	1:B:172:VAL:CB	2.46	0.42
1:A:314:LEU:H	1:A:316:PHE:HE2	1.66	0.42
1:B:181:SER:HA	1:B:209:TRP:CZ3	2.54	0.42
1:C:308:ILE:HB	1:C:336:LEU:HD23	2.00	0.42
1:B:196:SER:HB2	5:B:660:HOH:O	2.20	0.42
1:C:408:LYS:O	1:C:410:THR:CG2	2.68	0.42
1:C:397:PHE:HZ	1:D:347:PHE:CD1	2.38	0.42
1:C:116:TYR:OH	1:C:420:LEU:HD13	2.19	0.41
1:A:143:GLN:HA	1:A:211:ARG:HH12	1.85	0.41
1:B:82:GLY:HA3	1:B:118:ILE:O	2.20	0.41
1:B:451:HIS:ND1	1:B:452:PRO:HD2	2.35	0.41
1:B:7:LYS:HE3	1:B:9:PHE:CZ	2.56	0.41
1:C:92:ASN:ND2	1:C:385:LEU:HA	2.35	0.41
1:A:349:GLU:CB	1:A:350:GLN:HB2	2.50	0.41
1:D:138:THR:HA	1:D:139:PRO:HD3	1.89	0.41
1:D:341:ALA:HB2	5:D:661:HOH:O	2.21	0.41
1:C:312:TRP:CE3	1:C:313:TYR:N	2.88	0.41
1:D:326:GLU:OE1	1:D:329:ARG:NH1	2.54	0.41
1:B:128:PHE:HZ	1:B:398:VAL:HG22	1.86	0.41
1:A:354:LEU:HA	1:A:414:GLN:OE1	2.20	0.41
1:A:381:TRP:HA	1:A:381:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LYS:HB2	1:A:242:SER:HA	2.01	0.41
1:C:341:ALA:HB1	1:C:378:TRP:CH2	2.56	0.41
1:C:95:ALA:HB1	1:C:406:ILE:HG23	2.02	0.41
1:B:345:SER:HA	1:B:346:LYS:HA	1.84	0.41
1:A:316:PHE:O	1:B:317:LEU:HD13	2.21	0.41
1:C:165:LEU:HD22	1:C:172:VAL:HB	2.02	0.41
1:B:387:PRO:HD3	1:B:404:VAL:O	2.21	0.41
1:C:386:ASN:HB2	1:C:387:PRO:CD	2.50	0.41
1:B:176:ALA:HB2	1:B:227:PHE:CE2	2.55	0.41
1:B:253:PRO:HB3	1:B:291:TRP:CD2	2.56	0.41
1:B:390:GLY:HA3	1:B:391:PRO:HA	1.78	0.41
1:C:272:THR:HG23	5:C:715:HOH:O	2.22	0.40
1:C:209:TRP:CZ3	1:C:212:TYR:CD2	3.09	0.40
1:B:155:LYS:HD3	5:B:786:HOH:O	2.19	0.40
1:D:314:LEU:N	1:D:315:ASP:HB2	2.36	0.40
1:A:146:ASN:ND2	5:A:797:HOH:O	2.53	0.40
1:B:224:LYS:HE3	5:B:610:HOH:O	2.21	0.40
1:C:176:ALA:HB2	1:C:227:PHE:CE2	2.56	0.40
1:C:235:GLU:OE2	1:C:311:HIS:ND1	2.49	0.40
1:A:157:LYS:O	1:A:161:ILE:HG13	2.20	0.40
1:A:349:GLU:HB3	1:A:350:GLN:HB2	2.02	0.40
1:C:138:THR:HA	1:C:139:PRO:HD3	1.81	0.40
1:A:169:GLN:NE2	5:A:799:HOH:O	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:784:HOH:O	5:C:610:HOH:O[2_656]	2.06	0.14

## 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	492/497 (99%)	464 (94%)	26 (5%)	2 (0%)	39	56
1	B	495/497 (100%)	465 (94%)	22 (4%)	8 (2%)	12	16
1	C	492/497 (99%)	462 (94%)	26 (5%)	4 (1%)	24	35
1	D	495/497 (100%)	464 (94%)	23 (5%)	8 (2%)	12	16
All	All	1974/1988 (99%)	1855 (94%)	97 (5%)	22 (1%)	17	25

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	63	THR
1	B	233	GLU
1	C	313	TYR
1	C	345	SER
1	D	71	PRO
1	D	233	GLU
1	D	315	ASP
1	B	313	TYR
1	B	315	ASP
1	D	31	PHE
1	A	233	GLU
1	B	314	LEU
1	D	62	GLY
1	D	346	LYS
1	A	281	LEU
1	B	124	ALA
1	B	281	LEU
1	C	124	ALA
