



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:25 AM UTC

PDB ID : 1OD5 / pdb_00001od5
Title : Crystal structure of glycinin A3B4 subunit homohexamer
Authors : Adachi, M.; Kanamori, J.; Masuda, T.; Yagasaki, K.; Kitamura, K.; Mikami, B.; Utsumi, S.
Deposited on : 2003-02-13
Resolution : 2.10 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:

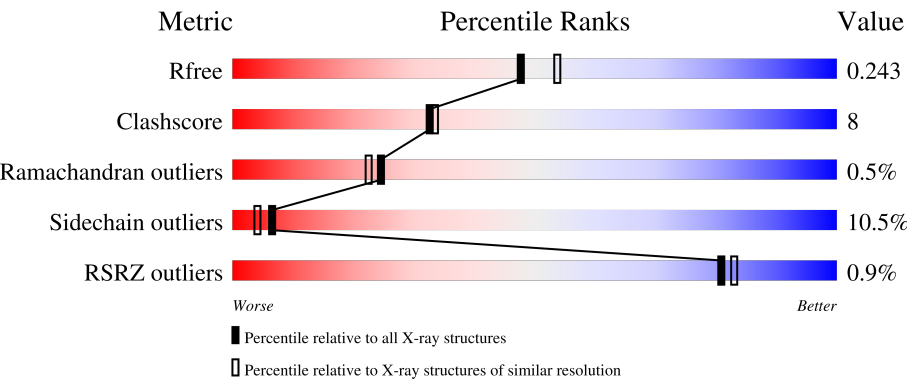
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	492	% 54%18%••22%
1	B	492	% 54%19%••22%

2 Entry composition [i](#)

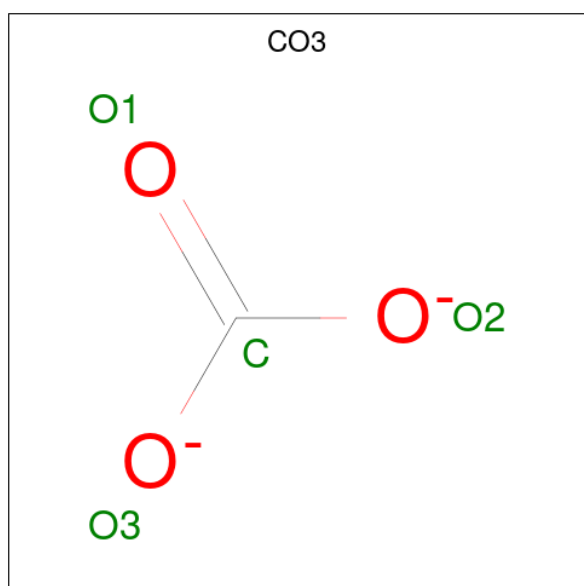
There are 4 unique types of molecules in this entry. The entry contains 6220 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLYCININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2998	1885	534	571	8			
1	B	382	Total	C	N	O	S	0	0	0
			2998	1885	534	571	8			

- Molecule 2 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



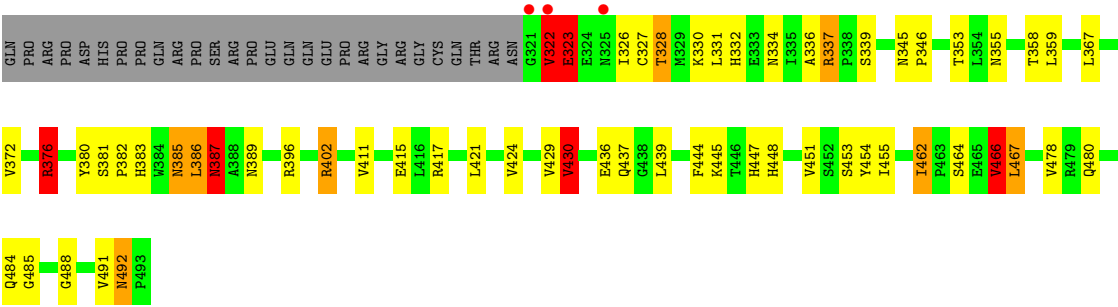
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	102	Total 102	O 102	0	0
4	B	112	Total 112	O 112	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	114.84Å 114.84Å 191.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.10 10.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.3 (10.00-2.10) 87.6 (10.00-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.09Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.201 , 0.254 0.193 , 0.243	Depositor DCC
R_{free} test set	4894 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 69.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6220	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CO3

