



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:27 PM GMT

PDB ID : 1P49  
Title : Structure of Human Placental Estrone/DHEA Sulfatase  
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Deposited on : 2003-04-21  
Resolution : 2.60 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

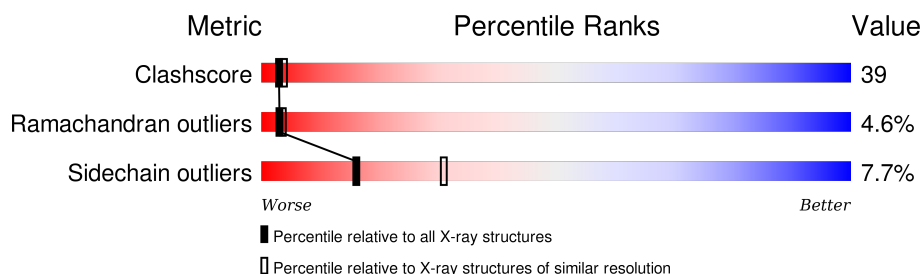
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	562	<div>46% 44% 7% ..</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
3	NAG	A	603	-	-	X	-
5	PO4	A	606	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4539 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.

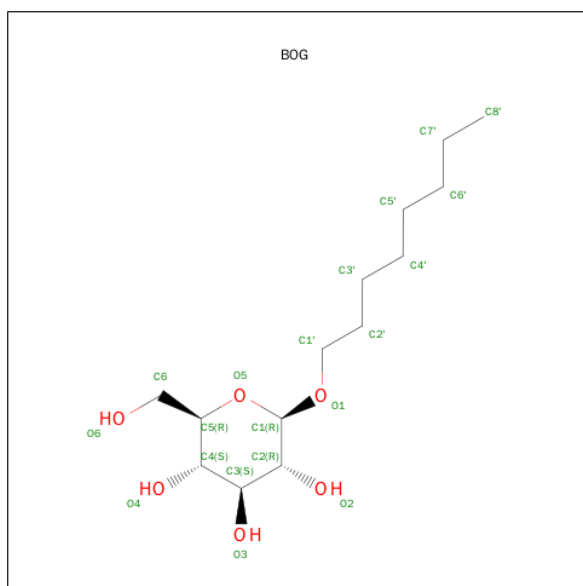
- Molecule 1 is a protein called STERYL-SULFATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4337	2786	743	782	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	ALS	CYS	MODIFIED RESIDUE	UNP P08842

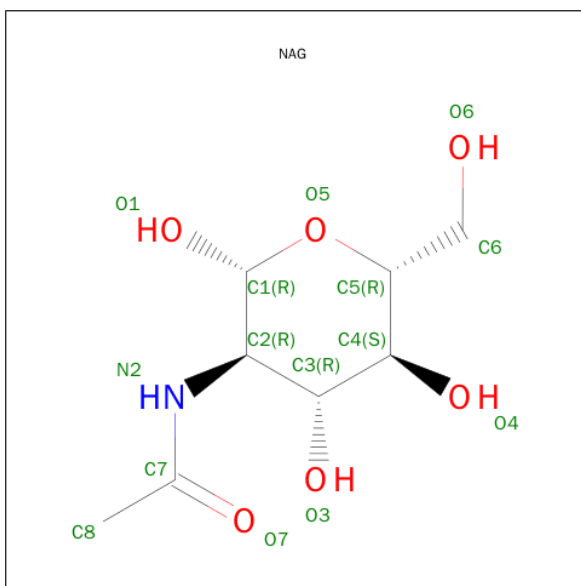
- Molecule 2 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula:  $C_{14}H_{28}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			3	2	1		

- Molecule 6 is water.

