



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:37 PM UTC

PDB ID : 1GBT / pdb_00001gbt
Title : STRUCTURE OF AN ACYL-ENZYME INTERMEDIATE DURING
CATALYSIS: (GUANIDINOBENZOYL) TRYPSIN
Authors : Singer, P.T.; Sweet, R.M.
Deposited on : 1991-09-17
Resolution : 2.00 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

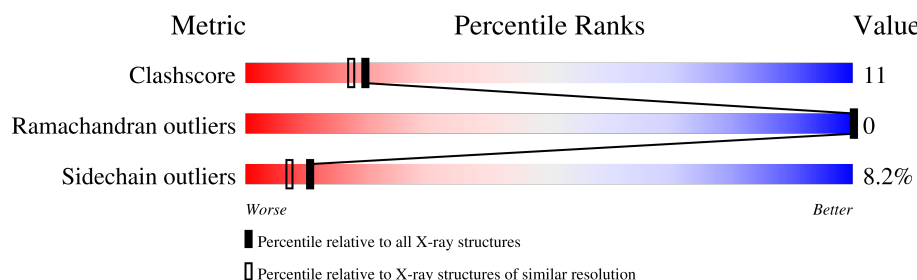
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	223	46% 42% 11% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1761 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.

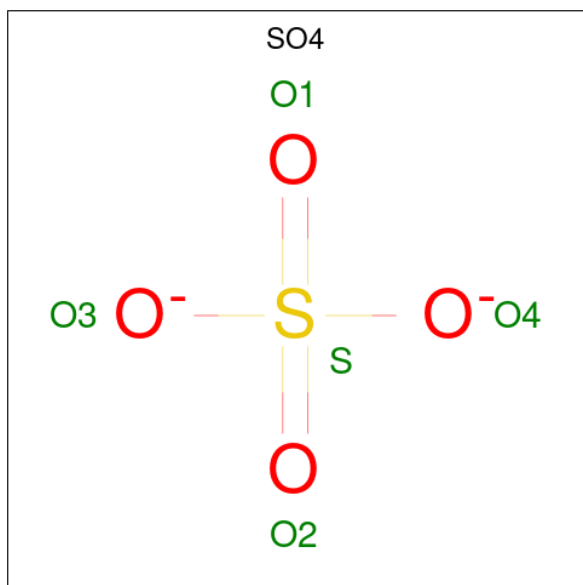
- Molecule 1 is a protein called BETA-TRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

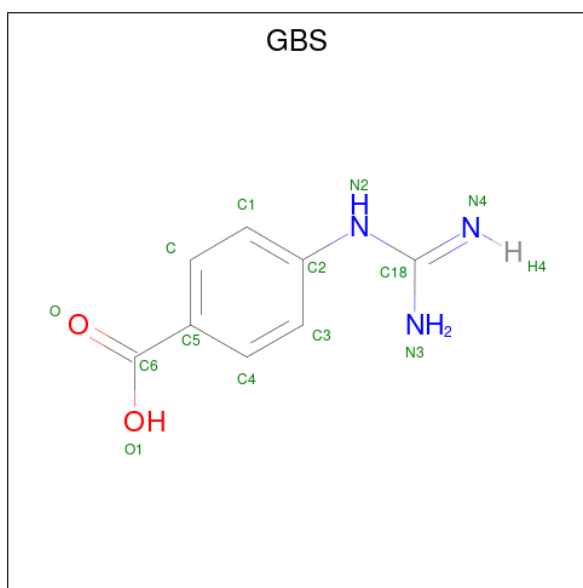
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is 4-carbamimidamidobenzoic acid (CCD ID: GBS) (formula: $C_8H_9N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	8	3	1		

- Molecule 5 is water.

