



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:11 AM UTC

PDB ID : 1BYA / pdb_00001bya
Title : CRYSTAL STRUCTURES OF SOYBEAN BETA-AMYLASE REACTED WITH BETA-MALTOSE AND MALTAL: ACTIVE SITE COMPONENTS AND THEIR APPARENT ROLE IN CATALYSIS
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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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

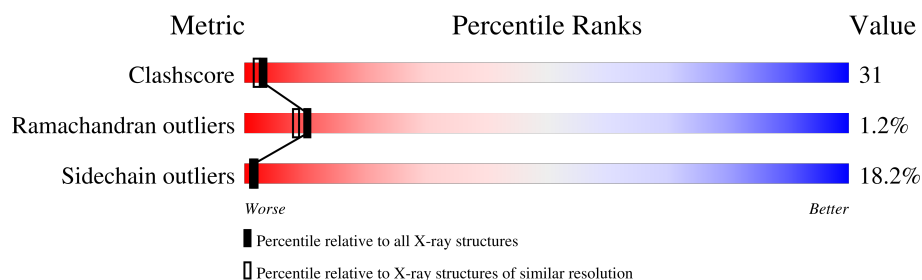
1 Overall quality at a glance

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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	495	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4254 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
			Total	C	N	O	S			
1	A	491	3929	2520	662	730	17	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

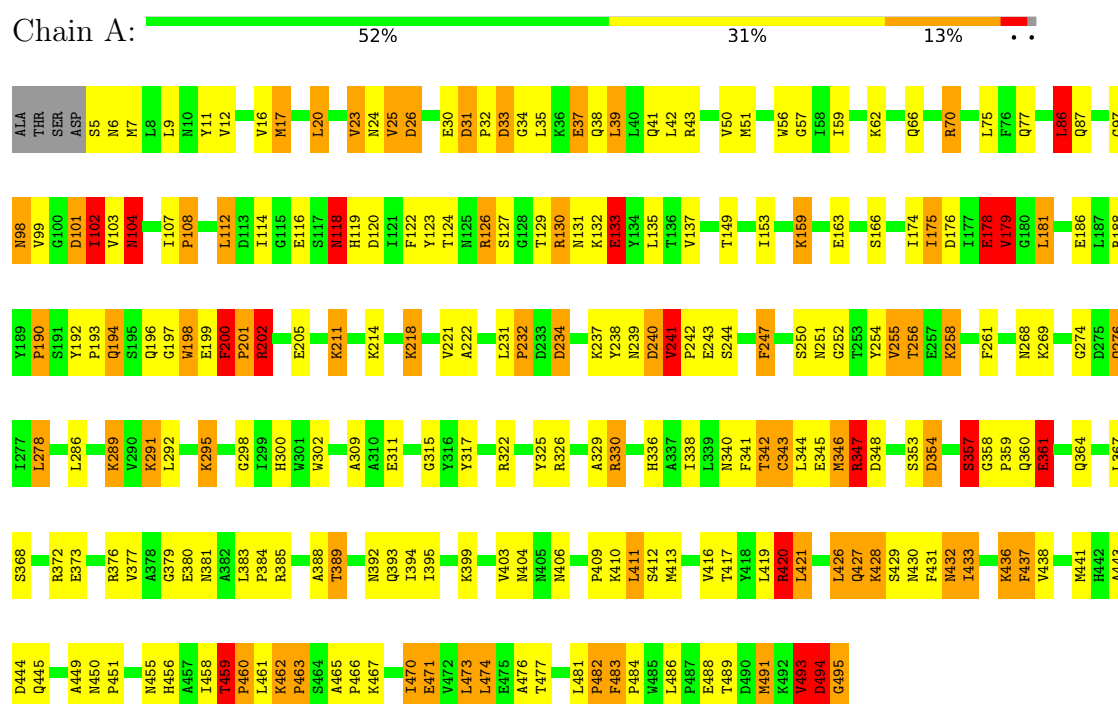
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	320	320	320	0	0

3 Residue-property plots

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: BETA-AMYLASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4254	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	4.80	38/4036 (0.9%)	1.65	46/5482 (0.8%)