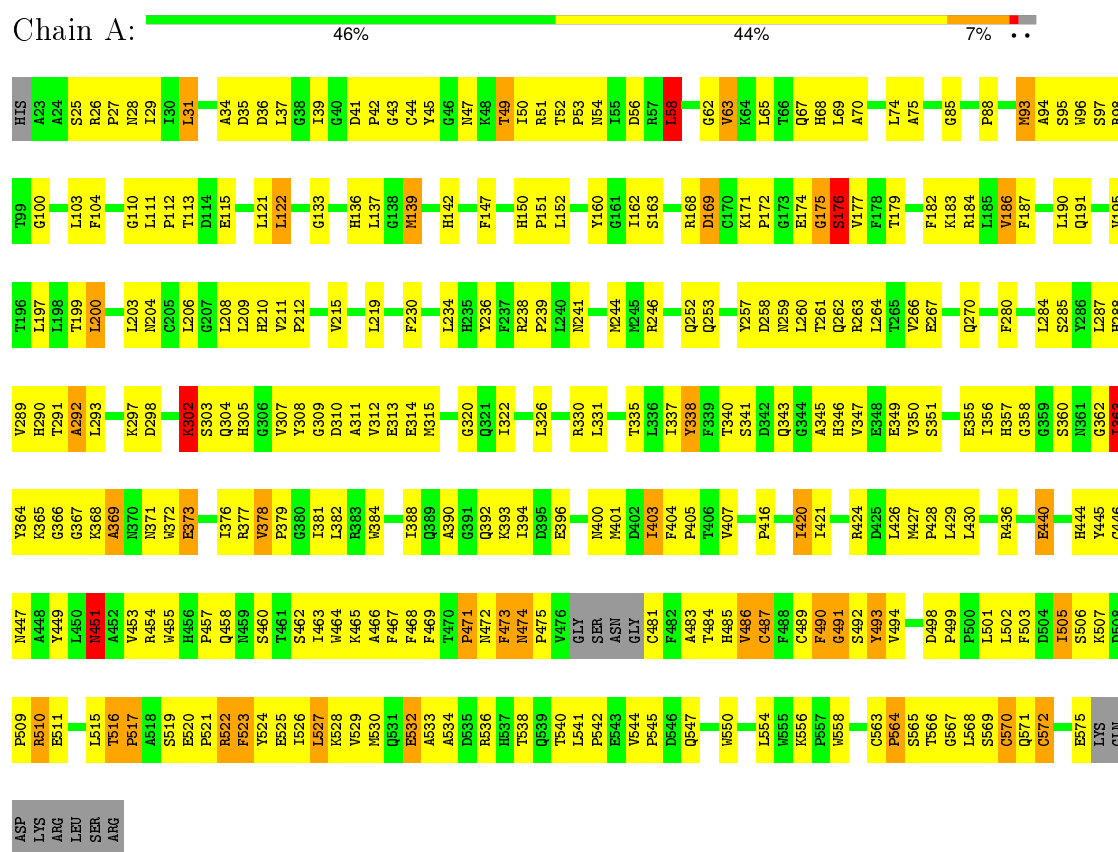
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	130	Total	O	0	0
			130	130		

### 3 Residue-property plots

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

Note EDS was not executed.

#### • Molecule 1: STERYL-SULFATASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.98Å 116.98Å 102.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.00 – 2.60	Depositor
% Data completeness (in resolution range)	96.7 (60.00-2.60)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.254 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4539	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, BOG, CA, NAG, ALS

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	0.40	0/4450	0.64	0/6049

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	338	TYR	Sidechain

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4337	0	4225	338	0
2	A	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	26	11	0
4	A	1	0	0	0	0
5	A	3	0	0	1	2
6	A	130	0	0	11	0
All	All	4539	0	4307	339	2

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 39.