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	1.07	16/3067 (0.5%)	1.81	64/4168 (1.5%)
1	B	1.08	17/3067 (0.6%)	1.80	79/4168 (1.9%)
All	All	1.07	33/6134 (0.5%)	1.81	143/8336 (1.7%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	458	VAL	CA-CB	7.83	1.64	1.54
1	B	37	HIS	CD2-NE2	-7.71	1.29	1.37
1	B	332	HIS	CD2-NE2	-7.51	1.29	1.37
1	A	58	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	111	HIS	CD2-NE2	-6.81	1.30	1.37
1	A	447	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	332	HIS	CD2-NE2	-6.67	1.30	1.37
1	B	466	VAL	CA-CB	6.59	1.62	1.54
1	B	58	HIS	CD2-NE2	-6.57	1.30	1.37
1	A	116	HIS	CD2-NE2	-6.49	1.30	1.37
1	B	111	HIS	CD2-NE2	-6.39	1.30	1.37
1	A	37	HIS	CD2-NE2	-6.37	1.30	1.37
1	B	21	HIS	CD2-NE2	-6.36	1.30	1.37
1	A	21	HIS	CD2-NE2	-6.34	1.30	1.37
1	A	111	HIS	CG-ND1	-6.28	1.31	1.38
1	A	372	VAL	CA-CB	6.25	1.65	1.55
1	A	144	ILE	CA-CB	6.09	1.61	1.54
1	A	211	HIS	CD2-NE2	-6.06	1.31	1.37
1	B	116	HIS	CD2-NE2	-6.05	1.31	1.37
1	A	383	HIS	CD2-NE2	-6.01	1.31	1.37
1	B	173	HIS	CD2-NE2	-6.00	1.31	1.37
1	B	322	VAL	CA-CB	5.95	1.62	1.54
1	B	447	HIS	CD2-NE2	-5.77	1.31	1.37
1	B	383	HIS	CD2-NE2	-5.76	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	HIS	CD2-NE2	-5.71	1.31	1.37
1	B	129	VAL	CA-CB	5.71	1.59	1.53
1	A	448	HIS	CD2-NE2	-5.62	1.31	1.37
1	B	211	HIS	CD2-NE2	-5.59	1.31	1.37
1	B	144	ILE	CA-CB	5.58	1.60	1.54
1	B	332	HIS	CG-ND1	-5.55	1.32	1.38
1	B	448	HIS	CD2-NE2	-5.34	1.31	1.37
1	B	111	HIS	CG-ND1	-5.21	1.32	1.38
1	A	446	THR	CA-CB	5.14	1.59	1.52

