Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 06:28 PM EDT

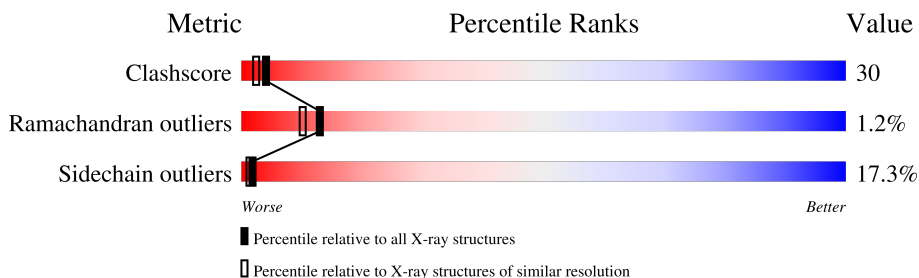|		
PDB ID	:	1BYA
Title	:	CRYSTAL STRUCTURES OF SOYBEAN BETA-AMYLASE REACTED WITH BETA-MALTOSE AND MALTAL: ACTIVE SITE COMPONENTS AND THEIR APPARENT ROLE IN CATALYSIS
Authors	:	Mikami, B.; Degano, M.; Hehre, E.J.; Sacchettini, J.C.
Deposited on	:	1994-01-25
Resolution	:	2.20 Å(reported)

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	Percentile Ranks	Value
Clashscore		30
Ramachandran outliers		1.2%
Sidechain outliers		17.3%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	495	49% 36% 11% • •

2 Entry composition ⓘ

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
1	A	491	Total 3929	C 2520	N 662	O 730	S 17	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	320	Total 320	O 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
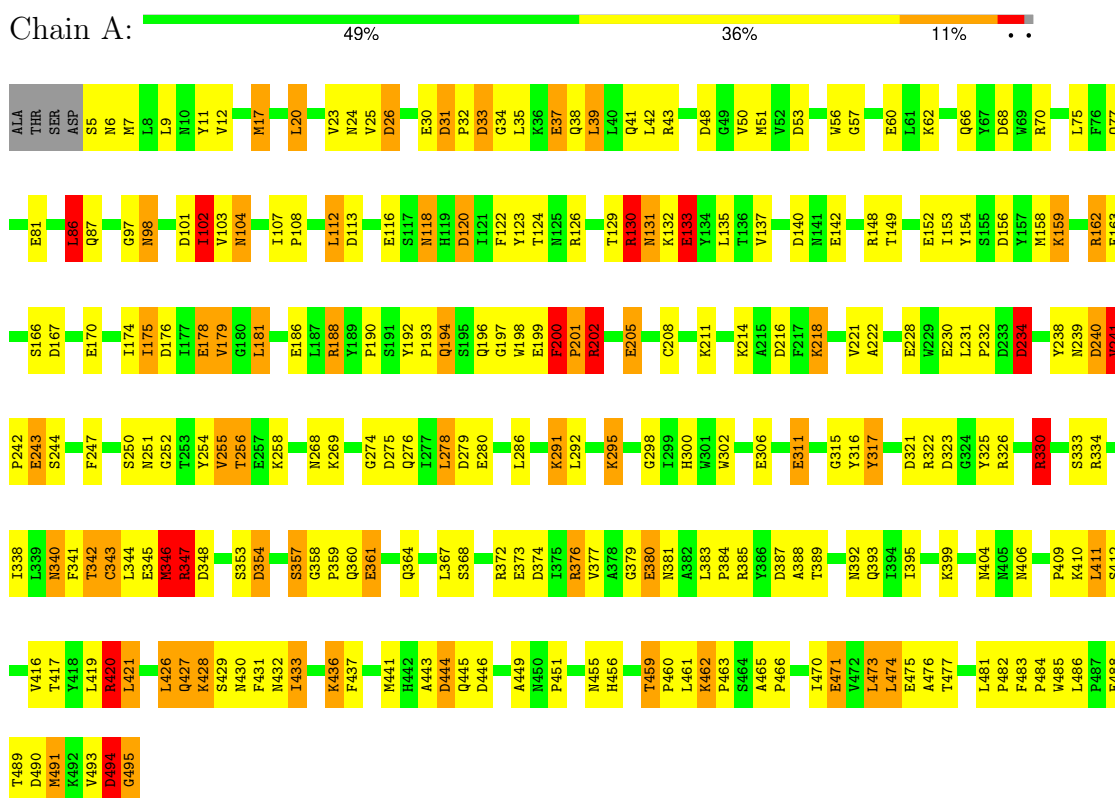
4 Data and refinement statistics ⓘ