All (339) 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:A:28:ASN:HB2	1:A:335:THR:HG22	1.33	1.09
1:A:49:THR:HB	1:A:304:GLN:HG3	1.42	1.02
1:A:204:ASN:HD22	1:A:211:VAL:H	1.12	0.94
1:A:304:GLN:NE2	3:A:603:NAG:H5	1.84	0.93
1:A:521:PRO:HG2	1:A:522:ARG:HD2	1.54	0.88
1:A:305:HIS:HB2	3:A:603:NAG:H62	1.54	0.87
1:A:70:ALA:HA	1:A:400:ASN:HB2	1.57	0.87
1:A:564:PRO:HG2	1:A:571:GLN:H	1.41	0.86
1:A:289:VAL:HG11	1:A:312:VAL:HG12	1.58	0.85
1:A:168:ARG:NH2	1:A:176:SER:HB3	1.94	0.83
1:A:260:LEU:HD21	1:A:287:LEU:HD22	1.62	0.81
1:A:350:VAL:HG13	1:A:356:ILE:HA	1.62	0.81
1:A:204:ASN:ND2	1:A:211:VAL:H	1.78	0.80
1:A:258:ASP:HB2	6:A:746:HOH:O	1.82	0.79
1:A:304:GLN:CD	3:A:603:NAG:H5	2.03	0.78
1:A:510:ARG:H	1:A:510:ARG:HD2	1.47	0.78
1:A:168:ARG:HB2	1:A:175:GLY:HA2	1.66	0.78
1:A:526:ILE:HG13	1:A:527:LEU:N	2.00	0.77
1:A:195:VAL:O	1:A:199:THR:HG22	1.85	0.76
1:A:516:THR:H	1:A:517:PRO:CD	2.01	0.74
1:A:472:ASN:HA	6:A:772:HOH:O	1.88	0.74
1:A:377:ARG:O	1:A:378:VAL:HB	1.87	0.73
1:A:305:HIS:CB	3:A:603:NAG:H62	2.18	0.73
1:A:501:LEU:HD23	1:A:502:LEU:N	2.03	0.73
1:A:567:GLY:C	1:A:568:LEU:HD12	2.08	0.73
1:A:503:PHE:HA	1:A:515:LEU:HD23	1.69	0.73
1:A:74:LEU:HD12	1:A:447:ASN:HD21	1.55	0.72
1:A:449:TYR:HD1	1:A:489:CYS:HB2	1.55	0.71
1:A:564:PRO:HG3	1:A:571:GLN:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ILE:H	1:A:506:SER:HB2	1.55	0.70
1:A:304:GLN:HE22	3:A:603:NAG:H3	1.57	0.70
1:A:304:GLN:OE1	1:A:305:HIS:HB2	1.91	0.70
1:A:142:HIS:ND1	5:A:606:PO4:O1	2.21	0.70
1:A:184:ARG:HH21	1:A:184:ARG:HG2	1.57	0.69
1:A:420:ILE:HD12	1:A:421:ILE:N	2.07	0.69
1:A:388:ILE:HD13	1:A:430:LEU:HD23	1.75	0.69
1:A:67:GLN:NE2	1:A:454:ARG:HE	1.91	0.69
1:A:526:ILE:O	1:A:529:VAL:HG12	1.92	0.69
1:A:363:ILE:HG13	1:A:510:ARG:HG3	1.75	0.69
1:A:85:GLY:HA2	1:A:401:MET:HB3	1.76	0.68
1:A:186:VAL:O	1:A:190:LEU:HB2	1.96	0.66
1:A:463:ILE:N	1:A:506:SER:HB2	2.11	0.66
1:A:63:VAL:HG23	1:A:382:LEU:HB2	1.77	0.66
1:A:309:GLY:O	1:A:313:GLU:HG3	1.96	0.66
1:A:505:ILE:H	1:A:505:ILE:HD12	1.59	0.66
1:A:168:ARG:HG2	1:A:291:THR:HG21	1.78	0.66
1:A:160:TYR:HE2	1:A:264:LEU:HD23	1.60	0.65
1:A:25:SER:HB2	1:A:27:PRO:HD3	1.79	0.65
1:A:384:TRP:HB3	1:A:388:ILE:HG13	1.78	0.65
1:A:567:GLY:O	1:A:568:LEU:HD12	1.97	0.65
1:A:331:LEU:O	1:A:335:THR:HG23	1.95	0.65
1:A:520:GLU:N	1:A:521:PRO:HD2	2.11	0.65
1:A:122:LEU:HD21	1:A:407:VAL:HG12	1.79	0.65
1:A:63:VAL:HG21	1:A:430:LEU:HG	1.80	0.64
1:A:474:ASN:H	1:A:481:CYS:HA	1.63	0.64
1:A:355:GLU:HB3	1:A:357:HIS:CE1	2.33	0.64
1:A:182:PHE:O	1:A:186:VAL:HG13	1.99	0.63
1:A:42:PRO:HA	1:A:52:THR:HG21	1.81	0.63
1:A:457:PRO:HD2	1:A:462:SER:O	1.98	0.63
1:A:307:VAL:HA	1:A:310:ASP:OD2	1.98	0.63
1:A:371:ASN:OD1	1:A:444:HIS:HB3	1.99	0.62
1:A:519:SER:C	1:A:521:PRO:HD2	2.20	0.62
1:A:204:ASN:HD22	1:A:211:VAL:N	1.91	0.62
1:A:238:ARG:HB3	1:A:239:PRO:HD3	1.81	0.62
2:A:602:BOG:H4	6:A:711:HOH:O	1.99	0.61
1:A:184:ARG:NH2	1:A:184:ARG:HG2	2.14	0.61
1:A:371:ASN:HA	1:A:376:ILE:HD11	1.83	0.61