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	4

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	495	GLY	C-O	248.36	6.20	1.23
1	A	495	GLY	CA-C	95.42	3.23	1.52
1	A	495	GLY	C-OXT	77.77	2.79	1.23
1	A	495	GLY	N-CA	76.57	2.68	1.45
1	A	493	VAL	CA-C	-7.21	1.44	1.52
1	A	176	ASP	CA-C	-7.17	1.43	1.52
1	A	460	PRO	C-O	-7.08	1.15	1.23
1	A	470	ILE	CA-CB	-6.68	1.46	1.54
1	A	178	GLU	CD-OE1	6.31	1.37	1.25
1	A	276	GLN	C-O	-6.23	1.16	1.24
1	A	104	ASN	N-CA	-5.97	1.39	1.46
1	A	488	GLU	CD-OE2	5.95	1.36	1.25
1	A	33	ASP	CG-OD1	5.89	1.36	1.25
1	A	31	ASP	C-N	-5.84	1.26	1.34
1	A	16	VAL	CA-C	-5.82	1.45	1.52
1	A	493	VAL	CA-CB	-5.78	1.47	1.54
1	A	37	GLU	CD-OE2	5.75	1.36	1.25
1	A	494	ASP	CG-OD2	5.75	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	GLU	CD-OE2	5.67	1.36	1.25
1	A	289	LYS	CA-CB	-5.66	1.45	1.52
1	A	190	PRO	CA-C	5.55	1.57	1.52
1	A	118	ASN	CA-C	-5.45	1.46	1.53
1	A	114	ILE	CA-CB	-5.45	1.46	1.54
1	A	16	VAL	N-CA	-5.43	1.39	1.46
1	A	86	LEU	N-CA	-5.36	1.39	1.46
1	A	198	TRP	NE1-CE2	-5.36	1.31	1.37
1	A	336	HIS	CG-ND1	5.34	1.44	1.38
1	A	459	THR	N-CA	-5.24	1.37	1.45
1	A	26	ASP	CG-OD1	5.20	1.35	1.25
1	A	471	GLU	CD-OE2	5.20	1.35	1.25
1	A	394	ILE	N-CA	-5.18	1.40	1.46
1	A	104	ASN	CG-OD1	5.14	1.33	1.23
1	A	460	PRO	CA-C	-5.09	1.46	1.52
1	A	357	SER	CA-C	-5.07	1.46	1.52
1	A	240	ASP	C-N	-5.06	1.27	1.33
1	A	329	ALA	C-N	-5.03	1.27	1.33
1	A	108	PRO	N-CA	-5.02	1.40	1.47
1	A	176	ASP	N-CA	-5.01	1.39	1.45

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	GLY	CA-C-O	15.63	167.90	121.00
1	A	495	GLY	N-CA-C	-14.13	72.33	113.30
1	A	354	ASP	CA-CB-CG	-9.41	103.19	112.60
1	A	202	ARG	CB-CA-C	8.87	124.38	109.48
1	A	309	ALA	N-CA-C	7.68	119.29	111.07
1	A	23	VAL	N-CA-CB	7.60	121.53	111.64
1	A	30	GLU	N-CA-C	7.42	119.05	110.97
1	A	86	LEU	CB-CA-C	7.41	122.41	109.80
1	A	458	ILE	N-CA-CB	7.28	121.15	111.25
1	A	483	PHE	CA-C-N	7.15	127.41	119.90
1	A	483	PHE	C-N-CA	7.15	127.41	119.90
1	A	389	THR	N-CA-CB	6.63	119.69	110.07
1	A	126	ARG	N-CA-C	6.63	119.51	111.82
1	A	416	VAL	CB-CA-C	-6.51	101.63	110.42
1	A	70	ARG	N-CA-CB	6.50	119.39	109.91
1	A	450	ASN	CA-CB-CG	-6.40	106.20	112.60
1	A	86	LEU	N-CA-CB	-6.40	100.08	110.71
1	A	119	HIS	CA-CB-CG	-6.31	107.49	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	ASP	N-CA-CB	5.99	120.60	110.49
1	A	59	ILE	N-CA-C	5.98	117.52	111.00
1	A	232	PRO	N-CA-CB	5.90	108.50	103.19
1	A	463	PRO	N-CA-CB	5.70	108.63	103.33
1	A	70	ARG	N-CA-C	5.69	117.17	110.97
1	A	437	PHE	N-CA-C	-5.68	104.99	111.07
1	A	438	VAL	N-CA-CB	5.60	117.10	110.55
1	A	116	GLU	CA-C-N	-5.55	112.65	122.26
1	A	116	GLU	C-N-CA	-5.55	112.65	122.26
1	A	179	VAL	N-CA-C	5.50	116.31	107.73
1	A	101	ASP	CA-CB-CG	-5.42	107.18	112.60
1	A	133	GLU	CB-CA-C	-5.37	99.08	110.31
1	A	99	VAL	N-CA-C	5.33	117.13	109.51
1	A	420	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	179	VAL	CB-CA-C	5.31	117.99	111.25
1	A	25	VAL	CB-CA-C	-5.31	102.59	111.29
1	A	361	GLU	N-CA-CB	5.30	118.46	110.30
1	A	389	THR	CB-CA-C	5.27	119.22	110.90
1	A	200	PHE	CB-CA-C	5.24	120.49	110.17
1	A	347	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	176	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	247	PHE	CA-CB-CG	5.17	118.97	113.80
1	A	202	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	A	179	VAL	N-CA-CB	5.16	117.66	111.31
1	A	482	PRO	CB-CA-C	-5.16	103.46	111.40
1	A	493	VAL	O-C-N	5.10	127.39	121.94
1	A	198	TRP	CB-CA-C	5.09	116.78	109.71
1	A	104	ASN	OD1-CG-ND2	5.03	127.63	122.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	489	THR	CB