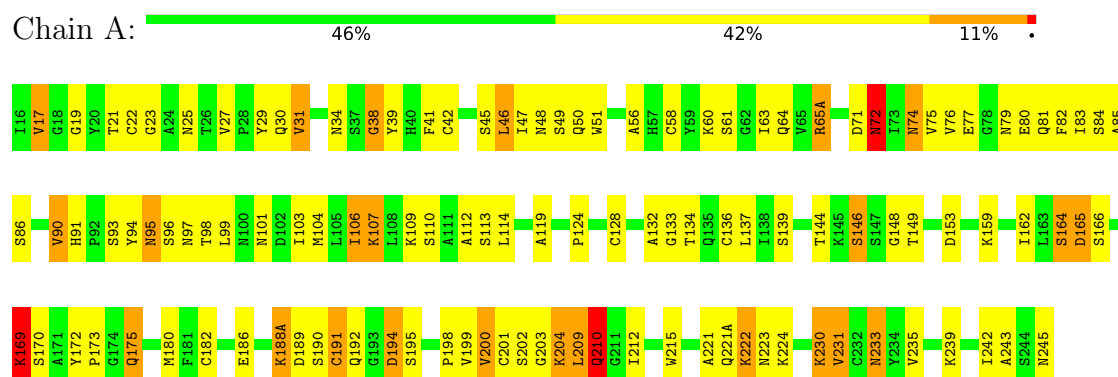
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	117	Total	O	0	0
			117	117		

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: BETA-TRYPSIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.74Å 63.54Å 68.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1761	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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, GBS, CA

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	1.35	4/1660 (0.2%)	2.49	128/2250 (5.7%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	SER	CB-OG	8.68	1.59	1.42
1	A	198	PRO	N-CD	6.14	1.56	1.47
1	A	230	LYS	N-CA	-5.98	1.39	1.46
1	A	21	THR	C-O	-5.56	1.17	1.23