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	GLY	O-C-N	-16.65	109.06	122.88
1	B	220	ASN	CA-CB-CG	11.29	123.89	112.60
1	A	322	VAL	O-C-N	-11.10	108.69	122.57
1	A	430	VAL	CB-CA-C	-10.05	96.82	111.19
1	B	485	GLY	O-C-N	-9.90	114.47	123.88
1	B	236	GLN	N-CA-C	8.92	123.72	113.01
1	B	430	VAL	CB-CA-C	-8.55	99.42	111.38
1	B	336	ALA	N-CA-C	8.38	122.79	112.23
1	A	221	GLU	CA-CB-CG	-8.27	97.56	114.10
1	A	8	GLU	N-CA-C	8.03	122.77	112.34
1	A	336	ALA	N-CA-C	7.97	122.27	112.23
1	B	380	TYR	N-CA-C	-7.77	91.72	107.41
1	A	326	ILE	N-CA-C	7.59	119.28	110.62
1	B	385	ASN	CA-CB-CG	-7.33	105.27	112.60
1	B	46	THR	CA-CB-OG1	-7.30	98.65	109.60
1	A	485	GLY	CA-C-N	7.20	134.66	121.70
1	A	485	GLY	C-N-CA	7.20	134.66	121.70
1	A	220	ASN	CA-CB-CG	7.11	119.71	112.60
1	B	37	HIS	CB-CG-CD2	-7.11	121.96	131.20
1	A	17	LEU	N-CA-C	7.04	121.31	109.76
1	B	429	VAL	N-CA-CB	-7.00	103.12	110.95
1	A	236	GLN	N-CA-C	6.95	120.86	112.38
1	B	118	ASN	CA-CB-CG	6.87	119.47	112.60
1	A	380	TYR	N-CA-C	-6.85	94.29	107.57
1	B	326	ILE	N-CA-C	6.84	118.42	110.62
1	A	324	GLU	N-CA-C	-6.83	104.95	113.28
1	A	170	ASP	N-CA-C	-6.81	99.49	110.32
1	B	323	GLU	CA-C-O	6.75	130.17	120.51
1	B	135	ASN	OD1-CG-ND2	-6.74	115.86	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ASN	CA-CB-CG	6.70	119.30	112.60
1	A	447	HIS	CB-CG-CD2	-6.69	122.50	131.20
1	B	447	HIS	CB-CG-CD2	-6.58	122.64	131.20
1	B	46	THR	CA-CB-CG2	6.56	121.66	110.50
1	B	221	GLU	N-CA-C	6.55	120.37	112.38
1	B	387	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	B	332	HIS	CB-CG-CD2	-6.46	122.80	131.20
1	B	376	ARG	CB-CG-CD	6.43	126.09	111.30
1	B	111	HIS	CA-CB-CG	6.39	120.19	113.80
1	B	144	ILE	CB-CG1-CD1	-6.36	100.45	113.80
1	B	462	ILE	CA-C-N	6.29	126.31	119.90
1	B	462	ILE	C-N-CA	6.29	126.31	119.90
1	B	148	ASP	CA-CB-CG	6.27	118.87	112.60
1	B	466	VAL	N-CA-C	-6.25	103.81	112.50
1	A	135	ASN	OD1-CG-ND2	-6.25	116.35	122.60
1	A	229	SER	CA-C-N	6.22	125.44	118.97
1	A	229	SER	C-N-CA	6.22	125.44	118.97
1	A	386	LEU	N-CA-C	6.20	118.11	111.36
1	A	69	ILE	N-CA-C	6.18	116.77	107.75
1	A	387	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	A	455	ILE	N-CA-C	6.14	118.73	111.05
1	B	69	ILE	N-CA-C	6.10	116.71	108.17
1	B	214	ALA	N-CA-C	-6.09	104.56	111.14
1	A	332	HIS	CB-CG-CD2	-6.09	123.29	131.20
1	B	455	ILE	CA-C-O	-6.05	113.93	120.47
1	B	145	SER	N-CA-C	6.00	119.02	109.24
1	B	462	ILE	CA-C-O	-5.99	115.29	119.19
1	A	350	ARG	NE-CZ-NH2	5.97	124.57	119.20
1	A	326	ILE	N-CA-CB	-5.96	103.02	110.47
1	B	218	ASN	CA-CB-CG	5.96	118.56	112.60
1	B	381	SER	CA-C-N	5.91	127.22	119.84
1	B	381	SER	C-N-CA	5.91	127.22	119.84
1	B	355	ASN	CA-CB-CG	5.90	118.50	112.60
1	B	135	ASN	CB-CG-ND2	5.84	125.16	116.40
1	A	21	HIS	CB-CG-CD2	-5.83	123.61	131.20
1	B	221	GLU	CA-CB-CG	-5.81	102.49	114.10
1	B	332	HIS	CA-CB-CG	5.77	119.57	113.80
1	A	111	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	A	328	THR	N-CA-CB	-5.76	101.70	111.27
1	B	326	ILE	N-CA-CB	-5.76	103.27	110.47
1	B	21	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	B	455	ILE	N-CA-C	5.68	118.19	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	VAL	CB-CA-C	-5.66	103.63	110.99