1	C	281	LEU
1	B	381	TRP
1	D	281	LEU
1	D	345	SER

### 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	423/424 (100%)	405 (96%)	18 (4%)	35	55
1	B	424/424 (100%)	409 (96%)	15 (4%)	43	64
1	C	423/424 (100%)	400 (95%)	23 (5%)	27	43
1	D	424/424 (100%)	410 (97%)	14 (3%)	45	66
All	All	1694/1696 (100%)	1624 (96%)	70 (4%)	37	57

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

Mol	Chain	Res	Type
1	A	36	THR
1	A	44	ARG
1	A	57	GLN
1	A	63	THR
1	A	278	LEU
1	A	311	HIS
1	A	312	TRP
1	A	335	MET
1	A	366	SER
1	A	378	TRP
1	A	381	TRP
1	A	396	ASN
1	A	398	VAL
1	A	406	ILE
1	A	410	THR
1	A	433	ARG
1	A	457	VAL
1	A	480	LEU
1	B	44	ARG
1	B	61	THR
1	B	313	TYR
1	B	314	LEU
1	B	316	PHE
1	B	317	LEU
1	B	329	ARG
1	B	335	MET
1	B	350	GLN
1	B	378	TRP
1	B	406	ILE
1	B	410	THR
1	B	420	LEU
1	B	457	VAL
1	B	477	VAL

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Mol	Chain	Res	Type
1	C	36	THR
1	C	44	ARG
1	C	57	GLN
1	C	63	THR
1	C	77	LYS
1	C	286	LEU
1	C	303	LYS
1	C	312	TRP
1	C	314	LEU
1	C	315	ASP
1	C	316	PHE
1	C	335	MET
1	C	346	LYS
1	C	366	SER
1	C	378	TRP
1	C	381	TRP
1	C	396	ASN
1	C	398	VAL
1	C	406	ILE
1	C	410	THR
1	C	433	ARG
1	C	450	MET
1	C	480	LEU
1	D	31	PHE
1	D	63	THR
1	D	110	SER
1	D	242	SER
1	D	312	TRP
1	D	314	LEU
1	D	317	LEU
1	D	329	ARG
1	D	335	MET
1	D	350	GLN
1	D	420	LEU
1	D	457	VAL
1	D	470	LEU
1	D	480	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN

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Mol	Chain	Res	Type
1	A	311	HIS
1	A	328	HIS
1	A	350	GLN
1	B	19	ASN
1	B	350	GLN
1	C	57	GLN
1	C	92	ASN
1	C	146	ASN
1	C	270	ASN
1	C	328	HIS
1	D	19	ASN
1	D	270	ASN
1	D	350	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

44 ligands 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	SO4	A	501	-	4,4,4	0.47	0	6,6,6	0.55	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	502	-	4,4,4	0.35	0	6,6,6	0.55	0
2	SO4	A	503	-	4,4,4	0.49	0	6,6,6	0.48	0
2	SO4	A	504	-	4,4,4	0.92	0	6,6,6	0.58	0
2	SO4	A	505	-	4,4,4	0.24	0	6,6,6	0.43	0
2	SO4	A	506	-	4,4,4	0.59	0	6,6,6	1.31	1 (16%)
2	SO4	A	507	-	4,4,4	0.53	0	6,6,6	0.48	0
2	SO4	A	508	-	4,4,4	0.56	0	6,6,6	0.54	0
2	SO4	A	509	-	4,4,4	0.53	0	6,6,6	0.80	0
2	SO4	A	510	-	4,4,4	0.56	0	6,6,6	0.68	0
2	SO4	A	511	-	4,4,4	0.46	0	6,6,6	0.34	0
3	NAG	A	512	1	14,14,15	2.42	8 (57%)	15,19,21	1.60	3 (20%)
4	3RK	A	513	-	5,11,11	1.02	0	2,15,15	0.92	0
2	SO4	B	501	-	4,4,4	0.54	0	6,6,6	0.50	0
2	SO4	B	502	-	4,4,4	0.49	0	6,6,6	0.33	0
2	SO4	B	503	-	4,4,4	0.46	0	6,6,6	0.82	0
2	SO4	B	504	-	4,4,4	0.44	0	6,6,6	0.83	0
2	SO4	B	505	-	4,4,4	0.61	0	6,6,6	0.39	0
