Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 11:54 AM EDT

PDB ID	:	1P49
Title	:	Structure of Human Placental Estrone/DHEA Sulfatase
Authors	:	Hernandez-Guzman, F.G.; Higashiyama, T.; Pangborn, W.; Osawa, Y.; Ghosh, D.
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

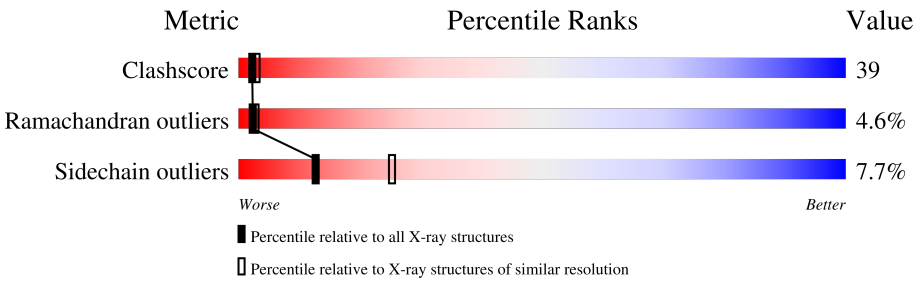
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	562	46% 44% 7% • •

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.

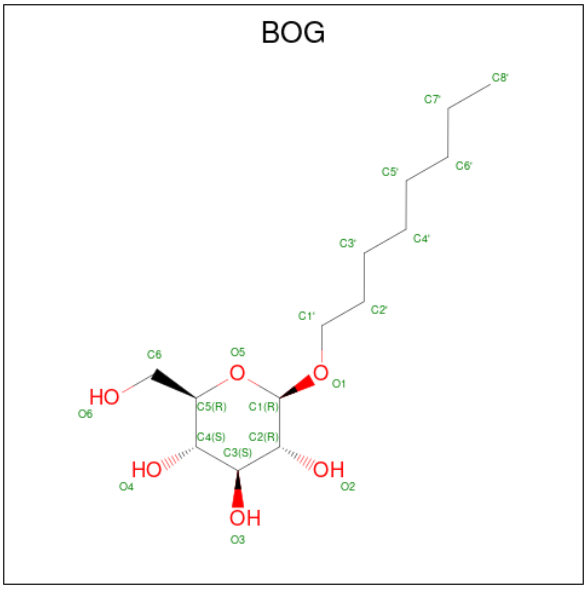
- Molecule 1 is a protein called STERYL-SULFATASE.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	ALS	CYS	modified residue	UNP P08842

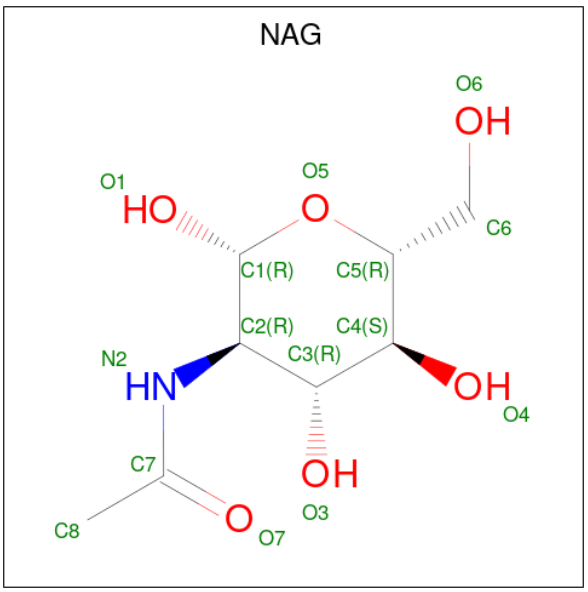
- Molecule 2 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).