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	86.20Å 86.20Å 144.20Å 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	5.63	26/4036 (0.6%)	1.47	69/5482 (1.3%)

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 (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	495	GLY	C-O	310.39	6.20	1.23
1	A	495	GLY	CA-C	107.48	3.23	1.51
1	A	495	GLY	C-OXT	81.97	2.79	1.23
1	A	495	GLY	N-CA	81.34	2.68	1.46
1	A	178	GLU	CD-OE1	10.62	1.37	1.25
1	A	488	GLU	CD-OE2	10.01	1.36	1.25
1	A	37	GLU	CD-OE2	9.67	1.36	1.25
1	A	163	GLU	CD-OE2	9.52	1.36	1.25
1	A	471	GLU	CD-OE2	8.71	1.35	1.25
1	A	306	GLU	CD-OE1	8.09	1.34	1.25
1	A	116	GLU	CD-OE1	7.67	1.34	1.25
1	A	30	GLU	CD-OE1	7.56	1.33	1.25
1	A	170	GLU	CD-OE1	7.43	1.33	1.25
1	A	475	GLU	CD-OE1	7.38	1.33	1.25
1	A	243	GLU	CD-OE1	7.16	1.33	1.25
1	A	230	GLU	CD-OE2	6.96	1.33	1.25
1	A	205	GLU	CD-OE1	6.81	1.33	1.25
1	A	311	GLU	CD-OE2	6.72	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	GLU	CD-OE2	6.58	1.32	1.25
1	A	152	GLU	CD-OE2	6.37	1.32	1.25
1	A	361	GLU	CD-OE1	6.36	1.32	1.25
1	A	280	GLU	CD-OE1	6.25	1.32	1.25
1	A	228	GLU	CD-OE1	6.09	1.32	1.25
1	A	142	GLU	CD-OE2	-5.45	1.19	1.25
1	A	81	GLU	CD-OE2	-5.18	1.20	1.25
1	A	380	GLU	CD-OE1	5.09	1.31	1.25

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	GLY	CA-C-O	26.28	167.90	120.60
1	A	495	GLY	N-CA-C	-16.31	72.33	113.10
1	A	330	ARG	NE-CZ-NH1	11.03	125.81	120.30
1	A	330	ARG	NE-CZ-NH2	-10.48	115.06	120.30
1	A	279	ASP	CB-CG-OD1	-9.67	109.59	118.30
1	A	240	ASP	CB-CG-OD2	8.28	125.75	118.30
1	A	446	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	A	240	ASP	CB-CG-OD1	-7.87	111.22	118.30
1	A	156	ASP	CB-CG-OD2	7.84	125.36	118.30
1	A	140	ASP	CB-CG-OD2	7.78	125.31	118.30
1	A	70	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	321	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	A	279	ASP	CB-CG-OD2	7.58	125.12	118.30
1	A	446	ASP	CB-CG-OD1	7.46	125.02	118.30
1	A	321	ASP	CB-CG-OD1	7.44	124.99	118.30
1	A	31	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	A	420	ARG	NE-CZ-NH2	7.37	123.99	120.30
1	A	33	ASP	CB-CG-OD1	-7.37	111.67	118.30
1	A	120	ASP	CB-CG-OD2	7.26	124.83	118.30
1	A	347	ARG	NE-CZ-NH2	7.19	123.90	120.30
1	A	234	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	387	ASP	CB-CG-OD1	-7.11	111.90	118.30
1	A	202	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	A	202	ARG	CB-CA-C	6.99	124.38	110.40
1	A	188	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	70	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	385	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	323	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	A	167	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	156	ASP	CB-CG-OD1	-6.61	112.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	162	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	86	LEU	CB-CA-C	6.42	122.41	110.20
1	A	323	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	167	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	374	ASP	CB-CG-OD2	6.14	123.82	118.30
1	A	346	MET	CG-SD-CE	6.13	110.01	100.20
1	A	316	TYR	CB-CG-CD1	6.12	124.67	121.00
1	A	148	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	216	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	385	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	176	ASP	CB-CG-OD1	-5.97	112.93	118.30
1	A	31	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	490	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	275	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	188	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	53	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	113	ASP	CB-CG-OD2	5.75	123.48	118.30
1	A	354	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	387	ASP	CB-CG-OD2	5.71	123.43	118.30
1	A	133	GLU	CB-CA-C	-5.66	99.08	110.40
1	A	334	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	494	ASP	N-CA-CB	5.56	120.60	110.60
1	A	48	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	374	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	130	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	216	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	48	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	316	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	A	334	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	376	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	26	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	A	444	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	A	86	LEU	N-CA-CB	-5.16	100.08	110.40
1	A	416	VAL	CB-CA-C	-5.14	101.63	111.40
1	A	68	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	A	158	MET	CG-SD-CE	5.06	108.30	100.20
1	A	200	PHE	CB-CA-C	5.05	120.49	110.40
1	A	154	TYR	CB-CG-CD1	5.03	124.02	121.00

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	233	0
2	A	5	0	0	0	0
3	A	320	0	0	23	0
All	All	4254	0	3827	233	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 30.

