



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:40 PM GMT

PDB ID : 1BYD
Title : CRYSTAL STRUCTURES OF SOYBEAN BETA-AMYLASE REACTED WITH BETA-MALTOSE AND MALTAL: ACTIVE SITE COMPONENTS AND THEIR APPARENT ROLE IN CATALYSIS
Authors : Mikami, B.; Degano, M.; Hehre, E.J.; Sacchettini, J.C.
Deposited on : 1994-01-25
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **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

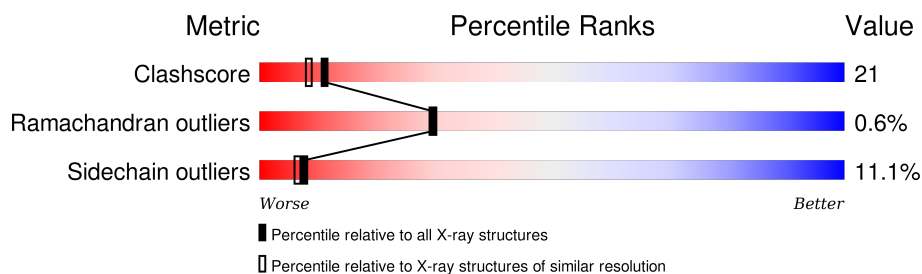
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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 ≥ 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	495	

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	DOM	A	496	X	-	-	-

2 Entry composition [i](#)

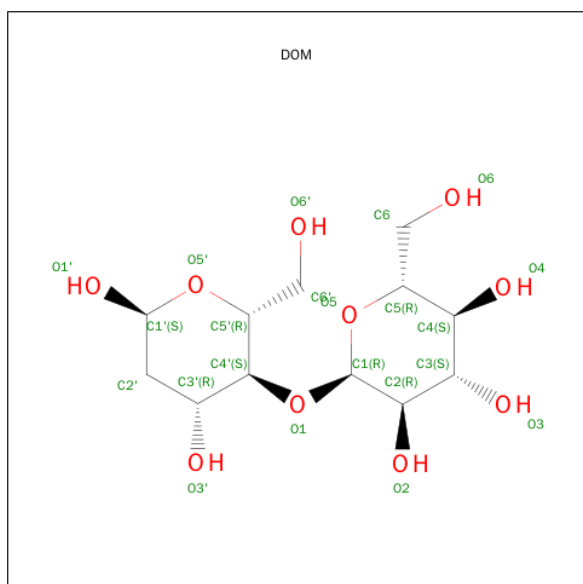
There are 4 unique types of molecules in this entry. The entry contains 4305 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-AMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	1
			3925	2518	662	728	17			

- Molecule 2 is SUGAR (2'-DEOXYMALTOSE) (three-letter code: DOM) (formula: C₁₂H₂₂O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			22	12	10		
2	A	1	Total	C	O	0	0
			22	12	10		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is water.