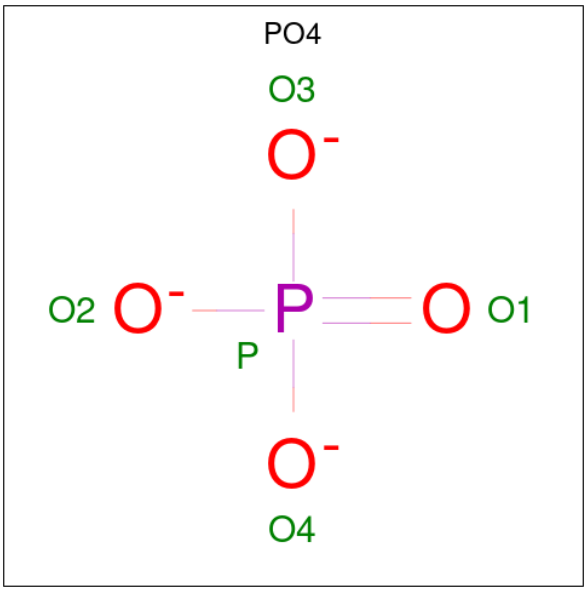


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- 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_4P).



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

- Molecule 6 is water.

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

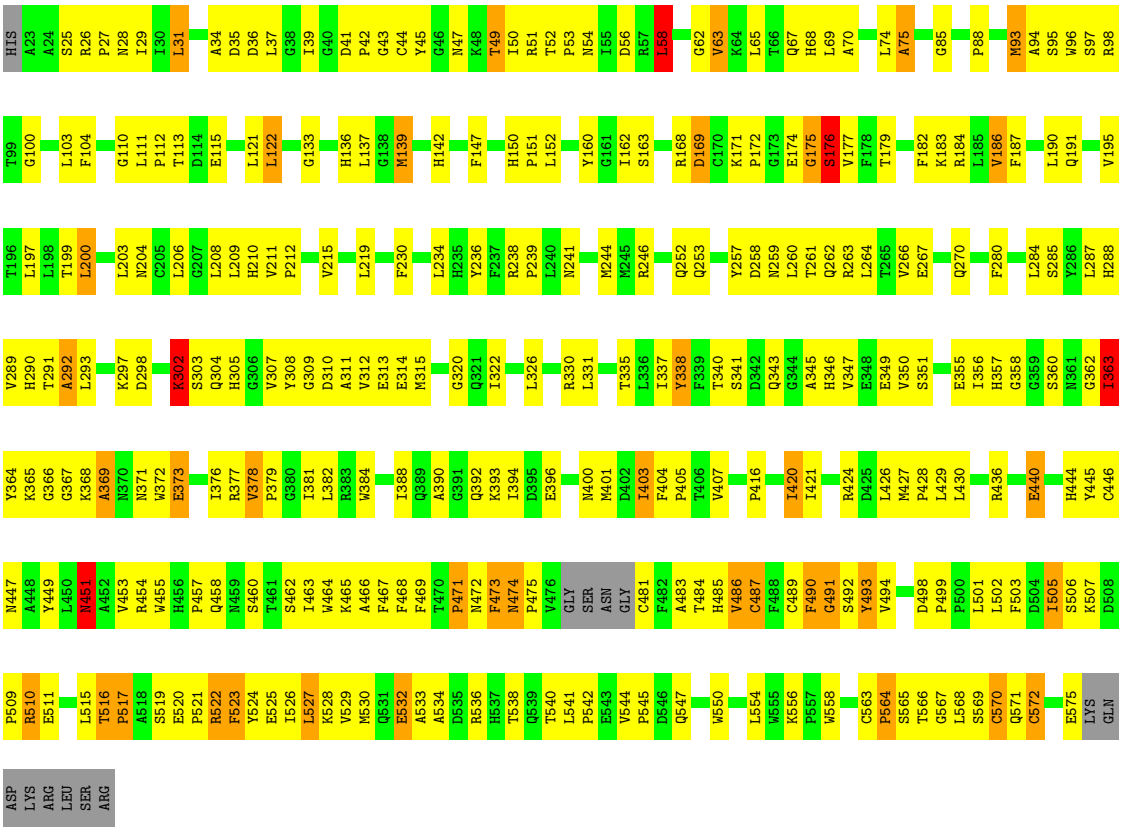
3 Residue-property plots (i)

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

Note EDS was not executed.