1:A:463:ILE:H	1:A:506:SER:CB	2.12	0.61
1:A:505:ILE:H	1:A:505:ILE:CD1	2.14	0.61
1:A:136:HIS:O	1:A:137:LEU:HD23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ARG:HH12	1:A:458:GLN:CD	2.04	0.60
1:A:168:ARG:HG2	1:A:291:THR:CG2	2.31	0.60
1:A:526:ILE:C	1:A:528:LYS:H	2.05	0.60
1:A:526:ILE:HG13	1:A:527:LEU:H	1.65	0.60
1:A:49:THR:CB	1:A:304:GLN:HG3	2.27	0.60
1:A:516:THR:H	1:A:517:PRO:HD3	1.66	0.60
1:A:54:ASN:CG	1:A:320:GLY:HA3	2.21	0.60
1:A:394:ILE:HD13	1:A:429:LEU:HG	1.83	0.60
1:A:365:LYS:O	1:A:372:TRP:HB3	2.02	0.59
1:A:502:LEU:HD22	1:A:503:PHE:H	1.67	0.59
1:A:236:TYR:O	1:A:239:PRO:HD2	2.03	0.59
1:A:520:GLU:N	1:A:521:PRO:CD	2.66	0.59
1:A:474:ASN:HB3	1:A:475:PRO:CD	2.32	0.59
1:A:376:ILE:HG21	1:A:444:HIS:CE1	2.38	0.59
1:A:67:GLN:HE21	1:A:454:ARG:HE	1.50	0.59
1:A:314:GLU:OE1	6:A:824:HOH:O	2.16	0.59
1:A:544:VAL:HG22	1:A:545:PRO:HD2	1.84	0.59
1:A:484:THR:O	1:A:485:HIS:HB3	2.03	0.59
1:A:505:ILE:HD12	1:A:505:ILE:N	2.17	0.58
1:A:472:ASN:HD22	1:A:493:TYR:C	2.06	0.58
1:A:28:ASN:C	1:A:29:ILE:HD12	2.24	0.58
1:A:378:VAL:HG22	1:A:379:PRO:HD2	1.84	0.58
1:A:502:LEU:HD22	1:A:503:PHE:N	2.19	0.58
1:A:93:MET:HE3	1:A:137:LEU:HD22	1.84	0.58
1:A:349:GLU:HG3	1:A:349:GLU:O	2.03	0.58
1:A:501:LEU:HD21	1:A:503:PHE:CE1	2.39	0.57
1:A:168:ARG:HG3	1:A:177:VAL:HG23	1.84	0.57
1:A:533:ALA:O	1:A:536:ARG:HG3	2.05	0.57
1:A:529:VAL:O	1:A:532:GLU:HG3	2.04	0.57
1:A:368:LYS:O	1:A:369:ALA:CB	2.52	0.57
1:A:95:SER:O	1:A:447:ASN:HB3	2.04	0.57
1:A:363:ILE:CG1	1:A:510:ARG:HG3	2.35	0.57
1:A:451:ASN:HA	1:A:469:PHE:CE1	2.40	0.57
1:A:345:ALA:HB1	1:A:358:GLY:O	2.05	0.57
1:A:564:PRO:HD2	1:A:570:CYS:HA	1.87	0.57
1:A:309:GLY:HA2	1:A:312:VAL:HG22	1.87	0.57
1:A:291:THR:O	1:A:292:ALA:HB3	2.04	0.57
1:A:175:GLY:C	1:A:177:VAL:H	2.08	0.56
1:A:502:LEU:C	1:A:502:LEU:HD13	2.25	0.56
1:A:516:THR:O	1:A:520:GLU:HB2	2.04	0.56
1:A:263:ARG:HD2	1:A:575:GLU:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:TRP:O	1:A:530:MET:HE3	2.06	0.55
1:A:183:LYS:HB3	1:A:184:ARG:NH1	2.22	0.55
1:A:302:LYS:HD3	1:A:302:LYS:H	1.70	0.55
1:A:175:GLY:O	1:A:177:VAL:N	2.40	0.55
1:A:110:GLY:H	1:A:547:GLN:HG3	1.70	0.55
1:A:424:ARG:HD3	6:A:749:HOH:O	2.07	0.54
1:A:516:THR:HG22	1:A:517:PRO:HD3	1.88	0.54
1:A:382:LEU:HG	1:A:430:LEU:HD21	1.89	0.54
1:A:455:TRP:CH2	1:A:529:VAL:HG11	2.43	0.54
1:A:396:GLU:OE2	1:A:436:ARG:HG3	2.07	0.54
1:A:110:GLY:O	1:A:547:GLN:HG2	2.06	0.54
1:A:291:THR:O	1:A:292:ALA:CB	2.55	0.54
1:A:491:GLY:C	1:A:493:TYR:H	2.11	0.54
1:A:39:ILE:HD11	1:A:45:TYR:CE2	2.42	0.54
1:A:34:ALA:O	1:A:341:SER:HA	2.08	0.53
1:A:29:ILE:N	1:A:29:ILE:HD12	2.23	0.53
1:A:368:LYS:O	1:A:369:ALA:HB3	2.09	0.53
1:A:326:LEU:CD1	1:A:337:ILE:HD11	2.38	0.53
1:A:471:PRO:HB3	1:A:487:CYS:SG	2.49	0.53
1:A:204:ASN:HB2	1:A:211:VAL:HG23	1.91	0.53
1:A:490:PHE:HB2	1:A:493:TYR:HE1	1.74	0.52
1:A:516:THR:CG2	1:A:517:PRO:HD3	2.39	0.52
1:A:293:LEU:HD22	1:A:293:LEU:H	1.74	0.52