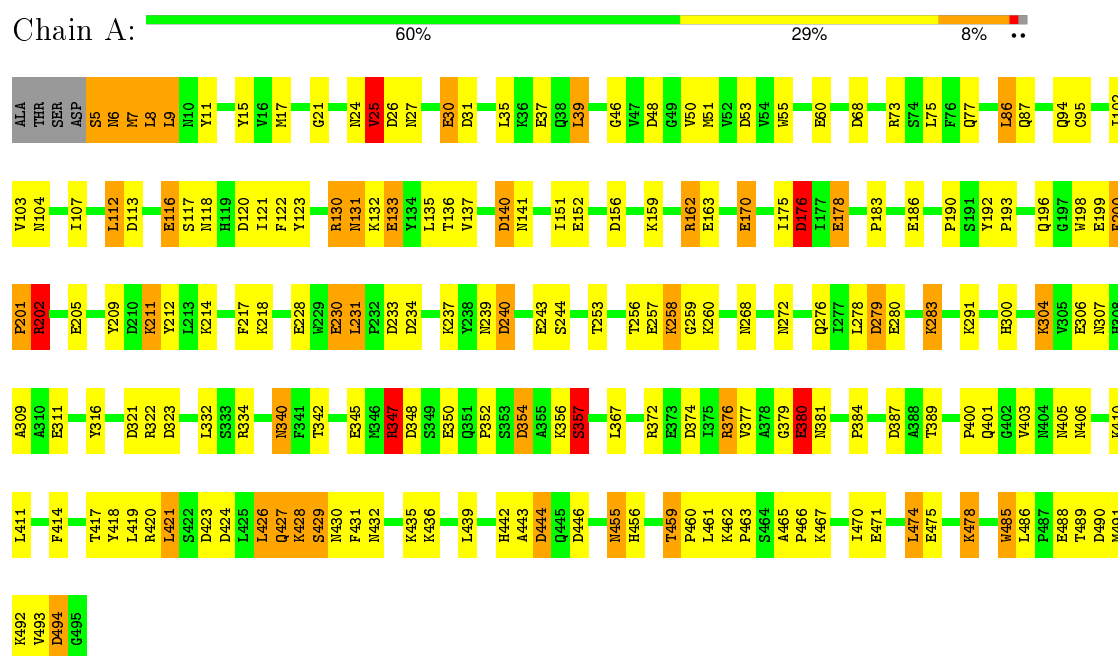
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	331	Total	O	0	0
			331	331		

3 Residue-property plots [i](#)

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: BETA-AMYLASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.20 Å 86.20 Å 144.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	9.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (9.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.145 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4305	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: SO4, DOM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.44	29/4032 (0.7%)	1.49	58/5479 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	GLU	CD-OE1	11.37	1.38	1.25
1	A	163	GLU	CD-OE1	10.83	1.37	1.25
1	A	257	GLU	CD-OE2	10.23	1.36	1.25
1	A	475	GLU	CD-OE1	10.00	1.36	1.25
1	A	306	GLU	CD-OE2	9.83	1.36	1.25
1	A	37	GLU	CD-OE2	9.71	1.36	1.25
1	A	488	GLU	CD-OE2	9.32	1.35	1.25
1	A	471	GLU	CD-OE2	8.76	1.35	1.25
1	A	243	GLU	CD-OE1	8.39	1.34	1.25
1	A	186	GLU	CD-OE2	7.98	1.34	1.25
1	A	60	GLU	CD-OE2	7.91	1.34	1.25
1	A	30	GLU	CD-OE1	7.62	1.34	1.25
1	A	205	GLU	CD-OE1	7.43	1.33	1.25
1	A	116	GLU	CD-OE2	7.19	1.33	1.25
1	A	152	GLU	CD-OE2	7.09	1.33	1.25
1	A	162	ARG	NE-CZ	6.96	1.42	1.33
1	A	228	GLU	CD-OE2	6.50	1.32	1.25
1	A	311	GLU	CD-OE2	6.30	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	GLU	CD-OE1	6.08	1.32	1.25
1	A	380	GLU	CD-OE1	5.88	1.32	1.25
1	A	350	GLU	CD-OE2	-5.80	1.19	1.25
1	A	357	SER	CB-OG	-5.58	1.34	1.42
1	A	133	GLU	CD-OE2	5.55	1.31	1.25
1	A	178	GLU	CD-OE1	5.39	1.31	1.25
1	A	104	ASN	N-CA	-5.21	1.35	1.46
1	A	37	GLU	CG-CD	5.18	1.59	1.51
1	A	380	GLU	CD-OE2	-5.08	1.20	1.25
1	A	347	ARG	NE-CZ	5.08	1.39	1.33
1	A	186	GLU	CD-OE1	-5.05	1.20	1.25