1	A	383	HIS	CB-CG-CD2	-5.65	123.86	131.20
1	B	33	TRP	N-CA-C	-5.64	101.36	110.32
1	A	337	ARG	CA-C-N	5.61	125.71	119.32
1	A	337	ARG	C-N-CA	5.61	125.71	119.32
1	B	491	VAL	N-CA-C	5.53	115.91	108.17
1	B	381	SER	N-CA-C	5.50	117.98	110.01
1	B	211	HIS	CB-CG-CD2	-5.49	124.07	131.20
1	A	325	ASN	CA-C-N	5.48	128.25	120.53
1	A	325	ASN	C-N-CA	5.48	128.25	120.53
1	B	328	THR	N-CA-CB	-5.47	102.41	111.49
1	B	485	GLY	CA-C-N	5.47	131.54	121.70
1	B	485	GLY	C-N-CA	5.47	131.54	121.70
1	A	322	VAL	CG1-CB-CG2	-5.45	98.81	110.80
1	A	421	LEU	N-CA-CB	-5.45	101.53	110.68
1	B	386	LEU	N-CA-C	5.42	118.11	111.82
1	B	447	HIS	CA-CB-CG	-5.42	108.38	113.80
1	A	54	ARG	CA-CB-CG	5.40	124.91	114.10
1	B	323	GLU	O-C-N	5.40	129.78	122.59
1	A	159	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	B	170	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	383	HIS	CB-CG-CD2	-5.39	124.19	131.20
1	B	462	ILE	N-CA-CB	-5.38	104.37	111.21
1	A	483	TYR	N-CA-C	5.38	119.99	113.38
1	A	46	THR	CA-CB-OG1	-5.37	101.55	109.60
1	B	488	GLY	CA-C-N	5.36	125.05	119.64
1	B	488	GLY	C-N-CA	5.36	125.05	119.64
1	A	385	ASN	CA-CB-CG	-5.36	107.24	112.60
1	B	216	SER	N-CA-C	5.36	117.20	111.36
1	A	448	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	B	337	ARG	CA-C-N	5.33	125.40	119.32
1	B	337	ARG	C-N-CA	5.33	125.40	119.32
1	B	13	ASN	CA-CB-CG	5.32	117.92	112.60
1	A	151	ASN	N-CA-C	5.31	117.93	110.23
1	A	222	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	359	LEU	CA-C-N	5.30	125.11	119.28
1	B	359	LEU	C-N-CA	5.30	125.11	119.28
1	A	376	ARG	CB-CG-CD	5.29	123.46	111.30
1	A	37	HIS	CA-C-N	5.28	125.34	119.32
1	A	37	HIS	C-N-CA	5.28	125.34	119.32
1	B	437	GLN	CA-CB-CG	5.28	124.65	114.10
1	B	119	GLU	N-CA-C	5.27	117.87	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	GLU	N-CA-C	5.25	118.47	111.75
1	B	222	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	59	LEU	N-CA-C	5.23	117.10	109.84
1	B	111	HIS	CB-CG-CD2	-5.22	124.41	131.20
1	A	118	ASN	CA-CB-CG	5.21	117.81	112.60
1	A	447	HIS	CB-CG-ND1	5.20	130.50	122.70
1	A	359	LEU	CA-C-N	5.19	124.99	119.28
1	A	359	LEU	C-N-CA	5.19	124.99	119.28
1	B	158	GLN	N-CA-C	5.19	120.53	113.37
1	B	444	PHE	O-C-N	-5.17	117.16	123.16
1	A	173	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	B	157	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	132	TRP	CE2-CD2-CG	-5.14	101.03	107.20
1	A	322	VAL	CA-C-O	-5.12	114.38	120.78
1	A	416	LEU	N-CA-C	-5.12	100.12	108.76
1	B	402	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	A	337	ARG	N-CA-C	5.10	115.46	109.60
1	A	211	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	A	125	ILE	CA-C-N	5.09	123.33	119.66
1	A	125	ILE	C-N-CA	5.09	123.33	119.66
1	A	216	SER	N-CA-C	5.09	116.83	111.28
1	B	389	ASN	N-CA-C	-5.09	102.95	110.48
1	B	145	SER	N-CA-CB	-5.06	102.18	110.43
1	B	155	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	B	53	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	A	429	VAL	N-CA-CB	-5.04	105.31	110.95
1	B	129	VAL	CA-C-N	5.03	124.94	119.76
1	B	129	VAL	C-N-CA	5.03	124.94	119.76
1	A	465	GLU	CA-C-O	-5.03	114.19	119.97
1	B	132	TRP	CG-CD2-CE3	5.02	138.92	133.90