- Molecule 1: STERYL-SULFATASE

Chain A: 46% 44% 7% • •



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	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^2)	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: BOG, NAG, ALS, CA, PO4

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	4228	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	4310	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:142:HIS:ND1	5:A:606:PO4:O1	2.21	0.70
1:A:304:GLN:OE1	1:A:305:HIS:HB2	1.91	0.70
1:A:184:ARG:HG2	1:A:184:ARG:HH21	1.57	0.69
1:A:67:GLN:NE2	1:A:454:ARG:HE	1.91	0.69
1:A:388:ILE:HD13	1:A:430:LEU:HD23	1.75	0.69
1:A:420:ILE:HD12	1:A:421:ILE:N	2.07	0.69
1:A:363:ILE:HG13	1:A:510:ARG:HG3	1.75	0.69
1:A:526:ILE:O	1:A:529:VAL:HG12	1.92	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:HD12	1:A:505:ILE:H	1.59	0.66
1:A:168:ARG:HG2	1:A:291:THR:HG21	1.78	0.66
1:A:25:SER:HB2	1:A:27:PRO:HD3	1.79	0.65
1:A:160:TYR:HE2	1:A:264:LEU:HD23	1.60	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:307:VAL:HA	1:A:310:ASP:OD2	1.98	0.63
1:A:457:PRO:HD2	1:A:462:SER:O	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:HG2	1:A:184:ARG:NH2	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:HG13	1:A:527:LEU:H	1.65	0.60
1:A:526:ILE:C	1:A:528:LYS:H	2.05	0.60
1:A:49:THR:CB	1:A:304:GLN:HG3	2.27	0.60
1:A:54:ASN:CG	1:A:320:GLY:HA3	2.21	0.60
1:A:516:THR:H	1:A:517:PRO:HD3	1.66	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:236:TYR:O	1:A:239:PRO:HD2	2.03	0.59
1:A:502:LEU:HD22	1:A:503:PHE:H	1.67	0.59
1:A:474:ASN:HB3	1:A:475:PRO:CD	2.32	0.59
1:A:520:GLU:N	1:A:521:PRO:CD	2.66	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:376:ILE:HG21	1:A:444:HIS:CE1	2.38	0.59
1:A:484:THR:O	1:A:485:HIS:HB3	2.03	0.59
1:A:544:VAL:HG22	1:A:545:PRO:HD2	1.84	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:93:MET:HE3	1:A:137:LEU:HD22	1.84	0.58
1:A:502:LEU:HD22	1:A:503:PHE:N	2.19	0.58
1:A:349:GLU:O	1:A:349:GLU:HG3	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:368:LYS:O	1:A:369:ALA:CB	2.52	0.57
1:A:529:VAL:O	1:A:532:GLU:HG3	2.04	0.57
1:A:95:SER:O	1:A:447:ASN:HB3	2.04	0.57
1:A:345:ALA:HB1	1:A:358:GLY:O	2.05	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:309:GLY:HA2	1:A:312:VAL:HG22	1.87	0.57
1:A:564:PRO:HD2	1:A:570:CYS:HA	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:H	1:A:302:LYS:HD3	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:382:LEU:HG	1:A:430:LEU:HD21	1.89	0.54
1:A:516:THR:HG22	1:A:517:PRO:HD3	1.88	0.54
1:A:110:GLY:O	1:A:547:GLN:HG2	2.06	0.54
1:A:396:GLU:OE2	1:A:436:ARG:HG3	2.07	0.54
1:A:455:TRP:CH2	1:A:529:VAL:HG11	2.43	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:HD12	1:A:29:ILE:N	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:293:LEU:H	1:A:293:LEU:HD22	1.74	0.52
1:A:516:THR:CG2	1:A:517:PRO:HD3	2.39	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:503:PHE:CD2	1:A:511:GLU:HG2	2.45	0.52