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ARG	NE-CZ-NH2	-11.98	114.31	120.30
1	A	279	ASP	CB-CG-OD1	-11.77	107.71	118.30
1	A	233	ASP	CB-CG-OD2	-11.69	107.78	118.30
1	A	130	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	A	321	ASP	CB-CG-OD1	10.52	127.77	118.30
1	A	279	ASP	CB-CG-OD2	9.39	126.75	118.30
1	A	423	ASP	CB-CG-OD2	-8.94	110.25	118.30
1	A	233	ASP	CB-CG-OD1	8.52	125.97	118.30
1	A	240	ASP	CB-CG-OD1	-8.46	110.69	118.30
1	A	240	ASP	CB-CG-OD2	8.38	125.85	118.30
1	A	156	ASP	CB-CG-OD1	-8.36	110.78	118.30
1	A	316	TYR	CB-CG-CD1	8.27	125.96	121.00
1	A	162	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	A	156	ASP	CB-CG-OD2	8.23	125.70	118.30
1	A	202	ARG	CB-CA-C	8.22	126.84	110.40
1	A	321	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	A	334	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	A	202	ARG	NE-CZ-NH2	7.74	124.17	120.30
1	A	376	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	494	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	A	420	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	A	176	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	48	ASP	CB-CG-OD1	7.03	124.63	118.30
1	A	176	ASP	CB-CG-OD1	6.97	124.58	118.30
1	A	140	ASP	CB-CG-OD2	6.88	124.49	118.30
1	A	316	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	A	372	ARG	NE-CZ-NH2	-6.29	117.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	THR	N-CA-CB	-6.21	98.50	110.30
1	A	130	ARG	CD-NE-CZ	6.17	132.24	123.60
1	A	7	MET	CG-SD-CE	6.12	109.99	100.20
1	A	68	ASP	CB-CG-OD1	6.04	123.73	118.30
1	A	73	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	424	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	494	ASP	O-C-N	-5.85	113.25	123.20
1	A	209	TYR	CB-CG-CD2	5.85	124.51	121.00
1	A	494	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	376	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	209	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	A	348	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	120	ASP	CB-CG-OD2	5.53	123.27	118.30
1	A	322	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	113	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	322	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	26	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	A	230	GLU	CG-CD-OE1	-5.36	107.57	118.30
1	A	31	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	5	SER	CB-CA-C	5.31	120.19	110.10
1	A	490	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	A	444	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	48	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	A	31	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	323	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	446	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	A	374	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	A	354	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	446	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	323	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	68	ASP	CB-CG-OD2	-5.03	113.77	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	256	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ASN	Mainchain
1	A	25	VAL	Mainchain

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	3925	0	3824	160	1
2	A	44	0	44	3	0
3	A	5	0	0	0	0
4	A	331	0	0	22	2
All	All	4305	0	3868	163	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 21.