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	TYR	Sidechain
1	A	133	GLU	Mainchain
1	A	241	VAL	Mainchain
1	A	276	GLN	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	3929	0	3827	243	0
2	A	5	0	0	0	0
3	A	320	0	0	23	0
All	All	4254	0	3827	243	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (243) 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:202:ARG:HG3	1:A:239:ASN:CA	1.64	1.27
1:A:202:ARG:HG3	1:A:239:ASN:HA	1.23	1.13
1:A:200:PHE:O	1:A:202:ARG:N	1.82	1.12
1:A:202:ARG:HG3	1:A:239:ASN:C	1.80	1.06
1:A:421:LEU:C	1:A:421:LEU:HD22	1.81	1.05
1:A:20:LEU:CD1	1:A:420:ARG:NH2	2.24	1.00
1:A:202:ARG:CG	1:A:239:ASN:HA	1.94	0.97
1:A:347:ARG:HH21	1:A:360:GLN:HE22	1.04	0.93
1:A:459:THR:HG22	1:A:460:PRO:HD2	1.50	0.93
1:A:347:ARG:NH2	1:A:360:GLN:HE22	1.66	0.92
1:A:20:LEU:HD13	1:A:420:ARG:NH2	1.83	0.92
1:A:17:MET:HG2	1:A:420:ARG:HH11	1.36	0.91
1:A:256:THR:HG22	1:A:258:LYS:H	1.37	0.89
1:A:202:ARG:HD2	1:A:240:ASP:O	1.73	0.88
1:A:347:ARG:HH21	1:A:360:GLN:NE2	1.70	0.88
1:A:131:ASN:HD22	1:A:132:LYS:N	1.76	0.84
1:A:346:MET:CE	1:A:383:LEU:HD12	2.08	0.82
1:A:395:ILE:HG22	1:A:489:THR:HG21	1.61	0.82
1:A:421:LEU:C	1:A:421:LEU:CD2	2.51	0.82
1:A:342:THR:O	1:A:343:CYS:SG	2.38	0.81
1:A:20:LEU:CD2	1:A:420:ARG:HH21	1.94	0.80
1:A:326:ARG:HG2	1:A:476:ALA:HB1	1.63	0.79
1:A:427:GLN:HG2	1:A:428:LYS:N	1.97	0.79
1:A:20:LEU:HD11	1:A:420:ARG:NH2	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:MET:HE3	1:A:87:GLN:NE2	1.97	0.78
1:A:200:PHE:C	1:A:202:ARG:H	1.89	0.78
1:A:459:THR:CG2	1:A:460:PRO:HD2	2.13	0.77
1:A:102:ILE:HG21	3:A:753:HOH:O	1.85	0.77
1:A:97:GLY:H	1:A:104:ASN:ND2	1.84	0.76
1:A:193:PRO:HG3	3:A:555:HOH:O	1.83	0.76
1:A:344:LEU:HD11	1:A:413:MET:HE1	1.67	0.75
1:A:199:GLU:H	1:A:239:ASN:HD21	1.34	0.75
1:A:342:THR:C	1:A:343:CYS:SG	2.70	0.74
1:A:489:THR:HG22	1:A:491:MET:H	1.52	0.74
1:A:17:MET:HG2	1:A:420:ARG:NH1	2.03	0.73
1:A:120:ASP:CG	1:A:211:LYS:HG2	2.13	0.73
1:A:202:ARG:HG3	1:A:239:ASN:CB	2.19	0.72
1:A:202:ARG:HG2	1:A:239:ASN:HD22	1.53	0.72
1:A:381:ASN:HD21	1:A:419:LEU:HB3	1.55	0.72
1:A:202:ARG:CB	1:A:239:ASN:HA	2.19	0.71
1:A:178:GLU:OE2	1:A:295:LYS:HE2	1.89	0.71
1:A:330:ARG:HD3	1:A:373:GLU:OE1	1.91	0.71