1:A:564:PRO:HG2	1:A:571:GLN:N	2.17	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:404:PHE:HB3	1:A:405:PRO:CD	2.40	0.52
1:A:474:ASN:CG	1:A:483:ALA:HB2	2.30	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:112:PRO:HB2	1:A:115:GLU:HG2	1.91	0.52
1:A:168:ARG:HB3	1:A:174:GLU:HG2	1.92	0.52
1:A:308:TYR:CE1	1:A:312:VAL:HG11	2.45	0.52
1:A:366:GLY:HA3	1:A:372:TRP:HB2	1.91	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:NH2	6:A:796:HOH:O	2.43	0.51
1:A:312:VAL:HG23	1:A:313:GLU:N	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:246:ARG:NH1	6:A:750:HOH:O	2.44	0.50
1:A:396:GLU:HG3	1:A:436:ARG:HA	1.93	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:266:VAL:O	1:A:270:GLN:HG3	2.12	0.49
1:A:340:THR:HA	1:A:379:PRO:O	2.12	0.49
1:A:440:GLU:O	1:A:455:TRP:HD1	1.95	0.49
1:A:307:VAL:O	1:A:310:ASP:HB2	2.12	0.49
1:A:474:ASN:CB	1:A:475:PRO:CD	2.90	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: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:519:SER:HA	1:A:522:ARG:HH11	1.79	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:74:LEU:HD13	1:A:100:GLY:HA3	1.95	0.48
1:A:501:LEU:HD23	1:A:501:LEU:C	2.33	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:75:ALS:OS3	1:A:290:HIS:CD2	2.66	0.48
1:A:426:LEU:O	1:A:430:LEU:HD13	2.14	0.48
1:A:490:PHE:HB2	1:A:493:TYR:CE1	2.47	0.48
1:A:147:PHE:HB3	1:A:150:HIS:HB2	1.96	0.48
1:A:392:GLN:HG3	1:A:393:LYS:H	1.79	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:197:LEU:HD12	1:A:219:LEU:HB2	1.96	0.47
1:A:445:TYR:OH	1:A:541:LEU:HD21	2.14	0.47
1:A:230:PHE:CZ	1:A:234:LEU:HD11	2.50	0.47
1:A:260:LEU:HD21	1:A:287:LEU:CD2	2.40	0.47
1:A:56:ASP:C	1:A:58:LEU:H	2.18	0.47
1:A:147:PHE:HB3	1:A:150:HIS:CB	2.45	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:53:PRO:HG2	1:A:54:ASN:H	1.80	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:491:GLY:HA2	1:A:494:VAL:HB	1.96	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:HA	1:A:458:GLN:NE2	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: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:449:TYR:CD1	1:A:489:CYS:HB2	2.43	0.46
1:A:526:ILE:O	1:A:528:LYS:N	2.47	0.46
1:A:28:ASN:CB	1:A:335:THR:HG22	2.24	0.46
1:A:330:ARG:NH2	1:A:330:ARG:HG2	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:163:SER:HB3	6:A:777:HOH:O	2.15	0.45
1:A:446:CYS:HB2	1:A:451:ASN:HB2	1.97	0.45
1:A:37:LEU:HD22	1:A:315:MET:HE3	1.98	0.45
1:A:303:SER:HB3	1:A:310:ASP:CG	2.37	0.45
1:A:356:ILE:HG23	1:A:356:ILE:O	2.16	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: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:523:PHE:HD1	1:A:524:TYR:HD2	1.63	0.45
1:A:25:SER:O	1:A:26:ARG:HB2	2.17	0.45
1:A:97:SER:HA	1:A:490:PHE:CZ	2.52	0.45
1:A:162:ILE:HG13	1:A:162:ILE:O	2.17	0.45
1:A:449:TYR:HD1	1:A:489:CYS:CB	2.24	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:330:ARG:HG2	1:A:330:ARG:HH21	1.81	0.44
1:A:371:ASN:OD1	1:A:376:ILE:HD11	2.16	0.44
1:A:507:LYS:O	1:A:509:PRO:HD3	2.17	0.44