All (163) 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:200:PHE:HB3	1:A:201:PRO:HD3	1.24	1.11
1:A:202:ARG:HG3	1:A:239:ASN:CA	1.82	1.08
1:A:421:LEU:O	1:A:421:LEU:HG	1.51	1.05
1:A:200:PHE:HB3	1:A:201:PRO:CD	1.88	1.03
1:A:200:PHE:CB	1:A:201:PRO:HD3	1.91	0.99
1:A:6:ASN:HD21	1:A:8:LEU:HB2	1.23	0.98
1:A:199:GLU:O	1:A:202:ARG:HB2	1.65	0.97
1:A:202:ARG:HG3	1:A:239:ASN:CB	1.93	0.96
1:A:202:ARG:HG3	1:A:239:ASN:HA	1.41	0.96
1:A:199:GLU:H	1:A:239:ASN:HD21	1.02	0.95
1:A:367:LEU:HD22	1:A:377:VAL:HG11	1.51	0.92
1:A:200:PHE:O	1:A:202:ARG:N	2.01	0.92
1:A:202:ARG:CB	1:A:239:ASN:HD22	1.87	0.88
1:A:141:ASN:HD21	1:A:276:GLN:HE22	1.18	0.88
1:A:381:ASN:HD21	1:A:419:LEU:HB3	1.40	0.87
1:A:253:THR:O	1:A:256:THR:HG22	1.75	0.86
1:A:427:GLN:HG2	1:A:428:LYS:N	1.90	0.85
1:A:6:ASN:OD1	1:A:7:MET:N	2.09	0.84
1:A:199:GLU:H	1:A:239:ASN:ND2	1.77	0.83
1:A:202:ARG:HG3	1:A:239:ASN:HB3	1.58	0.82
1:A:199:GLU:N	1:A:239:ASN:HD21	1.76	0.82
1:A:459:THR:HG23	1:A:460:PRO:HD2	1.62	0.80
1:A:6:ASN:ND2	1:A:8:LEU:HB2	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:CG	1:A:239:ASN:HA	2.13	0.79
1:A:380:GLU:HB2	4:A:505:HOH:O	1.84	0.78
1:A:200:PHE:CG	1:A:201:PRO:HD3	2.18	0.78
1:A:202:ARG:CG	1:A:239:ASN:HD22	1.96	0.78
1:A:230:GLU:HG3	4:A:692:HOH:O	1.85	0.77
1:A:347:ARG:HH11	1:A:347:ARG:HG3	1.51	0.76
1:A:478:LYS:HZ2	1:A:478:LYS:HB3	1.52	0.75
1:A:25:VAL:HG13	4:A:689:HOH:O	1.84	0.75
1:A:202:ARG:CG	1:A:239:ASN:HB3	2.19	0.71
1:A:202:ARG:CG	1:A:239:ASN:CB	2.68	0.70
1:A:200:PHE:CD2	1:A:201:PRO:HD3	2.26	0.70
1:A:256:THR:HG23	1:A:259:GLY:H	1.56	0.69
1:A:342:THR:HB	4:A:505:HOH:O	1.94	0.67
1:A:200:PHE:CB	1:A:201:PRO:CD	2.51	0.67
1:A:367:LEU:HD22	1:A:377:VAL:CG1	2.21	0.67
2:A:496:DOM:O1'	4:A:505:HOH:O	2.13	0.67
1:A:131:ASN:C	1:A:131:ASN:HD22	1.97	0.67
1:A:123:TYR:OH	1:A:137:VAL:HG23	1.95	0.66
1:A:381:ASN:ND2	1:A:419:LEU:HB3	2.09	0.66
1:A:11:TYR:N	4:A:690:HOH:O	2.29	0.65
1:A:200:PHE:C	1:A:202:ARG:H	1.97	0.65
1:A:380:GLU:HB3	1:A:417:THR:O	1.98	0.64
1:A:465:ALA:HB1	1:A:466:PRO:HD2	1.79	0.64
1:A:459:THR:CG2	1:A:460:PRO:HD2	2.29	0.63
1:A:276:GLN:O	1:A:279:ASP:HB2	1.98	0.62
1:A:465:ALA:HB1	1:A:466:PRO:CD	2.29	0.62
1:A:202:ARG:HB3	1:A:239:ASN:HA	1.82	0.61
1:A:117:SER:HA	4:A:722:HOH:O	1.99	0.61
1:A:6:ASN:CG	1:A:7:MET:N	2.54	0.61
1:A:460:PRO:O	1:A:462:LYS:HE3	2.01	0.60
1:A:340:ASN:ND2	1:A:379:GLY:HA2	2.17	0.59
1:A:384:PRO:HD3	1:A:419:LEU:CD2	2.31	0.59