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ASN	CA-CB-CG	-10.10	102.50	112.60
1	A	95	ASN	OD1-CG-ND2	-9.30	113.30	122.60
1	A	189	ASP	CA-CB-CG	8.59	121.19	112.60
1	A	45	SER	CA-C-O	-8.46	110.93	120.66
1	A	21	THR	CA-CB-OG1	-8.36	97.06	109.60
1	A	98	THR	OG1-CB-CG2	-8.32	92.66	109.30
1	A	132	ALA	CA-C-O	-8.29	112.48	121.44
1	A	103	ILE	O-C-N	-8.27	113.87	123.05
1	A	139	SER	O-C-N	-8.19	113.77	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ASN	CA-CB-CG	-8.18	104.42	112.60
1	A	49	SER	N-CA-C	8.14	122.64	112.87
1	A	42	CYS	CA-C-N	-8.08	113.08	122.85
1	A	42	CYS	C-N-CA	-8.08	113.08	122.85
1	A	86	SER	N-CA-C	-8.07	103.57	113.50
1	A	79	ASN	N-CA-CB	8.05	122.16	114.10
1	A	194	ASP	N-CA-C	-7.86	103.83	113.50
1	A	113	SER	CA-CB-OG	-7.82	95.45	111.10
1	A	169	LYS	CA-CB-CG	-7.78	98.54	114.10
1	A	210	GLN	OE1-CD-NE2	-7.77	114.83	122.60
1	A	49	SER	CA-C-O	7.63	128.71	119.10
1	A	72	ASN	CA-C-O	7.42	129.09	120.49
1	A	50	GLN	OE1-CD-NE2	7.39	129.99	122.60
1	A	186	GLU	CB-CA-C	-7.29	96.66	110.67
1	A	137	LEU	CA-C-N	7.29	132.11	122.93
1	A	137	LEU	C-N-CA	7.29	132.11	122.93
1	A	49	SER	CA-CB-OG	-7.24	96.62	111.10
1	A	199	VAL	CA-C-O	-7.22	111.30	120.69
1	A	149	THR	CA-CB-OG1	-7.14	98.89	109.60
1	A	149	THR	N-CA-C	7.12	120.70	108.02
1	A	46	LEU	CA-C-N	-7.10	113.21	122.16
1	A	46	LEU	C-N-CA	-7.10	113.21	122.16
1	A	85	ALA	CA-C-N	-7.06	109.70	121.92
1	A	85	ALA	C-N-CA	-7.06	109.70	121.92
1	A	199	VAL	N-CA-CB	7.00	120.61	112.15
1	A	27	VAL	CA-C-N	6.84	126.52	119.82
1	A	27	VAL	C-N-CA	6.84	126.52	119.82
1	A	19	GLY	CA-C-O	-6.79	114.97	121.90
1	A	169	LYS	N-CA-CB	6.73	120.71	110.28
1	A	164	SER	CA-C-O	6.70	129.65	121.87
1	A	106	ILE	CA-C-O	-6.66	113.42	120.48
1	A	106	ILE	CA-CB-CG1	-6.63	99.13	110.40
1	A	74	ASN	CA-C-O	-6.61	111.62	119.15
1	A	144	THR	CA-CB-OG1	-6.51	99.83	109.60
1	A	200	VAL	CA-C-O	-6.48	113.64	120.57
1	A	25	ASN	CA-CB-CG	-6.48	106.12	112.60
1	A	195	SER	N-CA-CB	6.44	119.56	109.83
1	A	221(A)	GLN	CB-CA-C	-6.43	97.71	109.54
1	A	153	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	107	LYS	CA-CB-CG	-6.37	101.37	114.10
1	A	46	LEU	CA-C-O	6.36	127.56	120.43
1	A	38	GLY	N-CA-C	-6.36	106.30	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	VAL	N-CA-C	6.36	117.03	110.36
1	A	22	CYS	N-CA-C	6.33	118.26	111.36
1	A	242	ILE	CB-CG1-CD1	-6.30	100.57	113.80
1	A	91	HIS	CA-C-O	6.29	125.67	119.75
1	A	82	PHE	O-C-N	-6.22	115.30	123.13
1	A	112	ALA	N-CA-CB	-6.20	100.86	110.29
1	A	99	LEU	CA-C-N	-6.19	112.57	121.42
1	A	99	LEU	C-N-CA	-6.19	112.57	121.42
1	A	119	ALA	CA-C-N	-6.15	112.03	122.67
1	A	119	ALA	C-N-CA	-6.15	112.03	122.67
1	A	233	ASN	CB-CA-C	-6.14	97.72	109.95
1	A	106	ILE	O-C-N	6.05	129.53	123.18
1	A	84	SER	CB-CA-C	-6.03	97.04	110.19
1	A	93	SER	CB-CA-C	-6.00	101.37	111.02
1	A	173	PRO	N-CA-CB	5.98	108.65	103.27