1:A:63:VAL:HG13	1:A:392:GLN:HB3	1.99	0.44
1:A:350:VAL:HG22	1:A:356:ILE:HD12	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:297:LYS:HG3	1:A:298:ASP:N	2.32	0.44
1:A:474:ASN:HB3	1:A:475:PRO:HD3	1.98	0.44
1:A:493:TYR:N	1:A:493:TYR:CD1	2.86	0.44
1:A:304:GLN:HE22	3:A:603:NAG:C3	2.27	0.44
1:A:484:THR:O	1:A:485:HIS:CB	2.66	0.44
1:A:503:PHE:CA	1:A:515:LEU:HD23	2.44	0.44
1:A:36:ASP:OD1	1:A:368:LYS:HD2	2.18	0.44
1:A:509:PRO:C	1:A:511:GLU:N	2.71	0.44
1:A:67:GLN:HE21	1:A:454:ARG:NE	2.13	0.43
1:A:253:GLN:N	1:A:572:CYS:HB3	2.33	0.43
1:A:302:LYS:H	1:A:302:LYS:CD	2.30	0.43
1:A:516:THR:N	1:A:517:PRO:HD3	2.31	0.43
1:A:96:TRP:HE3	1:A:449:TYR:CE2	2.36	0.43
1:A:515:LEU:N	1:A:515:LEU:HD22	2.33	0.43
1:A:362:GLY:O	1:A:364:TYR:N	2.51	0.43
1:A:371:ASN:ND2	1:A:451:ASN:HB3	2.33	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:37:LEU:HD22	1:A:315:MET:CE	2.48	0.43
1:A:52:THR:O	1:A:56:ASP:OD2	2.37	0.43
1:A:453:VAL:HG13	1:A:466:ALA:HB3	2.00	0.43
1:A:175:GLY:C	1:A:177:VAL:N	2.73	0.42
1:A:427:MET:N	1:A:428:PRO:CD	2.81	0.42
1:A:436:ARG:NH2	1:A:458:GLN:O	2.52	0.42
1:A:564:PRO:CG	1:A:571:GLN:O	2.65	0.42
1:A:462:SER:HA	1:A:506:SER:CB	2.50	0.42
1:A:532:GLU:CD	1:A:532:GLU:C	2.78	0.42
1:A:142:HIS:HD2	2:A:602:BOG:H2'1	1.84	0.42
1:A:312:VAL:CG2	1:A:313:GLU:N	2.82	0.42
1:A:190:LEU:HD12	1:A:190:LEU:HA	1.83	0.42
1:A:261:THR:OG1	1:A:288:HIS:CD2	2.72	0.42
1:A:458:GLN:HA	1:A:458:GLN:HE21	1.85	0.42
1:A:200:LEU:HD12	1:A:200:LEU:HA	1.79	0.42
1:A:522:ARG:O	1:A:526:ILE:HG23	2.20	0.42
1:A:88:PRO:HB2	6:A:770:HOH:O	2.19	0.42
1:A:171:LYS:HB2	1:A:257:TYR:CE1	2.55	0.42
1:A:363:ILE:CD1	1:A:510:ARG:HG3	2.50	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:171:LYS:HA	1:A:172:PRO:HD2	1.93	0.42
1:A:346:HIS:NE2	1:A:486:VAL:HG23	2.35	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:39:ILE:HD12	1:A:379:PRO:HG3	2.02	0.41
1:A:298:ASP:O	1:A:302:LYS:HE2	2.20	0.41
1:A:372:TRP:O	1:A:373:GLU:C	2.58	0.41
1:A:378:VAL:HG22	1:A:379:PRO:CD	2.48	0.41
1:A:346:HIS:HA	1:A:368:LYS:HB3	2.02	0.41
1:A:505:ILE:CD1	1:A:505:ILE:N	2.80	0.41
1:A:168:ARG:HB2	1:A:175:GLY:CA	2.44	0.41
1:A:519:SER:HA	1:A:522:ARG:NH1	2.35	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:179:THR:HG22	1:A:183:LYS:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:PRO:C	1:A:511:GLU:H	2.24	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:338:TYR:HA	1:A:381:ILE:O	2.21	0.41
1:A:349:GLU:HG3	1:A:357:HIS:HB2	2.02	0.41
1:A:51:ARG:C	1:A:53:PRO:HD3	2.41	0.41
1:A:63:VAL:CG2	1:A:382:LEU:HB2	2.49	0.41
1:A:150:HIS:CE1	1:A:151:PRO:HG2	2.56	0.41
1:A:246:ARG:HG2	1:A:246:ARG:HH11	1.86	0.41
1:A:484:THR:HG23	1:A:486:VAL:O	2.21	0.41
1:A:491:GLY:O	1:A:493:TYR:N	2.53	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:43:GLY:O	1:A:45:TYR:N	2.54	0.40
1:A:50:ILE:HD11	3:A:603:NAG:O6	2.21	0.40
1:A:183:LYS:HE2	1:A:184:ARG:HH22	1.86	0.40
1:A:520:GLU:HA	1:A:523:PHE:HB2	2.03	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%)	2 3