1:A:20:LEU:HD11	1:A:420:ARG:HH22	1.52	0.71
1:A:202:ARG:CG	1:A:239:ASN:HD22	2.04	0.70
1:A:202:ARG:HG3	1:A:239:ASN:O	1.91	0.70
1:A:202:ARG:HB3	1:A:239:ASN:HA	1.74	0.70
1:A:256:THR:CG2	1:A:258:LYS:H	2.05	0.70
1:A:201:PRO:HB2	1:A:202:ARG:NH1	2.06	0.70
1:A:17:MET:CG	1:A:420:ARG:HH11	2.03	0.69
1:A:51:MET:HE3	1:A:87:GLN:HE22	1.55	0.69
1:A:298:GLY:HA3	1:A:343:CYS:SG	2.32	0.69
1:A:179:VAL:O	1:A:181:LEU:HD22	1.93	0.69
1:A:421:LEU:HD22	1:A:421:LEU:O	1.93	0.69
1:A:20:LEU:CD1	1:A:420:ARG:HH22	2.06	0.68
1:A:256:THR:HG23	3:A:707:HOH:O	1.90	0.68
1:A:269:LYS:HE2	3:A:778:HOH:O	1.93	0.68
1:A:341:PHE:O	1:A:379:GLY:HA2	1.93	0.68
1:A:493:VAL:HG12	1:A:494:ASP:N	2.08	0.68
1:A:17:MET:HE2	3:A:670:HOH:O	1.94	0.67
1:A:97:GLY:H	1:A:104:ASN:HD21	1.43	0.67
1:A:403:VAL:HG21	1:A:491:MET:HE3	1.76	0.66
1:A:178:GLU:OE2	1:A:340:ASN:OD1	2.13	0.66
1:A:122:PHE:HB3	1:A:131:ASN:O	1.96	0.66
1:A:388:ALA:HB1	1:A:494:ASP:HB2	1.76	0.66
1:A:388:ALA:O	1:A:392:ASN:ND2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ASN:HD22	1:A:131:ASN:C	2.04	0.65
1:A:17:MET:HE3	1:A:51:MET:O	1.95	0.65
1:A:202:ARG:CG	1:A:239:ASN:CA	2.56	0.64
1:A:231:LEU:HB3	1:A:232:PRO:HD2	1.80	0.64
1:A:364:GLN:NE2	3:A:770:HOH:O	2.29	0.64
1:A:474:LEU:O	1:A:477:THR:HG23	1.98	0.64
1:A:241:VAL:HG22	1:A:302:TRP:CH2	2.33	0.64
1:A:178:GLU:HG2	1:A:295:LYS:CE	2.28	0.64
1:A:17:MET:CG	1:A:420:ARG:NH1	2.60	0.63
1:A:202:ARG:CG	1:A:239:ASN:C	2.66	0.63
1:A:409:PRO:HG2	1:A:412:SER:HB3	1.80	0.63
1:A:462:LYS:HG2	3:A:790:HOH:O	1.98	0.62
1:A:256:THR:HG22	1:A:258:LYS:N	2.13	0.62
1:A:98:ASN:N	1:A:101:ASP:OD2	2.33	0.62
1:A:346:MET:HE2	1:A:383:LEU:HD12	1.82	0.62
1:A:443:ALA:O	1:A:444:ASP:HB2	2.00	0.62
1:A:347:ARG:NH2	1:A:360:GLN:NE2	2.37	0.62
1:A:300:HIS:H	1:A:300:HIS:CD2	2.18	0.61
1:A:330:ARG:HG2	1:A:473:LEU:HD12	1.82	0.61
1:A:470:ILE:HG12	1:A:474:LEU:HD22	1.82	0.61
1:A:86:LEU:C	1:A:86:LEU:HD13	2.25	0.61
1:A:357:SER:HB3	1:A:359:PRO:HD3	1.83	0.61
1:A:489:THR:HG22	1:A:491:MET:N	2.16	0.61
1:A:159:LYS:HE2	3:A:549:HOH:O	2.00	0.60
1:A:192:TYR:HB2	1:A:198:TRP:CD2	2.37	0.60
1:A:107:ILE:HB	1:A:108:PRO:HD2	1.82	0.60
1:A:199:GLU:O	1:A:202:ARG:HB2	2.02	0.59
1:A:51:MET:HB2	1:A:87:GLN:HE21	1.68	0.58
1:A:20:LEU:HD21	1:A:420:ARG:HH21	1.68	0.58