1	A	170	SER	CA-CB-OG	-5.97	99.15	111.10
1	A	58	CYS	CA-C-O	5.97	126.50	119.28
1	A	48	ASN	CB-CG-ND2	-5.89	107.57	116.40
1	A	172	TYR	O-C-N	5.89	126.00	121.23
1	A	25	ASN	CB-CG-ND2	5.88	125.23	116.40
1	A	90	VAL	CA-C-O	-5.85	114.97	121.23
1	A	203	GLY	CA-C-N	-5.83	113.43	122.59
1	A	203	GLY	C-N-CA	-5.83	113.43	122.59
1	A	190	SER	O-C-N	-5.79	115.53	122.65
1	A	22	CYS	N-CA-CB	-5.78	101.61	110.16
1	A	209	LEU	CA-C-O	-5.77	114.75	120.98
1	A	39	TYR	CA-C-O	-5.76	114.66	121.06
1	A	148	GLY	CA-C-O	-5.74	114.55	121.55
1	A	165	ASP	N-CA-CB	-5.72	101.41	110.28
1	A	79	ASN	OD1-CG-ND2	5.72	128.32	122.60
1	A	21	THR	O-C-N	-5.71	115.87	122.95
1	A	189	ASP	N-CA-CB	-5.70	101.47	111.49
1	A	136	CYS	CA-C-O	-5.65	115.18	121.51
1	A	75	VAL	CA-C-N	-5.57	114.01	121.80
1	A	75	VAL	C-N-CA	-5.57	114.01	121.80
1	A	146	SER	CA-CB-OG	-5.56	99.98	111.10
1	A	198	PRO	CA-C-O	-5.48	115.28	122.19
1	A	50	GLN	CB-CA-C	-5.47	100.34	109.75
1	A	83	ILE	O-C-N	-5.45	117.37	123.26
1	A	166	SER	N-CA-CB	5.45	117.91	110.01
1	A	79	ASN	CA-C-O	5.44	123.64	119.18
1	A	81	GLN	CG-CD-NE2	5.42	124.53	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	VAL	CA-C-N	5.40	128.27	120.38
1	A	231	VAL	C-N-CA	5.40	128.27	120.38
1	A	31	VAL	CA-CB-CG2	5.39	119.56	110.40
1	A	61	SER	CA-CB-OG	-5.38	100.35	111.10
1	A	242	ILE	CA-C-O	-5.36	115.37	120.95
1	A	58	CYS	CA-CB-SG	-5.36	102.08	114.40
1	A	46	LEU	O-C-N	-5.35	116.98	123.13
1	A	191	CYS	O-C-N	-5.34	116.58	122.72
1	A	180	MET	CA-C-O	-5.32	115.38	121.40
1	A	204	LYS	N-CA-CB	5.32	120.81	111.55
1	A	204	LYS	CB-CG-CD	-5.32	99.07	111.30
1	A	222	LYS	O-C-N	5.30	128.95	122.96
1	A	23	GLY	N-CA-C	-5.29	100.64	113.18
1	A	215	TRP	O-C-N	-5.29	116.73	122.92
1	A	182	CYS	CA-C-O	-5.24	115.24	121.16
1	A	82	PHE	CA-C-O	5.22	126.05	120.46
1	A	239	LYS	CA-C-O	5.21	126.08	120.55
1	A	221	ALA	CB-CA-C	5.21	120.91	111.06
1	A	164	SER	CA-CB-OG	-5.18	100.73	111.10
1	A	77	GLU	O-C-N	5.17	128.71	122.35
1	A	74	ASN	O-C-N	5.17	129.19	122.42
1	A	91	HIS	CG-CD2-NE2	-5.14	102.06	107.20
1	A	65(A)	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A	72	ASN	O-C-N	-5.13	116.70	123.02
1	A	133	GLY	N-CA-C	-5.13	108.97	115.08
1	A	243	ALA	CA-C-O	5.13	125.70	119.49
1	A	71	ASP	N-CA-C	-5.12	99.90	110.80
1	A	42	CYS	CA-C-O	-5.12	115.96	121.38
1	A	17	VAL	CA-C-O	-5.10	114.68	120.65
1	A	71	ASP	CA-CB-CG	-5.09	107.50	112.60
1	A	50	GLN	CG-CD-OE1	-5.07	110.67	120.80
1	A	128	CYS	N-CA-CB	-5.03	102.93	110.17
1	A	169	LYS	CA-C-N	-5.02	111.24	121.18
1	A	169	LYS	C-N-CA	-5.02	111.24	121.18
1	A	186	GLU	CA-C-O	-5.01	114.20	119.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	ASN	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	1629	0	1587	37	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	12	0	0	0	0
5	A	117	0	0	4	0
All	All	1761	0	1587	37	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 11.