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 (i)

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%)	13 25

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

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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	4,1	7,10,11	1.15	1 (14%)	6,14,16	0.78	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
1	ALS	A	75	4,1	-	0/3/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	ALS	OS1-S	-2.49	1.49	1.57

There are no bond angle outliers.

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 monosaccharides 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	$\#\|Z\| > 2$
3	NAG	A	603	1	14,14,15	0.48	0	17,19,21	0.83	1 (5%)
5	PO4	A	606	-	0,2,4	-	-	0,1,6	-	-
2	BOG	A	602	-	20,20,20	1.18	2 (10%)	25,25,25	0.63	0
3	NAG	A	604	1	14,14,15	0.63	0	17,19,21	0.81	0
2	BOG	A	601	-	20,20,20	1.27	3 (15%)	25,25,25	0.65	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	BOG	A	602	-	-	1/11/31/31	0/1/1/1
3	NAG	A	603	1	-	4/6/23/26	0/1/1/1
2	BOG	A	601	-	-	4/11/31/31	0/1/1/1
3	NAG	A	604	1	-	3/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	BOG	O5-C1	3.16	1.49	1.41
2	A	602	BOG	O5-C1	3.16	1.49	1.41
2	A	601	BOG	O1-C1	2.80	1.45	1.40
2	A	602	BOG	O1-C1	2.34	1.44	1.40
2	A	601	BOG	C4-C5	2.26	1.57	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	603	NAG	C2-N2-C7	-2.24	119.71	122.90

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	BOG	C2'-C1'-O1-C1
2	A	602	BOG	C2'-C1'-O1-C1
3	A	603	NAG	C8-C7-N2-C2
3	A	603	NAG	O7-C7-N2-C2
3	A	604	NAG	C8-C7-N2-C2
3	A	604	NAG	O7-C7-N2-C2
2	A	601	BOG	O5-C5-C6-O6
2	A	601	BOG	C4-C5-C6-O6
3	A	603	NAG	O5-C5-C6-O6
3	A	604	NAG	O5-C5-C6-O6
2	A	601	BOG	C3'-C4'-C5'-C6'
3	A	603	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	NAG	11	0