1:A:381:ASN:ND2	1:A:419:LEU:HB3	2.17	0.58
1:A:5:SER:OG	1:A:6:ASN:N	2.33	0.58
1:A:214:LYS:O	1:A:218:LYS:HG3	2.04	0.57
1:A:342:THR:HG23	1:A:380:GLU:HB2	1.85	0.57
1:A:198:TRP:CH2	1:A:200:PHE:HA	2.40	0.57
1:A:367:LEU:HD22	1:A:377:VAL:HG11	1.87	0.57
1:A:495:GLY:N	1:A:495:GLY:CA	2.68	0.57
1:A:56:TRP:CE2	1:A:108:PRO:HG2	2.40	0.57
1:A:122:PHE:CD1	1:A:132:LYS:HA	2.40	0.57
1:A:348:ASP:OD2	1:A:361:GLU:OE2	2.23	0.57
1:A:393:GLN:HA	1:A:393:GLN:NE2	2.19	0.57
1:A:444:ASP:C	1:A:445:GLN:HE21	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:VAL:O	1:A:495:GLY:N	2.38	0.57
1:A:120:ASP:CB	1:A:211:LYS:HG2	2.35	0.56
1:A:268:ASN:ND2	3:A:559:HOH:O	2.38	0.56
1:A:427:GLN:OE1	1:A:429:SER:N	2.38	0.56
1:A:118:ASN:C	1:A:118:ASN:HD22	2.12	0.56
1:A:97:GLY:N	1:A:104:ASN:HD21	2.03	0.56
1:A:35:LEU:HG	1:A:39:LEU:HD22	1.86	0.56
1:A:202:ARG:CG	1:A:239:ASN:O	2.54	0.55
1:A:421:LEU:O	1:A:421:LEU:HD13	2.06	0.55
1:A:459:THR:HG22	1:A:460:PRO:CD	2.31	0.55
1:A:12:VAL:HG12	1:A:441:MET:HE3	1.88	0.55
1:A:98:ASN:O	1:A:101:ASP:HB2	2.07	0.55
1:A:342:THR:CG2	3:A:784:HOH:O	2.55	0.55
1:A:123:TYR:CD2	1:A:190:PRO:HG3	2.42	0.55
1:A:197:GLY:O	1:A:198:TRP:C	2.49	0.54
1:A:250:SER:O	1:A:251:ASN:HB2	2.06	0.54
1:A:24:ASN:OD1	1:A:26:ASP:N	2.39	0.54
1:A:421:LEU:HD21	1:A:426:LEU:CD2	2.37	0.54
1:A:346:MET:HE1	1:A:383:LEU:HD12	1.90	0.54
1:A:449:ALA:O	1:A:451:PRO:HD3	2.08	0.54
1:A:194:GLN:HB2	3:A:914:HOH:O	2.08	0.53
1:A:445:GLN:HE21	1:A:445:GLN:N	2.06	0.53
1:A:31:ASP:N	1:A:32:PRO:HD3	2.23	0.53
1:A:178:GLU:HG2	1:A:295:LYS:HE3	1.89	0.53
1:A:388:ALA:CB	1:A:494:ASP:HB2	2.39	0.53
1:A:427:GLN:OE1	1:A:430:ASN:N	2.32	0.53
1:A:465:ALA:HB1	1:A:466:PRO:CD	2.39	0.53
1:A:86:LEU:HD12	1:A:174:ILE:HG12	1.91	0.53
1:A:178:GLU:CD	1:A:295:LYS:HE2	2.34	0.53
1:A:202:ARG:CD	1:A:239:ASN:O	2.57	0.53
1:A:118:ASN:HD22	1:A:120:ASP:H	1.57	0.53
1:A:20:LEU:HD22	1:A:420:ARG:HH21	1.71	0.52
1:A:367:LEU:HD22	1:A:377:VAL:CG1	2.39	0.52
1:A:31:ASP:OD2	1:A:34:GLY:HA3	2.09	0.52
1:A:256:THR:CG2	1:A:258:LYS:HB3	2.39	0.52
1:A:489:THR:HG23	3:A:525:HOH:O	2.09	0.52
1:A:428:LYS:HD3	3:A:799:HOH:O	2.08	0.52
1:A:465:ALA:HB1	1:A:466:PRO:HD2	1.92	0.52
1:A:7:MET:HA	3:A:920:HOH:O	2.11	0.50