There are no chirality outliers.

There are no planarity outliers.

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	2998	0	2907	51	0
1	B	2998	0	2907	50	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	102	0	0	1	0
4	B	112	0	0	7	0
All	All	6220	0	5814	93	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 8.

All (93) 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:175:GLU:HG2	1:A:176:THR:HG23	1.64	0.78
1:B:334:ASN:HD21	1:B:337:ARG:H	1.31	0.78
1:B:76:GLY:HA2	1:B:136:THR:HB	1.67	0.77
1:A:322:VAL:HG22	4:B:2105:HOH:O	1.87	0.74
1:A:322:VAL:HB	1:A:323:GLU:HA	1.72	0.72
1:B:170:ASP:H	1:B:236:GLN:HE22	1.39	0.71
1:A:34:ASN:HD22	1:A:36:GLN:H	1.41	0.68
1:A:236:GLN:HE21	1:A:236:GLN:H	1.42	0.68
1:B:236:GLN:H	1:B:236:GLN:HE21	1.42	0.67
1:A:246:VAL:HG22	1:A:251:TRP:HZ3	1.59	0.66
1:B:47:VAL:HG21	1:B:421:LEU:HD21	1.78	0.64
1:A:334:ASN:HD21	1:A:337:ARG:H	1.43	0.64
1:B:34:ASN:HD22	1:B:36:GLN:H	1.45	0.64
1:A:387:ASN:HD21	1:A:451:VAL:H	1.44	0.63
1:A:170:ASP:H	1:A:236:GLN:HE22	1.45	0.62
1:B:323:GLU:HB3	1:B:327:CYS:HB2	1.83	0.60
1:A:480:GLN:O	1:A:484:GLN:HB2	2.01	0.60
1:B:376:ARG:HE	1:B:376:ARG:H	1.50	0.60
1:A:64:PRO:HG3	1:A:156:LEU:HD12	1.83	0.59
1:A:159:ASN:HD22	1:A:176:THR:HB	1.68	0.58
1:B:75:LYS:HG3	1:B:136:THR:HG22	1.85	0.57
1:B:387:ASN:HD21	1:B:451:VAL:H	1.52	0.57
1:A:467:LEU:HD23	1:A:478:VAL:HG13	1.86	0.57
1:B:387:ASN:HD22	1:B:387:ASN:H	1.53	0.57
1:A:358:THR:HG23	1:B:330:LYS:HD2	1.85	0.57
1:B:323:GLU:HA	4:B:2064:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HG12	1:A:324:GLU:HG3	1.86	0.56
1:A:387:ASN:HD22	1:A:387:ASN:H	1.52	0.56
1:A:330:LYS:HD2	1:B:358:THR:HG23	1.88	0.56
1:A:250:LYS:HD2	1:B:339:SER:HB3	1.87	0.56
1:B:417:ARG:HG2	4:B:2099:HOH:O	2.06	0.55
1:A:328:THR:HG23	4:B:2071:HOH:O	2.07	0.55
1:A:246:VAL:HG22	1:A:251:TRP:CZ3	2.39	0.54
1:A:90:GLU:O	1:B:346:PRO:HD2	2.07	0.54
1:A:373:VAL:HG22	1:A:440:GLU:HG2	1.89	0.54
4:A:2097:HOH:O	1:B:322:VAL:HB	2.06	0.54
1:A:401:VAL:HG21	1:A:416:LEU:HD12	1.89	0.54
1:A:321:GLY:HA3	4:B:2107:HOH:O	2.06	0.54
1:B:467:LEU:HD23	1:B:478:VAL:HG13	1.91	0.53
1:A:50:ARG:HH22	1:A:67:GLN:HE22	1.54	0.53
1:A:220:ASN:ND2	1:A:223:THR:H	2.06	0.53
1:B:173:HIS:HD2	4:B:2054:HOH:O	1.93	0.52
1:B:37:HIS:HD2	4:B:2011:HOH:O	1.93	0.51
1:A:34:ASN:ND2	1:A:36:GLN:H	2.08	0.51
1:A:323:GLU:HB2	1:A:327:CYS:HB2	1.92	0.51