All (233) 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	1.01
1:A:421:LEU:C	1:A:421:LEU:HD22	1.81	1.01
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:421:LEU:C	1:A:421:LEU:CD2	2.51	0.77
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:199:GLU:H	1:A:239:ASN:HD21	1.34	0.75
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: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:342:THR:C	1:A:343:CYS:SG	2.70	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:346:MET:HE2	1:A:383:LEU:HD12	1.74	0.69
1:A:120:ASP:CG	1:A:211:LYS:HG2	2.13	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:97:GLY:H	1:A:104:ASN:HD21	1.43	0.67
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
1:A:17:MET:HE1	3:A:670:HOH:O	1.96	0.64
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:200:PHE:C	1:A:202:ARG:H	1.89	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: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:5:SER:OG	1:A:6:ASN:N	2.33	0.62
1:A:98:ASN:N	1:A:101:ASP:OD2	2.33	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: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:131:ASN:HD22	1:A:131:ASN:C	2.04	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:51:MET:HE3	1:A:417:THR:HG21	1.84	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:214:LYS:O	1:A:218:LYS:HG3	2.04	0.57
1:A:51:MET:HE3	1:A:87:GLN:HE22	1.69	0.57
1:A:202:ARG:CG	1:A:239:ASN:C	2.66	0.57
1:A:342:THR:HG23	1:A:380:GLU:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASP:CB	1:A:211:LYS:HG2	2.35	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:493:VAL:O	1:A:495:GLY:N	2.38	0.57
1:A:86:LEU:C	1:A:86:LEU:HD13	2.25	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:51:MET:HE3	1:A:87:GLN:NE2	2.20	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: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: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: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:202:ARG:CD	1:A:239:ASN:O	2.57	0.53
1:A:12:VAL:HG12	1:A:441:MET:HE3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:444:ASP:C	1:A:445:GLN:HE21	2.13	0.51
1:A:118:ASN:HD22	1:A:118:ASN:C	2.12	0.51
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
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:197:GLY:O	1:A:198:TRP:C	2.49	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: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:51:MET:CE	1:A:87:GLN:NE2	2.77	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:178:GLU:CD	1:A:295:LYS:HE2	2.34	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:345:GLU:HG2	1:A:346:MET:N	2.29	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:255:VAL:O	1:A:255:VAL:CG1	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:376:ARG:NH2	3:A:652:HOH:O	2.49	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: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
1:A:199:GLU:H	1:A:239:ASN:ND2	2.10	0.45
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:51:MET:CE	1:A:417:THR:HG21	2.48	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: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: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:12:VAL:CG1	1:A:441:MET:HE3	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:178:GLU:HG2	1:A:295:LYS:CD	2.50	0.41
1:A:242:PRO:C	1:A:244:SER:H	2.24	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:243:GLU:CD	1:A:243:GLU:H	2.24	0.40

There are no symmetry-related clashes.

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%)	459 (94%)	24 (5%)	6 (1%)	13 10

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

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Mol	Chain	Res	Type
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%)	349 (83%)	73 (17%)	2 1

All (73) 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	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	130	ARG
1	A	131	ASN
1	A	135	LEU
1	A	137	VAL
1	A	159	LYS

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Mol	Chain	Res	Type
1	A	162	ARG
1	A	166	SER
1	A	175	ILE
1	A	179	VAL
1	A	181	LEU
1	A	194	GLN
1	A	202	ARG
1	A	208	CYS
1	A	218	LYS
1	A	234	ASP
1	A	241	VAL
1	A	255	VAL
1	A	256	THR
1	A	278	LEU
1	A	286	LEU
1	A	291	LYS
1	A	292	LEU
1	A	295	LYS
1	A	317	TYR
1	A	330	ARG
1	A	333	SER
1	A	340	ASN
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	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	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

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Mol	Chain	Res	Type
1	A	473	LEU
1	A	474	LEU
1	A	485	TRP
1	A	486	LEU
1	A	491	MET
1	A	494	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
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	239	ASN
1	A	268	ASN
1	A	276	GLN
1	A	282	ASN
1	A	307	ASN
1	A	340	ASN
1	A	364	GLN
1	A	393	GLN
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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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.