1:A:200:PHE:CD2	1:A:201:PRO:HD3	2.46	0.50
1:A:149:THR:O	1:A:153:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:HD23	1:A:102:ILE:HD12	1.92	0.50
1:A:178:GLU:HG2	1:A:295:LYS:HD2	1.94	0.50
1:A:462:LYS:NZ	1:A:462:LYS:HB3	2.18	0.50
1:A:186:GLU:HB3	1:A:188:ARG:HG2	1.94	0.49
1:A:24:ASN:OD1	1:A:26:ASP:HB2	2.11	0.49
1:A:462:LYS:HB3	1:A:462:LYS:HZ1	1.78	0.49
1:A:470:ILE:HG23	1:A:471:GLU:N	2.28	0.49
1:A:404:ASN:OD1	1:A:406:ASN:HB2	2.13	0.49
1:A:199:GLU:N	1:A:239:ASN:HD21	2.06	0.49
1:A:205:GLU:HG3	1:A:238:TYR:CD1	2.48	0.49
1:A:341:PHE:O	1:A:379:GLY:CA	2.60	0.49
1:A:202:ARG:CB	1:A:239:ASN:HD22	2.26	0.48
1:A:131:ASN:ND2	1:A:133:GLU:H	2.10	0.48
1:A:66:GLN:NE2	3:A:690:HOH:O	2.45	0.48
1:A:97:GLY:CA	1:A:104:ASN:HD21	2.26	0.48
1:A:462:LYS:HB3	1:A:462:LYS:HE3	1.66	0.48
1:A:426:LEU:CD1	1:A:431:PHE:CE1	2.96	0.48
1:A:50:VAL:O	1:A:86:LEU:HA	2.13	0.48
1:A:395:ILE:CG2	1:A:489:THR:HG21	2.40	0.48
1:A:427:GLN:HG2	1:A:428:LYS:H	1.75	0.47
1:A:57:GLY:HA2	1:A:108:PRO:HD3	1.96	0.47
1:A:120:ASP:OD1	1:A:130:ARG:NH2	2.45	0.47
1:A:360:GLN:O	1:A:364:GLN:HG3	2.15	0.47
1:A:344:LEU:HD11	1:A:379:GLY:HA3	1.96	0.46
1:A:123:TYR:CD2	1:A:190:PRO:CG	2.99	0.46
1:A:256:THR:CG2	3:A:707:HOH:O	2.57	0.46
1:A:462:LYS:NZ	1:A:462:LYS:CB	2.78	0.46
1:A:368:SER:O	1:A:372:ARG:HB2	2.16	0.46
1:A:241:VAL:HG13	1:A:243:GLU:OE2	2.16	0.46
1:A:383:LEU:HB3	1:A:384:PRO:HD2	1.98	0.46
1:A:124:THR:HA	1:A:129:THR:O	2.16	0.46
1:A:372:ARG:HD3	3:A:720:HOH:O	2.16	0.46
1:A:234:ASP:OD1	1:A:234:ASP:N	2.50	0.45
1:A:242:PRO:C	1:A:244:SER:H	2.24	0.45
1:A:376:ARG:NH2	3:A:652:HOH:O	2.49	0.45
1:A:12:VAL:CG1	1:A:441:MET:HE3	2.47	0.45
1:A:432:ASN:HB3	3:A:923:HOH:O	2.15	0.45
1:A:481:LEU:HB3	1:A:482:PRO:HD2	1.98	0.45
1:A:243:GLU:H	1:A:243:GLU:CD	2.24	0.45
1:A:358:GLY:N	1:A:359:PRO:CD	2.80	0.45
1:A:410:LYS:HG2	1:A:411:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLU:H	1:A:239:ASN:ND2	2.10	0.45
1:A:131:ASN:C	1:A:131:ASN:ND2	2.73	0.44
1:A:342:THR:HG21	3:A:784:HOH:O	2.17	0.44
1:A:399:LYS:HE2	3:A:524:HOH:O	2.16	0.44
1:A:445:GLN:CA	1:A:445:GLN:NE2	2.79	0.44
1:A:201:PRO:HB2	1:A:202:ARG:HH12	1.81	0.44
1:A:255:VAL:O	1:A:255:VAL:CG1	2.64	0.44
1:A:268:ASN:CG	1:A:470:ILE:HD11	2.43	0.44
1:A:51:MET:CE	1:A:417:THR:HG21	2.48	0.44