1:A:220:ASN:HD22	1:A:223:THR:H	1.59	0.50
1:B:462:ILE:CG2	1:B:466:VAL:HG22	2.42	0.50
1:A:321:GLY:N	1:B:454:TYR:HH	2.09	0.50
1:B:385:ASN:HD21	1:B:445:LYS:NZ	2.11	0.49
1:A:50:ARG:HH12	1:A:67:GLN:NE2	2.11	0.49
1:A:376:ARG:NE	1:A:376:ARG:H	2.11	0.49
1:A:387:ASN:ND2	1:A:451:VAL:H	2.11	0.49
1:A:34:ASN:O	1:A:37:HIS:HD2	1.96	0.48
1:A:322:VAL:CB	1:A:323:GLU:HA	2.40	0.48
1:B:220:ASN:HD22	1:B:223:THR:H	1.60	0.48
1:B:206:SER:HA	1:B:228:ARG:HB2	1.96	0.48
1:B:462:ILE:CG2	1:B:467:LEU:HD13	2.45	0.47
1:B:376:ARG:HE	1:B:376:ARG:N	2.12	0.47
1:B:376:ARG:H	1:B:376:ARG:NE	2.12	0.46
1:B:387:ASN:HD22	1:B:387:ASN:N	2.13	0.46
1:A:351:ILE:HG12	1:A:372:VAL:HB	1.97	0.46
1:B:225:GLU:O	1:B:228:ARG:HG2	2.15	0.46
1:B:20:ASP:OD1	1:B:37:HIS:HE1	1.99	0.45
1:B:334:ASN:ND2	1:B:337:ARG:HB2	2.31	0.45
1:A:454:TYR:CE2	1:B:322:VAL:HG22	2.51	0.45
1:B:250:LYS:O	1:B:251:TRP:HB2	2.16	0.45
1:A:334:ASN:ND2	1:A:337:ARG:HG3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASP:H	1:B:236:GLN:NE2	2.12	0.44
1:A:70:ILE:HG21	1:A:442:VAL:HG11	2.00	0.44
1:A:14:LEU:HD22	1:A:411:VAL:HG23	2.00	0.44
1:B:14:LEU:HD22	1:B:411:VAL:HG23	1.99	0.44
1:A:324:GLU:HB3	1:B:353:THR:HG21	2.00	0.43
1:A:376:ARG:HH21	1:A:438:GLY:HA3	1.83	0.43
1:B:345:ASN:HD21	1:B:492:ASN:ND2	2.17	0.43
1:B:424:VAL:HG11	1:B:430:VAL:HG22	2.00	0.43
1:A:424:VAL:HG11	1:A:430:VAL:HG22	2.01	0.43
1:A:82:PHE:HZ	1:A:331:LEU:HD21	1.83	0.43
1:A:462:ILE:CG2	1:A:466:VAL:HG22	2.48	0.43
1:B:235:LYS:HB3	1:B:236:GLN:HE21	1.84	0.43
1:B:492:ASN:ND2	1:B:492:ASN:H	2.17	0.42
1:B:64:PRO:HG3	1:B:156:LEU:HD12	2.01	0.42
1:B:91:LYS:O	1:B:108:GLN:HA	2.19	0.42
1:B:386:LEU:HD11	1:B:453:SER:HB2	2.01	0.42
1:A:454:TYR:CZ	1:A:457:ASP:HB2	2.55	0.42
1:A:403:VAL:HG22	1:A:430:VAL:HG13	2.01	0.41
1:B:334:ASN:HD21	1:B:337:ARG:HB2	1.85	0.41
1:B:322:VAL:HB	1:B:323:GLU:H	1.71	0.41
1:A:376:ARG:HG3	1:A:436:GLU:O	2.20	0.41
1:B:385:ASN:HD21	1:B:445:LYS:HZ3	1.67	0.41
1:A:344:TYR:CD2	1:B:249:PRO:HG3	2.56	0.40
1:A:170:ASP:HA	1:A:200:GLU:HA	2.04	0.40
1:A:175:GLU:HG2	1:A:176:THR:N	2.37	0.40
1:B:245:SER:HA	1:B:251:TRP:CZ3	2.56	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	374/492 (76%)	352 (94%)	20 (5%)	2 (0%)	24	22
1	B	374/492 (76%)	351 (94%)	21 (6%)	2 (0%)	24	22
All	All	748/984 (76%)	703 (94%)	41 (6%)	4 (0%)	24	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	VAL
1	B	323	GLU
1	B	484	GLN
1	A	158	GLN