1:A:260:LEU:CD2	1:A:287:LEU:HD22	2.36	0.52
1:A:540:THR:O	1:A:542:PRO:HD3	2.09	0.52
1:A:564:PRO:HG2	1:A:571:GLN:N	2.17	0.52
1:A:503:PHE:CD2	1:A:511:GLU:HG2	2.45	0.52
1:A:31:LEU:HG	1:A:403:ILE:CD1	2.38	0.52
1:A:212:PRO:HG2	1:A:215:VAL:HG23	1.91	0.52
1:A:139:MET:HE3	1:A:163:SER:HB2	1.92	0.52
1:A:68:HIS:O	1:A:378:VAL:HG12	2.10	0.52
1:A:474:ASN:CG	1:A:483:ALA:HB2	2.30	0.52
1:A:404:PHE:HB3	1:A:405:PRO:CD	2.40	0.52
1:A:457:PRO:HG2	1:A:460:SER:HB3	1.91	0.52
1:A:473:PHE:HD2	1:A:481:CYS:SG	2.33	0.52
1:A:308:TYR:CE1	1:A:312:VAL:HG11	2.45	0.52
1:A:168:ARG:HB3	1:A:174:GLU:HG2	1.92	0.52
1:A:366:GLY:HA3	1:A:372:TRP:HB2	1.91	0.52
1:A:112:PRO:HB2	1:A:115:GLU:HG2	1.91	0.52
1:A:312:VAL:HG23	1:A:313:GLU:N	2.24	0.51
1:A:168:ARG:NH2	6:A:796:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ILE:HA	1:A:379:PRO:HG3	1.91	0.51
1:A:65:LEU:HD13	1:A:68:HIS:ND1	2.24	0.51
1:A:186:VAL:HG22	1:A:187:PHE:N	2.25	0.51
1:A:168:ARG:HB3	1:A:174:GLU:CG	2.41	0.51
1:A:525:GLU:O	1:A:528:LYS:HB3	2.10	0.51
1:A:209:LEU:HD12	1:A:210:HIS:N	2.25	0.51
1:A:465:LYS:HE2	1:A:467:PHE:CZ	2.46	0.51
1:A:501:LEU:HD21	1:A:503:PHE:HE1	1.75	0.50
1:A:41:ASP:OD1	1:A:360:SER:O	2.29	0.50
1:A:396:GLU:HG3	1:A:436:ARG:HA	1.93	0.50
1:A:246:ARG:NH1	6:A:750:HOH:O	2.44	0.50
1:A:304:GLN:HE22	3:A:603:NAG:H5	1.70	0.50
1:A:426:LEU:HB3	6:A:733:HOH:O	2.12	0.50
1:A:28:ASN:HB3	1:A:280:PHE:CE1	2.47	0.50
1:A:160:TYR:CE2	1:A:264:LEU:HD23	2.45	0.49
1:A:404:PHE:HB3	1:A:405:PRO:HD3	1.93	0.49
1:A:253:GLN:HB3	1:A:572:CYS:HB2	1.94	0.49
1:A:440:GLU:O	1:A:455:TRP:HD1	1.95	0.49
1:A:340:THR:HA	1:A:379:PRO:O	2.12	0.49
1:A:266:VAL:O	1:A:270:GLN:HG3	2.12	0.49
1:A:474:ASN:CB	1:A:475:PRO:CD	2.90	0.49
1:A:307:VAL:O	1:A:310:ASP:HB2	2.12	0.49
1:A:69:LEU:HD22	1:A:376:ILE:HG22	1.95	0.49
1:A:392:GLN:HG3	1:A:393:LYS:N	2.27	0.49
1:A:289:VAL:HG11	1:A:312:VAL:CG1	2.37	0.49
1:A:526:ILE:C	1:A:528:LYS:N	2.66	0.49
1:A:519:SER:HA	1:A:522:ARG:HH11	1.79	0.48
1:A:258:ASP:O	1:A:259:ASN:HB2	2.13	0.48
1:A:259:ASN:HA	1:A:262:GLN:OE1	2.12	0.48
1:A:341:SER:HB3	1:A:378:VAL:CG2	2.43	0.48
1:A:47:ASN:HA	3:A:603:NAG:H83	1.95	0.48
1:A:62:GLY:HA2	1:A:390:ALA:HA	1.95	0.48
1:A:501:LEU:C	1:A:501:LEU:HD23	2.33	0.48
1:A:74:LEU:HD13	1:A:100:GLY:HA3	1.95	0.48
1:A:416:PRO:HG2	1:A:421:ILE:HD11	1.94	0.48
1:A:98:ARG:HD3	1:A:493:TYR:OH	2.13	0.48
1:A:426:LEU:O	1:A:430:LEU:HD13	2.14	0.48
1:A:75:ALS:OS3	1:A:290:HIS:CD2	2.66	0.48
1:A:490:PHE:HB2	1:A:493:TYR:CE1	2.47	0.48
1:A:392:GLN:HG3	1:A:393:LYS:H	1.79	0.48
1:A:147:PHE:HB3	1:A:150:HIS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:PHE:CD2	1:A:481:CYS:SG	3.06	0.48
1:A:455:TRP:HB3	1:A:464:TRP:HB2	1.96	0.47
1:A:133:GLY:HA3	1:A:285:SER:O	2.14	0.47
1:A:445:TYR:OH	1:A:541:LEU:HD21	2.14	0.47
1:A:197:LEU:HD12	1:A:219:LEU:HB2	1.96	0.47
1:A:260:LEU:HD21	1:A:287:LEU:CD2	2.40	0.47
1:A:230:PHE:CZ	1:A:234:LEU:HD11	2.50	0.47
1:A:56:ASP:C	1:A:58:LEU:H	2.18	0.47
1:A:253:GLN:HG2	1:A:570:CYS:O	2.15	0.47