2	SO4	B	506	-	4,4,4	0.55	0	6,6,6	0.34	0
2	SO4	B	507	-	4,4,4	0.57	0	6,6,6	0.50	0
3	NAG	B	508	1	14,14,15	2.04	2 (14%)	15,19,21	2.37	5 (33%)
4	3RK	B	509	-	5,11,11	0.97	0	2,15,15	1.00	0
2	SO4	C	501	-	4,4,4	0.47	0	6,6,6	0.50	0
2	SO4	C	502	-	4,4,4	0.34	0	6,6,6	0.75	0
2	SO4	C	503	-	4,4,4	0.32	0	6,6,6	0.34	0
2	SO4	C	504	-	4,4,4	0.90	0	6,6,6	0.73	0
2	SO4	C	505	-	4,4,4	0.34	0	6,6,6	0.56	0
2	SO4	C	506	-	4,4,4	0.49	0	6,6,6	0.41	0
2	SO4	C	507	-	4,4,4	0.60	0	6,6,6	0.24	0
2	SO4	C	508	-	4,4,4	0.47	0	6,6,6	0.18	0
2	SO4	C	509	-	4,4,4	0.66	0	6,6,6	0.57	0
2	SO4	C	510	-	4,4,4	0.62	0	6,6,6	0.69	0
2	SO4	C	511	-	4,4,4	0.69	0	6,6,6	0.91	0
3	NAG	C	512	1	14,14,15	2.01	5 (35%)	15,19,21	2.04	5 (33%)
4	3RK	C	513	-	5,11,11	0.64	0	2,15,15	0.46	0
2	SO4	D	501	-	4,4,4	0.46	0	6,6,6	0.44	0
2	SO4	D	502	-	4,4,4	0.30	0	6,6,6	0.23	0
2	SO4	D	503	-	4,4,4	0.74	0	6,6,6	0.41	0
2	SO4	D	504	-	4,4,4	0.39	0	6,6,6	0.69	0
2	SO4	D	505	-	4,4,4	0.50	0	6,6,6	0.57	0
2	SO4	D	506	-	4,4,4	0.53	0	6,6,6	0.41	0
2	SO4	D	507	-	4,4,4	0.47	0	6,6,6	0.20	0
3	NAG	D	508	1	14,14,15	2.08	4 (28%)	15,19,21	2.18	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	3RK	D	509	-	5,11,11	0.98	0	2,15,15	0.79	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	SO4	A	501	-	-	0/0/0/0	0/0/0/0
2	SO4	A	502	-	-	0/0/0/0	0/0/0/0
2	SO4	A	503	-	-	0/0/0/0	0/0/0/0
2	SO4	A	504	-	-	0/0/0/0	0/0/0/0
2	SO4	A	505	-	-	0/0/0/0	0/0/0/0
2	SO4	A	506	-	-	0/0/0/0	0/0/0/0
2	SO4	A	507	-	-	0/0/0/0	0/0/0/0
2	SO4	A	508	-	-	0/0/0/0	0/0/0/0
2	SO4	A	509	-	-	0/0/0/0	0/0/0/0
2	SO4	A	510	-	-	0/0/0/0	0/0/0/0
2	SO4	A	511	-	-	0/0/0/0	0/0/0/0
3	NAG	A	512	1	-	0/6/23/26	0/1/1/1
4	3RK	A	513	-	-	0/0/18/18	0/1/1/1
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	502	-	-	0/0/0/0	0/0/0/0
2	SO4	B	503	-	-	0/0/0/0	0/0/0/0
2	SO4	B	504	-	-	0/0/0/0	0/0/0/0
2	SO4	B	505	-	-	0/0/0/0	0/0/0/0
2	SO4	B	506	-	-	0/0/0/0	0/0/0/0
2	SO4	B	507	-	-	0/0/0/0	0/0/0/0
3	NAG	B	508	1	-	0/6/23/26	0/1/1/1
4	3RK	B	509	-	-	0/0/18/18	0/1/1/1
2	SO4	C	501	-	-	0/0/0/0	0/0/0/0
2	SO4	C	502	-	-	0/0/0/0	0/0/0/0
2	SO4	C	503	-	-	0/0/0/0	0/0/0/0
2	SO4	C	504	-	-	0/0/0/0	0/0/0/0
2	SO4	C	505	-	-	0/0/0/0	0/0/0/0
2	SO4	C	506	-	-	0/0/0/0	0/0/0/0
2	SO4	C	507	-	-	0/0/0/0	0/0/0/0
2	SO4	C	508	-	-	0/0/0/0	0/0/0/0
2	SO4	C	509	-	-	0/0/0/0	0/0/0/0
2	SO4	C	510	-	-	0/0/0/0	0/0/0/0
2	SO4	C	511	-	-	0/0/0/0	0/0/0/0
3	NAG	C	512	1	-	0/6/23/26	0/1/1/1
4	3RK	C	513	-	-	0/0/18/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	D	501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	502	-	-	0/0/0/0	0/0/0/0