1:A:404:ASN:C	1:A:406:ASN:H	2.26	0.44
1:A:345:GLU:HG2	1:A:346:MET:N	2.29	0.44
1:A:51:MET:HB2	1:A:87:GLN:NE2	2.33	0.44
1:A:175:ILE:HG23	3:A:543:HOH:O	2.18	0.43
1:A:268:ASN:OD1	1:A:470:ILE:HD11	2.18	0.43
1:A:317:TYR:HB3	1:A:322:ARG:NH1	2.32	0.43
1:A:419:LEU:O	1:A:420:ARG:HB2	2.17	0.43
1:A:311:GLU:HG2	1:A:325:TYR:OH	2.18	0.43
1:A:112:LEU:HD12	1:A:112:LEU:HA	1.74	0.43
1:A:175:ILE:HD12	1:A:175:ILE:HA	1.50	0.43
1:A:315:GLY:HA2	3:A:744:HOH:O	2.17	0.43
1:A:474:LEU:HD12	1:A:474:LEU:HA	1.72	0.43
1:A:193:PRO:HG2	1:A:196:GLN:HB2	2.01	0.43
1:A:218:LYS:HB3	1:A:218:LYS:HE3	1.62	0.43
1:A:256:THR:HG22	1:A:258:LYS:HB3	1.99	0.43
1:A:255:VAL:O	1:A:255:VAL:HG13	2.18	0.43
1:A:118:ASN:C	1:A:118:ASN:ND2	2.77	0.43
1:A:291:LYS:HE2	1:A:376:ARG:NH1	2.33	0.43
1:A:37:GLU:H	1:A:37:GLU:HG3	1.66	0.43
1:A:437:PHE:HA	1:A:493:VAL:CG2	2.49	0.43
1:A:199:GLU:HB2	1:A:239:ASN:HD21	1.83	0.43
1:A:247:PHE:O	1:A:254:TYR:HD1	2.02	0.43
1:A:51:MET:CE	1:A:87:GLN:NE2	2.77	0.42
1:A:123:TYR:CD2	1:A:190:PRO:CD	3.02	0.42
1:A:38:GLN:O	1:A:41:GLN:HB2	2.18	0.42
1:A:131:ASN:HD22	1:A:132:LYS:H	1.59	0.42
1:A:354:ASP:OD1	1:A:354:ASP:N	2.32	0.42
1:A:218:LYS:HA	1:A:221:VAL:HG22	2.03	0.41
1:A:274:GLY:O	1:A:278:LEU:HB2	2.20	0.41
1:A:462:LYS:CB	1:A:463:PRO:CD	2.96	0.41
1:A:123:TYR:HD2	1:A:190:PRO:HG3	1.82	0.41
1:A:202:ARG:CG	1:A:239:ASN:CB	2.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:MET:HE3	1:A:417:THR:HG21	2.02	0.41
1:A:178:GLU:HG2	1:A:295:LYS:CD	2.50	0.41
1:A:419:LEU:HD23	1:A:420:ARG:HB2	2.03	0.41
1:A:345:GLU:O	1:A:393:GLN:HG2	2.20	0.41
1:A:483:PHE:HB3	1:A:484:PRO:HD2	2.03	0.41
1:A:118:ASN:ND2	1:A:120:ASP:H	2.18	0.41
1:A:433:ILE:O	1:A:436:LYS:HB2	2.21	0.41
1:A:445:GLN:NE2	1:A:445:GLN:HA	2.36	0.41
1:A:20:LEU:HD13	1:A:420:ARG:CZ	2.45	0.40
1:A:338:ILE:HD13	1:A:338:ILE:HG21	1.86	0.40
1:A:202:ARG:CG	1:A:239:ASN:ND2	2.80	0.40
1:A:221:VAL:HG23	1:A:222:ALA:N	2.36	0.40
1:A:470:ILE:CG2	1:A:471:GLU:N	2.85	0.40
1:A:261:PHE:CD1	1:A:261:PHE:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	489/495 (99%)	459 (94%)	24 (5%)	6 (1%)	10 8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ILE
1	A	200	PHE
1	A	494	ASP
1	A	201	PRO
1	A	252	GLY
1	A	420	ARG