1:A:447:ASN:N	1:A:447:ASN:HD22	2.11	0.47
1:A:147:PHE:HB3	1:A:150:HIS:CB	2.45	0.47
1:A:491:GLY:HA2	1:A:494:VAL:HB	1.96	0.47
1:A:446:CYS:O	1:A:447:ASN:HB2	2.15	0.47
1:A:473:PHE:CD2	1:A:481:CYS:N	2.83	0.47
1:A:53:PRO:HG2	1:A:54:ASN:H	1.80	0.47
1:A:204:ASN:HA	1:A:209:LEU:O	2.13	0.47
1:A:122:LEU:HD11	1:A:407:VAL:CG1	2.44	0.47
1:A:458:GLN:NE2	1:A:458:GLN:HA	2.30	0.47
1:A:347:VAL:HG23	1:A:367:GLY:HA3	1.97	0.47
1:A:139:MET:CE	1:A:163:SER:HB2	2.45	0.46
1:A:526:ILE:O	1:A:528:LYS:N	2.47	0.46
1:A:449:TYR:CD1	1:A:489:CYS:HB2	2.43	0.46
1:A:93:MET:HE1	1:A:111:LEU:N	2.28	0.46
1:A:169:ASP:OD1	1:A:169:ASP:N	2.43	0.46
1:A:28:ASN:CB	1:A:335:THR:HG22	2.24	0.46
1:A:330:ARG:HG2	1:A:330:ARG:NH2	2.30	0.46
1:A:523:PHE:HD1	1:A:524:TYR:CD2	2.34	0.46
1:A:369:ALA:HB2	1:A:486:VAL:HG22	1.97	0.46
1:A:526:ILE:CG1	1:A:527:LEU:N	2.75	0.46
1:A:522:ARG:O	1:A:525:GLU:HB2	2.16	0.46
1:A:63:VAL:HG22	1:A:388:ILE:HG21	1.97	0.46
1:A:304:GLN:OE1	3:A:603:NAG:H5	2.16	0.45
1:A:446:CYS:HB2	1:A:451:ASN:HB2	1.97	0.45
1:A:163:SER:HB3	6:A:777:HOH:O	2.15	0.45
1:A:356:ILE:HG23	1:A:356:ILE:O	2.16	0.45
1:A:303:SER:HB3	1:A:310:ASP:CG	2.37	0.45
1:A:37:LEU:HD22	1:A:315:MET:HE3	1.98	0.45
1:A:150:HIS:HE1	1:A:152:LEU:HD13	1.80	0.45
1:A:534:ALA:O	1:A:538:THR:HG23	2.15	0.45
1:A:74:LEU:HD12	1:A:447:ASN:ND2	2.28	0.45
1:A:468:PHE:N	1:A:468:PHE:CD2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:PHE:HD1	1:A:524:TYR:HD2	1.63	0.45
1:A:26:ARG:N	1:A:27:PRO:CD	2.80	0.45
1:A:236:TYR:C	1:A:239:PRO:HD2	2.37	0.45
1:A:436:ARG:CZ	1:A:458:GLN:O	2.64	0.45
1:A:97:SER:HA	1:A:490:PHE:CZ	2.52	0.45
1:A:449:TYR:HD1	1:A:489:CYS:CB	2.24	0.45
1:A:25:SER:O	1:A:26:ARG:HB2	2.17	0.45
1:A:162:ILE:HG13	1:A:162:ILE:O	2.17	0.45
1:A:253:GLN:H	1:A:572:CYS:HB3	1.82	0.45
1:A:436:ARG:NH1	1:A:458:GLN:CD	2.70	0.45
1:A:394:ILE:CD1	1:A:430:LEU:HD12	2.46	0.44
1:A:544:VAL:CG2	1:A:545:PRO:HD2	2.46	0.44
1:A:308:TYR:O	1:A:312:VAL:HG13	2.16	0.44
1:A:491:GLY:C	1:A:493:TYR:N	2.70	0.44
1:A:104:PHE:HA	1:A:241:ASN:OD1	2.18	0.44
1:A:309:GLY:O	1:A:312:VAL:HG22	2.18	0.44
1:A:507:LYS:O	1:A:509:PRO:HD3	2.17	0.44
1:A:371:ASN:OD1	1:A:376:ILE:HD11	2.16	0.44
1:A:330:ARG:HG2	1:A:330:ARG:HH21	1.81	0.44
1:A:350:VAL:HG22	1:A:356:ILE:HD12	1.99	0.44
1:A:63:VAL:HG13	1:A:392:GLN:HB3	1.99	0.44
1:A:536:ARG:HD2	1:A:536:ARG:C	2.37	0.44
1:A:261:THR:OG1	1:A:288:HIS:NE2	2.50	0.44
1:A:493:TYR:CD1	1:A:493:TYR:N	2.86	0.44
1:A:474:ASN:HB3	1:A:475:PRO:HD3	1.98	0.44
1:A:297:LYS:HG3	1:A:298:ASP:N	2.32	0.44
1:A:304:GLN:HE22	3:A:603:NAG:C3	2.27	0.44
1:A:503:PHE:CA	1:A:515:LEU:HD23	2.44	0.44
1:A:484:THR:O	1:A:485:HIS:CB	2.66	0.44
1:A:509:PRO:C	1:A:511:GLU:N	2.71	0.44
1:A:36:ASP:OD1	1:A:368:LYS:HD2	2.18	0.44
1:A:516:THR:N	1:A:517:PRO:HD3	2.31	0.43
1:A:253:GLN:N	1:A:572:CYS:HB3	2.33	0.43
1:A:67:GLN:HE21	1:A:454:ARG:NE	2.13	0.43
1:A:302:LYS:CD	1:A:302:LYS:H	2.30	0.43
1:A:515:LEU:N	1:A:515:LEU:HD22	2.33	0.43
1:A:96:TRP:HE3	1:A:449:TYR:CE2	2.36	0.43