All (37) 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:64:GLN:HE21	1:A:65(A):ARG:HE	1.01	0.99
1:A:64:GLN:HE22	1:A:65(A):ARG:HH21	1.17	0.89
1:A:64:GLN:NE2	1:A:65(A):ARG:HE	1.71	0.89
1:A:72:ASN:HD22	1:A:74:ASN:H	1.31	0.76
1:A:64:GLN:HE21	1:A:65(A):ARG:NE	1.84	0.65
1:A:72:ASN:ND2	1:A:74:ASN:H	1.95	0.64
1:A:51:TRP:CZ2	1:A:107:LYS:HD3	2.33	0.63
1:A:64:GLN:NE2	1:A:65(A):ARG:NE	2.46	0.62
1:A:64:GLN:HE22	1:A:65(A):ARG:NH2	1.95	0.60
1:A:34:ASN:ND2	1:A:38:GLY:H	2.01	0.59
1:A:64:GLN:NE2	1:A:65(A):ARG:HH21	1.95	0.56
1:A:134:THR:HB	1:A:162:ILE:HD12	1.89	0.54
1:A:46:LEU:HD21	1:A:114:LEU:HD21	1.91	0.53
1:A:56:ALA:HB1	1:A:90:VAL:HG13	1.93	0.50
1:A:94:TYR:HA	1:A:101:ASN:HB2	1.94	0.49
1:A:95:ASN:OD1	1:A:97:ASN:N	2.44	0.48
1:A:230:LYS:NZ	5:A:365:HOH:O	2.46	0.48
1:A:41:PHE:CE2	1:A:60:LYS:HE2	2.49	0.48
1:A:191:CYS:O	1:A:194:ASP:HB2	2.15	0.46
1:A:29:TYR:CZ	1:A:200:VAL:HG21	2.51	0.46
1:A:17:VAL:O	1:A:188(A):LYS:HA	2.16	0.46
1:A:41:PHE:HZ	1:A:63:ILE:HG12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HG21	1:A:47:ILE:HD13	1.71	0.44
1:A:109:LYS:HE2	1:A:109:LYS:HB3	1.68	0.44
1:A:210:GLN:NE2	5:A:277:HOH:O	2.49	0.44
1:A:76:VAL:HA	1:A:80:GLU:OE2	2.18	0.44
1:A:192:GLN:H	1:A:192:GLN:HG2	1.48	0.43
1:A:223:ASN:O	1:A:224:LYS:HE2	2.19	0.43
1:A:164:SER:HB2	5:A:349:HOH:O	2.18	0.43
1:A:104:MET:HE3	1:A:106:ILE:HD11	2.01	0.43
1:A:175:GLN:HB3	5:A:289:HOH:O	2.18	0.42
1:A:212:ILE:HG13	1:A:231:VAL:CG2	2.50	0.41
1:A:124:PRO:HD3	1:A:209:LEU:O	2.19	0.41
1:A:72:ASN:HD22	1:A:72:ASN:C	2.29	0.41
1:A:72:ASN:HD22	1:A:74:ASN:N	2.10	0.41
1:A:165:ASP:O	1:A:169:LYS:HD3	2.21	0.41
1:A:56:ALA:HA	1:A:104:MET:HB2	2.03	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	221/223 (99%)	214 (97%)	7 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	184/184 (100%)	169 (92%)	15 (8%)	10 7

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	31	VAL
1	A	72	ASN
1	A	96	SER
1	A	110	SER
1	A	146	SER
1	A	159	LYS
1	A	169	LYS
1	A	175	GLN
1	A	188(A)	LYS
1	A	201	CYS
1	A	202	SER
1	A	204	LYS
1	A	210	GLN
1	A	222	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	34	ASN
1	A	64	GLN
1	A	72	ASN
1	A	74	ASN
1	A	97	ASN
1	A	210	GLN
1	A	240	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic and 2 are modelled with single atom - leaving 1 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	$\# Z > 2$
4	GBS	A	704	1	12,12,13	1.50	2 (16%)	14,15,17	1.14	1 (7%)

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
4	GBS	A	704	1	-	0/6/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	704	GBS	C18-N2	-3.81	1.33	1.38
4	A	704	GBS	O-C6	2.48	1.30	1.21

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	704	GBS	O-C6-C5	-2.27	116.88	124.56

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.

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.