2	SO4	D	503	-	-	0/0/0/0	0/0/0/0
2	SO4	D	504	-	-	0/0/0/0	0/0/0/0
2	SO4	D	505	-	-	0/0/0/0	0/0/0/0
2	SO4	D	506	-	-	0/0/0/0	0/0/0/0
2	SO4	D	507	-	-	0/0/0/0	0/0/0/0
3	NAG	D	508	1	-	0/6/23/26	0/1/1/1
4	3RK	D	509	-	-	0/0/18/18	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	508	NAG	C1-C2	-2.99	1.48	1.52
3	B	508	NAG	C8-C7	2.30	1.55	1.50
3	C	512	NAG	C2-N2	2.44	1.50	1.46
3	A	512	NAG	C4-C5	2.45	1.58	1.53
3	A	512	NAG	C1-C2	2.51	1.55	1.52
3	A	512	NAG	C3-C2	2.54	1.58	1.52
3	A	512	NAG	C8-C7	2.65	1.55	1.50
3	C	512	NAG	O5-C5	2.74	1.49	1.43
3	C	512	NAG	C4-C3	2.90	1.60	1.52
3	D	508	NAG	C8-C7	3.11	1.56	1.50
3	D	508	NAG	O5-C5	3.12	1.50	1.43
3	A	512	NAG	C2-N2	3.14	1.51	1.46
3	A	512	NAG	C4-C3	3.24	1.60	1.52
3	C	512	NAG	C8-C7	3.28	1.57	1.50
3	C	512	NAG	O4-C4	3.91	1.52	1.43
3	A	512	NAG	O4-C4	3.91	1.52	1.43
3	A	512	NAG	O5-C5	4.30	1.52	1.43
3	D	508	NAG	O4-C4	4.79	1.54	1.43
3	B	508	NAG	O4-C4	5.96	1.57	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	508	NAG	O5-C5-C6	-5.43	95.60	107.35
3	B	508	NAG	O5-C5-C6	-5.31	95.85	107.35
3	B	508	NAG	O6-C6-C5	-3.70	99.10	111.33
3	D	508	NAG	C6-C5-C4	-3.03	105.55	113.02
3	C	512	NAG	O3-C3-C2	-3.02	103.13	109.11
3	D	508	NAG	O6-C6-C5	-2.60	102.74	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	508	NAG	O3-C3-C4	-2.24	105.29	110.34
3	A	512	NAG	O4-C4-C5	2.04	114.64	109.24
3	C	512	NAG	C2-N2-C7	2.20	125.86	123.04
3	C	512	NAG	O4-C4-C5	2.40	115.59	109.24
3	A	512	NAG	O4-C4-C3	2.42	115.78	110.34
3	C	512	NAG	O4-C4-C3	2.51	115.99	110.34
2	A	506	SO4	O2-S-O1	2.58	117.69	109.50
3	D	508	NAG	O4-C4-C5	2.67	116.32	109.24
3	D	508	NAG	O4-C4-C3	2.74	116.52	110.34
3	B	508	NAG	O4-C4-C5	2.91	116.95	109.24
3	B	508	NAG	O4-C4-C3	2.94	116.96	110.34
3	A	512	NAG	C1-O5-C5	3.70	116.94	112.25
3	B	508	NAG	C1-O5-C5	4.11	117.46	112.25
3	C	512	NAG	C1-O5-C5	5.07	118.69	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	506	SO4	3	0
2	B	501	SO4	1	0
3	B	508	NAG	3	0
2	C	506	SO4	1	0
4	C	513	3RK	2	0
2	D	501	SO4	1	0
3	D	508	NAG	3	0
4	D	509	3RK	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	496/497 (99%)	-0.56	1 (0%) 95 95	12, 20, 41, 69	0
1	B	497/497 (100%)	-0.45	13 (2%) 59 58	13, 22, 49, 93	0
1	C	496/497 (99%)	-0.53	6 (1%) 81 81	11, 20, 39, 91	0
1	D	497/497 (100%)	-0.45	12 (2%) 62 61	12, 22, 50, 84	0
All	All	1986/1988 (99%)	-0.50	32 (1%) 74 74	11, 21, 44, 93	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	63	THR	5.2
1	B	344	GLY	4.2
1	B	63	THR	4.1
1	C	312	TRP	4.0
1	B	312	TRP	3.7
1	B	314	LEU	3.6
1	D	476	ALA	3.2
1	B	62	GLY	3.1