1:A:371:ASN:ND2	1:A:451:ASN:HB3	2.33	0.43
1:A:362:GLY:O	1:A:364:TYR:N	2.51	0.43
1:A:50:ILE:HG22	1:A:52:THR:HG23	2.01	0.43
1:A:47:ASN:OD1	1:A:50:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:HIS:HA	1:A:289:VAL:HA	1.75	0.43
1:A:365:LYS:HE3	1:A:372:TRP:NE1	2.34	0.43
1:A:498:ASP:HA	1:A:499:PRO:C	2.38	0.43
1:A:52:THR:O	1:A:56:ASP:OD2	2.37	0.43
1:A:37:LEU:HD22	1:A:315:MET:CE	2.48	0.43
1:A:453:VAL:HG13	1:A:466:ALA:HB3	2.00	0.43
1:A:564:PRO:CG	1:A:571:GLN:O	2.65	0.42
1:A:175:GLY:C	1:A:177:VAL:N	2.73	0.42
1:A:436:ARG:NH2	1:A:458:GLN:O	2.52	0.42
1:A:427:MET:N	1:A:428:PRO:CD	2.81	0.42
1:A:532:GLU:CD	1:A:532:GLU:C	2.78	0.42
1:A:462:SER:HA	1:A:506:SER:CB	2.50	0.42
1:A:312:VAL:CG2	1:A:313:GLU:N	2.82	0.42
1:A:142:HIS:HD2	2:A:602:BOG:H2'1	1.84	0.42
1:A:261:THR:OG1	1:A:288:HIS:CD2	2.72	0.42
1:A:190:LEU:HA	1:A:190:LEU:HD12	1.83	0.42
1:A:458:GLN:HA	1:A:458:GLN:HE21	1.85	0.42
1:A:522:ARG:O	1:A:526:ILE:HG23	2.20	0.42
1:A:200:LEU:HA	1:A:200:LEU:HD12	1.79	0.42
1:A:88:PRO:HB2	6:A:770:HOH:O	2.19	0.42
1:A:363:ILE:CD1	1:A:510:ARG:HG3	2.50	0.42
1:A:171:LYS:HB2	1:A:257:TYR:CE1	2.55	0.42
1:A:36:ASP:O	1:A:345:ALA:HA	2.19	0.42
1:A:110:GLY:N	1:A:547:GLN:HG3	2.34	0.42
1:A:346:HIS:NE2	1:A:486:VAL:HG23	2.35	0.42
1:A:171:LYS:HA	1:A:172:PRO:HD2	1.93	0.42
1:A:550:TRP:O	1:A:554:LEU:HG	2.19	0.42
1:A:304:GLN:NE2	3:A:603:NAG:H3	2.31	0.41
1:A:363:ILE:O	1:A:363:ILE:HG12	2.14	0.41
1:A:458:GLN:HE21	1:A:458:GLN:CA	2.32	0.41
1:A:378:VAL:HG22	1:A:379:PRO:CD	2.48	0.41
1:A:39:ILE:HD12	1:A:379:PRO:HG3	2.02	0.41
1:A:372:TRP:O	1:A:373:GLU:C	2.58	0.41
1:A:298:ASP:O	1:A:302:LYS:HE2	2.20	0.41
1:A:505:ILE:N	1:A:505:ILE:CD1	2.80	0.41
1:A:346:HIS:HA	1:A:368:LYS:HB3	2.02	0.41
1:A:519:SER:HA	1:A:522:ARG:NH1	2.35	0.41
1:A:168:ARG:HB2	1:A:175:GLY:CA	2.44	0.41
1:A:94:ALA:HB1	1:A:447:ASN:C	2.41	0.41
1:A:244:MET:HB2	1:A:252:GLN:HB3	2.03	0.41
1:A:509:PRO:C	1:A:511:GLU:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:THR:HG22	1:A:183:LYS:HD3	2.03	0.41
1:A:288:HIS:ND1	1:A:311:ALA:HB1	2.35	0.41
1:A:490:PHE:CB	1:A:493:TYR:HE1	2.33	0.41
1:A:505:ILE:HG23	1:A:509:PRO:HA	2.01	0.41
1:A:349:GLU:HG3	1:A:357:HIS:HB2	2.02	0.41
1:A:338:TYR:HA	1:A:381:ILE:O	2.21	0.41
1:A:491:GLY:O	1:A:493:TYR:N	2.53	0.41
1:A:63:VAL:CG2	1:A:382:LEU:HB2	2.49	0.41
1:A:51:ARG:C	1:A:53:PRO:HD3	2.41	0.41
1:A:484:THR:HG23	1:A:486:VAL:O	2.21	0.41
1:A:246:ARG:HH11	1:A:246:ARG:HG2	1.86	0.41
1:A:150:HIS:CE1	1:A:151:PRO:HG2	2.56	0.41
1:A:509:PRO:O	1:A:511:GLU:N	2.54	0.41
1:A:160:TYR:CD2	1:A:267:GLU:HG3	2.56	0.40
1:A:206:LEU:HB2	1:A:208:LEU:HD12	2.03	0.40
1:A:297:LYS:HG3	1:A:298:ASP:OD1	2.22	0.40
1:A:556:LYS:HD3	1:A:558:TRP:CZ2	2.56	0.40
1:A:50:ILE:HD11	3:A:603:NAG:O6	2.21	0.40
1:A:520:GLU:HA	1:A:523:PHE:HB2	2.03	0.40
1:A:43:GLY:O	1:A:45:TYR:N	2.54	0.40
1:A:183:LYS:HE2	1:A:184:ARG:HH22	1.86	0.40
1:A:35:ASP:O	1:A:289:VAL:N	2.46	0.40
1:A:420:ILE:HA	6:A:795:HOH:O	2.21	0.40