1:A:202:ARG:CB	1:A:239:ASN:HA	2.32	0.59
1:A:122:PHE:HB3	1:A:131:ASN:O	2.03	0.59
1:A:352:PRO:HB2	1:A:354:ASP:OD1	2.02	0.59
1:A:193:PRO:HG2	1:A:196:GLN:HB2	1.85	0.59
1:A:131:ASN:HD22	1:A:132:LYS:N	2.01	0.59
1:A:427:GLN:OE1	1:A:429:SER:N	2.36	0.58
1:A:258:LYS:HE2	4:A:795:HOH:O	2.04	0.57
1:A:200:PHE:CG	1:A:201:PRO:CD	2.85	0.57
2:A:496:DOM:H5	2:A:496:DOM:H6'1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:LYS:HE2	4:A:826:HOH:O	2.05	0.55
1:A:387:ASP:OD2	1:A:389:THR:HB	2.07	0.55
1:A:202:ARG:CG	1:A:239:ASN:ND2	2.69	0.54
1:A:202:ARG:HG2	1:A:239:ASN:HD22	1.69	0.54
1:A:462:LYS:HB3	1:A:463:PRO:HD2	1.90	0.54
1:A:198:TRP:CZ2	1:A:200:PHE:O	2.61	0.54
1:A:340:ASN:HD22	1:A:340:ASN:C	2.13	0.53
1:A:256:THR:HG21	4:A:629:HOH:O	2.08	0.52
1:A:381:ASN:ND2	1:A:419:LEU:CB	2.71	0.52
1:A:211:LYS:O	1:A:211:LYS:HG2	2.02	0.52
1:A:414:PHE:O	1:A:456:HIS:HE1	1.93	0.52
1:A:15:TYR:CE2	1:A:175:ILE:HD11	2.45	0.51
1:A:17:MET:HG3	1:A:418:TYR:O	2.11	0.51
1:A:403:VAL:HG21	1:A:491:MET:CE	2.41	0.51
1:A:170:GLU:HB2	4:A:809:HOH:O	2.10	0.51
1:A:202:ARG:HB2	1:A:239:ASN:HD22	1.72	0.50
1:A:421:LEU:CD1	1:A:426:LEU:HD21	2.41	0.50
1:A:202:ARG:HG2	1:A:239:ASN:ND2	2.27	0.50
1:A:230:GLU:HG3	1:A:231:LEU:H	1.77	0.50
1:A:200:PHE:CG	1:A:201:PRO:N	2.78	0.50
1:A:107:ILE:HG13	1:A:112:LEU:HD13	1.93	0.50
1:A:140:ASP:HB3	1:A:151:ILE:CD1	2.43	0.49
1:A:459:THR:HG22	1:A:460:PRO:O	2.13	0.49
1:A:443:ALA:O	1:A:444:ASP:HB2	2.12	0.49
1:A:21:GLY:N	4:A:849:HOH:O	2.40	0.48
1:A:459:THR:HG22	1:A:460:PRO:N	2.27	0.48
1:A:202:ARG:HG3	1:A:239:ASN:C	2.32	0.48
1:A:55:TRP:CH2	1:A:95:CYS:HB2	2.48	0.48
1:A:268:ASN:ND2	4:A:565:HOH:O	2.46	0.48
1:A:459:THR:CG2	1:A:460:PRO:CD	2.92	0.47
1:A:426:LEU:HD12	1:A:431:PHE:CE1	2.49	0.47
1:A:7:MET:C	1:A:9:LEU:H	2.18	0.47
1:A:304:LYS:HD2	1:A:357:SER:O	2.14	0.47
1:A:384:PRO:HD3	1:A:419:LEU:HD21	1.96	0.47
1:A:202:ARG:NE	1:A:239:ASN:O	2.46	0.46
1:A:459:THR:CG2	1:A:460:PRO:N	2.78	0.46
1:A:347:ARG:HG3	1:A:347:ARG:NH1	2.25	0.46
1:A:7:MET:O	1:A:9:LEU:N	2.49	0.46
1:A:389:THR:HG21	4:A:608:HOH:O	2.15	0.46
1:A:218:LYS:HD2	1:A:218:LYS:HA	1.75	0.46
1:A:340:ASN:HD22	1:A:379:GLY:HA2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LYS:HG3	1:A:231:LEU:CD2	2.46	0.45
1:A:94:GLN:HG2	1:A:95:CYS:N	2.29	0.45
1:A:340:ASN:ND2	1:A:340:ASN:C	2.69	0.45
1:A:131:ASN:ND2	1:A:133:GLU:H	2.14	0.45
1:A:291:LYS:HE3	1:A:376:ARG:CZ	2.46	0.45