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	422/425 (99%)	345 (82%)	77 (18%)	2 1

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	17	MET
1	A	20	LEU
1	A	23	VAL
1	A	25	VAL
1	A	33	ASP
1	A	39	LEU
1	A	42	LEU
1	A	43	ARG
1	A	62	LYS
1	A	70	ARG
1	A	75	LEU
1	A	77	GLN
1	A	86	LEU
1	A	98	ASN
1	A	102	ILE
1	A	103	VAL
1	A	104	ASN
1	A	112	LEU
1	A	118	ASN
1	A	126	ARG
1	A	127	SER
1	A	130	ARG
1	A	135	LEU
1	A	137	VAL
1	A	159	LYS
1	A	166	SER
1	A	175	ILE
1	A	178	GLU
1	A	179	VAL

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Mol	Chain	Res	Type
1	A	181	LEU
1	A	194	GLN
1	A	202	ARG
1	A	211	LYS
1	A	218	LYS
1	A	234	ASP
1	A	237	LYS
1	A	241	VAL
1	A	255	VAL
1	A	256	THR
1	A	258	LYS
1	A	278	LEU
1	A	286	LEU
1	A	289	LYS
1	A	291	LYS
1	A	292	LEU
1	A	295	LYS
1	A	330	ARG
1	A	342	THR
1	A	343	CYS
1	A	346	MET
1	A	347	ARG
1	A	353	SER
1	A	357	SER
1	A	361	GLU
1	A	385	ARG
1	A	389	THR
1	A	411	LEU
1	A	420	ARG
1	A	421	LEU
1	A	426	LEU
1	A	427	GLN
1	A	428	LYS
1	A	432	ASN
1	A	433	ILE
1	A	436	LYS
1	A	455	ASN
1	A	456	HIS
1	A	459	THR
1	A	461	LEU
1	A	462	LYS
1	A	467	LYS

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Mol	Chain	Res	Type
1	A	473	LEU
1	A	474	LEU
1	A	486	LEU
1	A	491	MET
1	A	493	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	87	GLN
1	A	104	ASN
1	A	118	ASN
1	A	119	HIS
1	A	131	ASN
1	A	141	ASN
1	A	207	GLN
1	A	239	ASN
1	A	268	ASN
1	A	276	GLN
1	A	340	ASN
1	A	364	GLN
1	A	393	GLN
1	A	406	ASN
1	A	445	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
2	SO4	A	951	-	4,4,4	0.35	0	6,6,6	0.63	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.