1	B	345	SER	3.1
1	D	317	LEU	3.1
1	B	476	ALA	3.1
1	B	313	TYR	3.0
1	A	312	TRP	3.0
1	B	61	THR	2.9
1	D	61	THR	2.8
1	D	316	PHE	2.8
1	B	347	PHE	2.7
1	C	344	GLY	2.7
1	D	345	SER	2.6
1	B	317	LEU	2.6
1	C	314	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	64	GLY	2.5
1	D	318	ALA	2.4
1	C	318	ALA	2.4
1	D	31	PHE	2.4
1	B	439	SER	2.2
1	C	316	PHE	2.2
1	D	62	GLY	2.1
1	D	59	ASN	2.1
1	D	347	PHE	2.1
1	C	10	GLY	2.1
1	D	64	GLY	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	SO4	C	511	5/5	0.89	0.28	12.36	64,72,76,82	0
2	SO4	C	508	5/5	0.91	0.34	9.30	68,81,85,87	0
2	SO4	D	503	5/5	0.98	0.17	3.63	40,43,46,47	0
4	3RK	C	513	11/11	0.91	0.18	2.09	31,35,41,55	0
2	SO4	C	504	5/5	0.96	0.18	1.96	42,42,47,49	0
2	SO4	A	504	5/5	0.97	0.18	1.76	35,37,42,47	0
2	SO4	B	503	5/5	0.98	0.14	0.66	43,46,48,49	0
4	3RK	A	513	11/11	0.95	0.14	0.04	29,33,34,34	0
4	3RK	D	509	11/11	0.97	0.12	0.03	27,32,36,36	0
4	3RK	B	509	11/11	0.97	0.12	-0.13	24,29,30,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	501	5/5	0.99	0.11	-0.82	22,23,23,23	0
2	SO4	D	501	5/5	0.99	0.10	-1.02	27,27,30,30	0
2	SO4	C	501	5/5	0.99	0.12	-1.09	24,24,25,26	0
2	SO4	B	501	5/5	0.99	0.09	-1.32	25,28,29,31	0
2	SO4	C	506	5/5	0.94	0.31	-	55,63,65,67	0
2	SO4	A	506	5/5	0.92	0.28	-	57,59,62,64	0
2	SO4	C	505	5/5	0.96	0.19	-	50,51,57,62	0
2	SO4	B	505	5/5	0.89	0.25	-	74,79,86,90	0
3	NAG	D	508	14/15	0.90	0.18	-	32,36,41,45	0
2	SO4	B	506	5/5	0.93	0.27	-	67,68,73,80	0
2	SO4	D	507	5/5	0.85	0.31	-	81,81,85,96	0
2	SO4	A	510	5/5	0.90	0.21	-	71,80,82,85	0
3	NAG	A	512	14/15	0.91	0.12	-	27,30,33,37	0
2	SO4	A	509	5/5	0.85	0.26	-	59,64,73,84	0
2	SO4	A	508	5/5	0.87	0.24	-	53,59,63,66	0
3	NAG	B	508	14/15	0.91	0.18	-	30,35,42,44	0
2	SO4	A	507	5/5	0.89	0.21	-	68,68,74,77	0
2	SO4	D	506	5/5	0.90	0.34	-	66,74,77,79	0
2	SO4	B	507	5/5	0.93	0.26	-	68,73,73,74	0
2	SO4	D	502	5/5	0.98	0.10	-	36,37,39,39	0
2	SO4	D	505	5/5	0.92	0.24	-	82,83,87,90	0
2	SO4	A	503	5/5	0.99	0.11	-	26,28,31,31	0
2	SO4	C	503	5/5	0.98	0.13	-	39,40,43,44	0
3	NAG	C	512	14/15	0.90	0.14	-	27,30,31,31	0
2	SO4	C	507	5/5	0.91	0.19	-	64,64,71,72	0
2	SO4	C	510	5/5	0.86	0.27	-	67,70,79,80	0
2	SO4	D	504	5/5	0.94	0.13	-	47,49,54,58	0
2	SO4	A	502	5/5	0.99	0.13	-	30,33,35,36	0
2	SO4	A	511	5/5	0.90	0.20	-	86,93,97,97	0
2	SO4	B	504	5/5	0.94	0.15	-	52,54,56,57	0
2	SO4	C	502	5/5	0.99	0.07	-	27,28,30,31	0
2	SO4	A	505	5/5	0.96	0.18	-	50,51,52,55	0
2	SO4	C	509	5/5	0.88	0.21	-	59,63,68,71	0
2	SO4	B	502	5/5	0.99	0.09	-	33,35,36,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.