1:A:462:LYS:HG2	4:A:796:HOH:O	2.17	0.45
1:A:116:GLU:HG3	4:A:611:HOH:O	2.17	0.45
1:A:7:MET:C	1:A:9:LEU:N	2.68	0.45
1:A:121:ILE:O	1:A:136:THR:HG22	2.17	0.45
1:A:421:LEU:HD11	1:A:426:LEU:HD21	1.99	0.44
1:A:478:LYS:HG2	1:A:478:LYS:HZ3	1.50	0.44
1:A:462:LYS:HB3	1:A:463:PRO:CD	2.47	0.44
2:A:496:DOM:H1'	2:A:498:DOM:O4	2.17	0.44
1:A:400:PRO:HB3	1:A:485:TRP:CD2	2.53	0.44
1:A:35:LEU:HG	1:A:39:LEU:HD22	2.00	0.44
1:A:200:PHE:C	1:A:202:ARG:N	2.62	0.44
1:A:474:LEU:HA	1:A:474:LEU:HD12	1.82	0.43
1:A:192:TYR:HB2	1:A:198:TRP:CD2	2.53	0.43
1:A:200:PHE:C	1:A:200:PHE:CD1	2.89	0.43
1:A:51:MET:HB2	1:A:87:GLN:HE21	1.84	0.43
1:A:455:ASN:HA	1:A:455:ASN:HD22	1.60	0.43
1:A:131:ASN:ND2	1:A:131:ASN:C	2.69	0.43
1:A:403:VAL:HG21	1:A:491:MET:HE3	2.00	0.43
1:A:234:ASP:N	1:A:234:ASP:OD1	2.51	0.43
1:A:427:GLN:OE1	1:A:430:ASN:N	2.43	0.43
1:A:410:LYS:N	4:A:659:HOH:O	2.25	0.43
1:A:381:ASN:OD1	1:A:419:LEU:N	2.51	0.43
1:A:410:LYS:O	1:A:410:LYS:HG2	2.19	0.43
1:A:7:MET:HE1	1:A:405:ASN:HB3	2.00	0.42
1:A:50:VAL:HG23	1:A:86:LEU:HD12	2.01	0.42
1:A:198:TRP:CH2	1:A:200:PHE:HA	2.55	0.42
1:A:278:LEU:HA	1:A:278:LEU:HD23	1.82	0.42
1:A:291:LYS:CE	1:A:376:ARG:CZ	2.98	0.42
1:A:237:LYS:N	1:A:240:ASP:OD2	2.43	0.42
1:A:283:LYS:HG2	4:A:556:HOH:O	2.18	0.42
1:A:300:HIS:H	1:A:300:HIS:CD2	2.37	0.42
1:A:122:PHE:CD1	1:A:132:LYS:HA	2.55	0.42
1:A:467:LYS:HD3	4:A:754:HOH:O	2.19	0.41
1:A:46:GLY:O	1:A:442:HIS:HE1	2.03	0.41
1:A:332:LEU:HD23	1:A:332:LEU:HA	1.73	0.41
1:A:9:LEU:HA	1:A:9:LEU:HD12	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:PHE:CD2	1:A:231:LEU:HD13	2.54	0.41
1:A:183:PRO:HG3	1:A:190:PRO:HB3	2.02	0.41
1:A:489:THR:CG2	1:A:492:LYS:HG2	2.50	0.41
1:A:175:ILE:HD13	1:A:175:ILE:HG21	1.85	0.41
1:A:470:ILE:HG13	1:A:474:LEU:HD22	2.02	0.41
1:A:159:LYS:HE3	4:A:556:HOH:O	2.20	0.41
1:A:403:VAL:HG21	1:A:491:MET:HE2	2.02	0.41
1:A:24:ASN:HD22	1:A:30:GLU:CD	2.24	0.41
1:A:53:ASP:CB	1:A:55:TRP:CE2	3.04	0.41
1:A:376:ARG:NH2	4:A:790:HOH:O	2.54	0.41
1:A:356:LYS:HE3	1:A:356:LYS:HA	2.03	0.41
1:A:401:GLN:HG2	4:A:811:HOH:O	2.21	0.41
1:A:304:LYS:HD2	1:A:357:SER:C	2.41	0.40
1:A:307:ASN:HD22	1:A:309:ALA:H	1.68	0.40
1:A:345:GLU:N	1:A:345:GLU:OE1	2.45	0.40
1:A:176:ASP:OD1	1:A:178:GLU:OE2	2.39	0.40
1:A:439:LEU:CD1	1:A:444:ASP:HA	2.52	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)
4:A:800:HOH:O	4:A:800:HOH:O[6_555]	2.01	0.19
1:A:212:TYR:OH	4:A:651:HOH:O[6_655]	2.19	0.01