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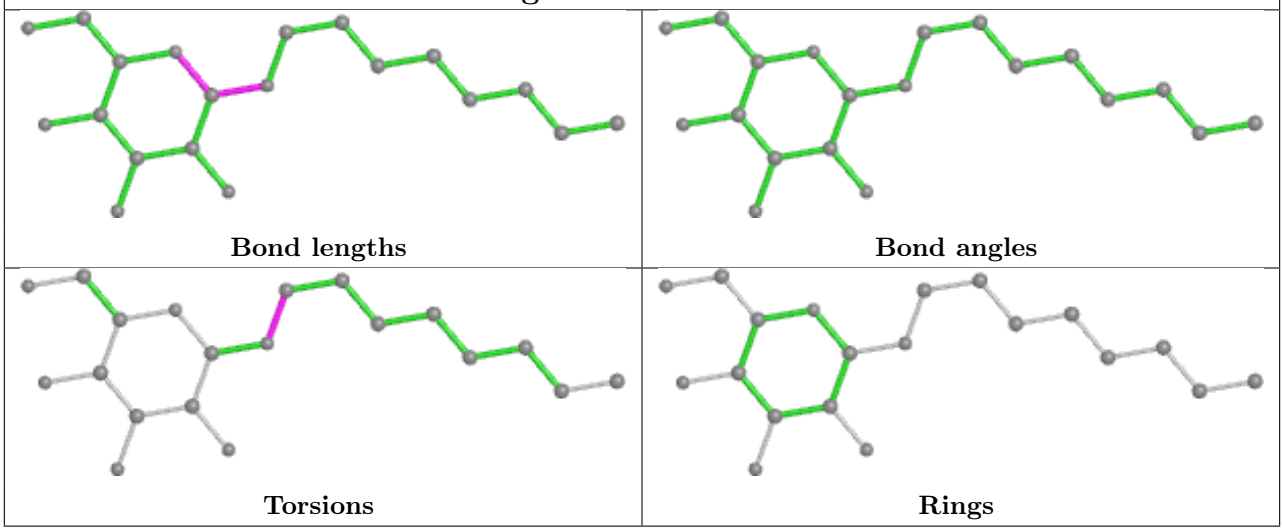
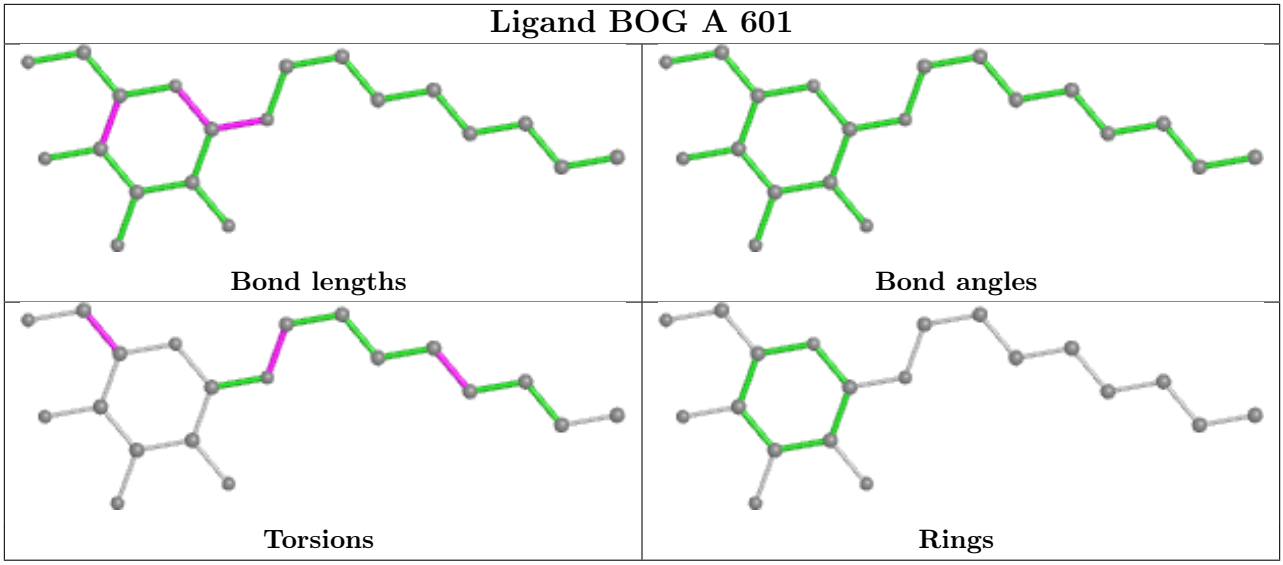
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	606	PO4	1	2
2	A	602	BOG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand BOG A 602





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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.