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	332/435 (76%)	296 (89%)	36 (11%)	6	4
1	B	332/435 (76%)	298 (90%)	34 (10%)	7	4
All	All	664/870 (76%)	594 (90%)	70 (10%)	6	4

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	14	LEU
1	A	34	ASN
1	A	54	ARG
1	A	57	LEU
1	A	87	GLU
1	A	118	ASN
1	A	144	ILE
1	A	158	GLN
1	A	177	MET
1	A	213	LEU
1	A	218	ASN

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Mol	Chain	Res	Type
1	A	220	ASN
1	A	236	GLN
1	A	322	VAL
1	A	323	GLU
1	A	325	ASN
1	A	328	THR
1	A	331	LEU
1	A	364	GLN
1	A	367	LEU
1	A	372	VAL
1	A	376	ARG
1	A	387	ASN
1	A	390	SER
1	A	417	ARG
1	A	418	ARG
1	A	430	VAL
1	A	458	VAL
1	A	466	VAL
1	A	467	LEU
1	A	468	SER
1	A	480	GLN
1	A	484	GLN
1	A	487	SER
1	A	492	ASN
1	B	14	LEU
1	B	34	ASN
1	B	54	ARG
1	B	57	LEU
1	B	108	GLN
1	B	118	ASN
1	B	136	THR
1	B	144	ILE
1	B	213	LEU
1	B	220	ASN
1	B	231	ASP
1	B	236	GLN
1	B	241	GLU
1	B	251	TRP
1	B	322	VAL
1	B	323	GLU
1	B	328	THR
1	B	331	LEU

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Mol	Chain	Res	Type
1	B	367	LEU
1	B	372	VAL
1	B	376	ARG
1	B	382	PRO
1	B	387	ASN
1	B	396	ARG
1	B	402	ARG
1	B	415	GLU
1	B	430	VAL
1	B	436	GLU
1	B	439	LEU
1	B	464	SER
1	B	466	VAL
1	B	467	LEU
1	B	480	GLN
1	B	492	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	37	HIS
1	A	67	GLN
1	A	108	GLN
1	A	135	ASN
1	A	159	ASN
1	A	220	ASN
1	A	236	GLN
1	A	325	ASN
1	A	334	ASN
1	A	364	GLN
1	A	385	ASN
1	A	387	ASN
1	A	484	GLN
1	A	492	ASN
1	B	7	ASN
1	B	15	ASN
1	B	21	HIS
1	B	34	ASN
1	B	37	HIS
1	B	53	ASN
1	B	73	GLN

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Mol	Chain	Res	Type
1	B	135	ASN
1	B	153	ASN
1	B	158	GLN
1	B	173	HIS
1	B	220	ASN
1	B	236	GLN
1	B	325	ASN
1	B	334	ASN
1	B	385	ASN
1	B	387	ASN
1	B	480	GLN
1	B	492	ASN

5.3.3 RNA [i](#)

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, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	CO3	A	496	-	3,3,3	1.13	0	2,3,3	0.39	0
2	CO3	B	497	-	3,3,3	1.00	0	2,3,3	0.49	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	382/492 (77%)	-0.47	4 (1%) 79 81	8, 20, 41, 60	0
1	B	382/492 (77%)	-0.47	3 (0%) 82 84	7, 19, 41, 58	0
All	All	764/984 (77%)	-0.47	7 (0%) 81 83	7, 20, 41, 60	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	321	GLY	4.2
1	B	322	VAL	3.8
1	B	325	ASN	2.5
1	A	322	VAL	2.5
1	A	321	GLY	2.2
1	A	178	GLN	2.1
1	A	176	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CO3	B	497	4/4	0.86	0.06	25,25,30,33	0
2	CO3	A	496	4/4	0.94	0.05	20,22,25,31	0
3	MG	A	498	1/1	0.97	0.03	6,6,6,6	0
3	MG	B	499	1/1	1.00	0.05	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.