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	489/495 (99%)	464 (95%)	22 (4%)	3 (1%)	30 29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	PHE
1	A	8	LEU
1	A	201	PRO

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	422/425 (99%)	375 (89%)	47 (11%)	8 6

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	6	ASN
1	A	9	LEU
1	A	25	VAL
1	A	27	ASN
1	A	39	LEU
1	A	75	LEU
1	A	77	GLN
1	A	86	LEU
1	A	102	ILE
1	A	103	VAL
1	A	112	LEU
1	A	130	ARG
1	A	131	ASN
1	A	135	LEU
1	A	162	ARG
1	A	176	ASP
1	A	202	ARG
1	A	211	LYS
1	A	231	LEU
1	A	244	SER
1	A	258	LYS
1	A	260	LYS
1	A	272	ASN

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Mol	Chain	Res	Type
1	A	283	LYS
1	A	304	LYS
1	A	340	ASN
1	A	347	ARG
1	A	357	SER
1	A	380	GLU
1	A	406	ASN
1	A	411	LEU
1	A	421	LEU
1	A	426	LEU
1	A	427	GLN
1	A	428	LYS
1	A	429	SER
1	A	432	ASN
1	A	436	LYS
1	A	455	ASN
1	A	461	LEU
1	A	474	LEU
1	A	478	LYS
1	A	485	TRP
1	A	486	LEU
1	A	493	VAL
1	A	494	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	38	GLN
1	A	87	GLN
1	A	131	ASN
1	A	194	GLN
1	A	239	ASN
1	A	268	ASN
1	A	276	GLN
1	A	307	ASN
1	A	340	ASN
1	A	455	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 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	DOM	A	496	-	23,23,23	1.11	2 (8%)	31,33,33	1.98	8 (25%)
2	DOM	A	498	-	23,23,23	1.00	2 (8%)	31,33,33	1.14	2 (6%)
3	SO4	A	860	-	4,4,4	0.92	0	6,6,6	0.29	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	DOM	A	496	-	1/1/9/9	0/8/44/44	0/2/2/2
2	DOM	A	498	-	-	0/8/44/44	0/2/2/2
3	SO4	A	860	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	496	DOM	C2'-C3'	-2.19	1.49	1.52
2	A	498	DOM	C3-C2	2.01	1.57	1.52
2	A	496	DOM	O5-C1	2.48	1.48	1.41
2	A	498	DOM	O5-C5	2.75	1.51	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	496	DOM	O1-C1-O5	-3.39	102.09	110.68
2	A	496	DOM	C6'-C5'-C4'	-2.90	104.82	113.25
2	A	498	DOM	O1-C1-C2	-2.58	101.83	108.10
2	A	498	DOM	C1-O1-C4'	-2.24	112.16	118.01
2	A	496	DOM	C1-O1-C4'	-2.16	112.37	118.01
2	A	496	DOM	C1'-C2'-C3'	-2.13	107.58	111.23
2	A	496	DOM	C6-C5-C4	-2.04	107.97	113.02
2	A	496	DOM	O3'-C3'-C4'	2.71	116.27	110.09
2	A	496	DOM	C1'-O5'-C5'	4.53	121.78	113.42
2	A	496	DOM	O5'-C1'-C2'	5.78	115.22	110.72

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	496	DOM	C1'

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	496	DOM	3	0
2	A	498	DOM	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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