All (2) 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:A:606:PO4:P	5:A:606:PO4:O2[5_556]	1.43	0.77
5:A:606:PO4:P	5:A:606:PO4:O1[5_556]	1.48	0.72

## 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	544/562 (97%)	443 (81%)	76 (14%)	25 (5%)	<b>3</b> <b>3</b>

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ALA
1	A	369	ALA
1	A	490	PHE
1	A	516	THR
1	A	564	PRO
1	A	44	CYS
1	A	176	SER
1	A	363	ILE
1	A	373	GLU
1	A	451	ASN
1	A	471	PRO
1	A	474	ASN
1	A	517	PRO
1	A	569	SER
1	A	175	GLY
1	A	302	LYS
1	A	351	SER
1	A	527	LEU
1	A	491	GLY
1	A	492	SER
1	A	523	PHE
1	A	565	SER
1	A	58	LEU
1	A	505	ILE
1	A	378	VAL

### 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	470/481 (98%)	434 (92%)	36 (8%)	16	31

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	49	THR
1	A	58	LEU
1	A	63	VAL
1	A	93	MET
1	A	103	LEU
1	A	113	THR
1	A	121	LEU
1	A	122	LEU
1	A	139	MET
1	A	169	ASP
1	A	176	SER
1	A	186	VAL
1	A	191	GLN
1	A	200	LEU
1	A	203	LEU
1	A	284	LEU
1	A	302	LYS
1	A	322	ILE
1	A	343	GLN
1	A	363	ILE
1	A	403	ILE
1	A	420	ILE
1	A	440	GLU
1	A	451	ASN
1	A	473	PHE
1	A	486	VAL
1	A	487	CYS
1	A	493	TYR
1	A	510	ARG
1	A	522	ARG
1	A	532	GLU
1	A	563	CYS
1	A	566	THR
1	A	570	CYS
1	A	572	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	191	GLN
1	A	204	ASN
1	A	247	ASN
1	A	321	GLN
1	A	357	HIS
1	A	435	GLN
1	A	447	ASN
1	A	458	GLN
1	A	472	ASN
1	A	531	GLN
1	A	571	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	ALS	A	75	1,4	7,10,11	1.09	1 (14%)	8,14,16	1.30	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ALS	A	75	1,4	-	0/3/11/13	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	ALS	OS1-S	-2.25	1.49	1.57

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ALS	C-CA-N	2.43	114.91	109.83

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
1	A	75	ALS	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z  > 2$
2	BOG	A	601	-	20,20,20	1.23	3 (15%)	25,25,25	0.65	0
2	BOG	A	602	-	20,20,20	1.14	2 (10%)	25,25,25	0.65	0
3	NAG	A	603	1	14,14,15	0.47	0	15,19,21	0.90	1 (6%)
3	NAG	A	604	1	14,14,15	0.61	0	15,19,21	0.86	1 (6%)
5	PO4	A	606	-	0,2,4	0.00	-	0,1,6	0.00	-

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	BOG	A	601	-	-	0/11/31/31	0/1/1/1
2	BOG	A	602	-	-	0/11/31/31	0/1/1/1
3	NAG	A	603	1	-	0/6/23/26	0/1/1/1
3	NAG	A	604	1	-	0/6/23/26	0/1/1/1
5	PO4	A	606	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	BOG	C4-C5	2.22	1.57	1.53
2	A	602	BOG	O1-C1	2.25	1.44	1.40
2	A	601	BOG	O1-C1	2.68	1.45	1.40
2	A	602	BOG	O5-C1	3.14	1.49	1.41
2	A	601	BOG	O5-C1	3.14	1.49	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	NAG	C2-N2-C7	-2.59	119.71	123.04
3	A	604	NAG	C2-N2-C7	-2.21	120.19	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	BOG	2	0
3	A	603	NAG	11	0
5	A	606	PO4	1	2

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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