Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:18 PM GMT

PDB ID	:	1OD5
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

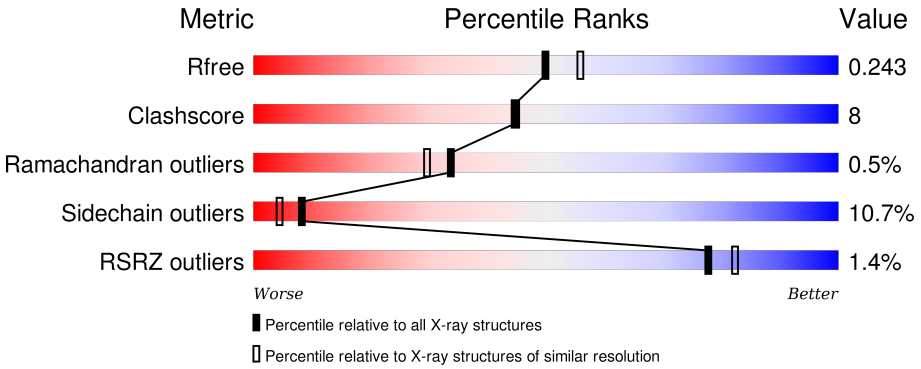
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	% 59% 14% • • 22%
1	B	492	% 59% 15% • • 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CO3	B	497	-	-	-	X

2 Entry composition

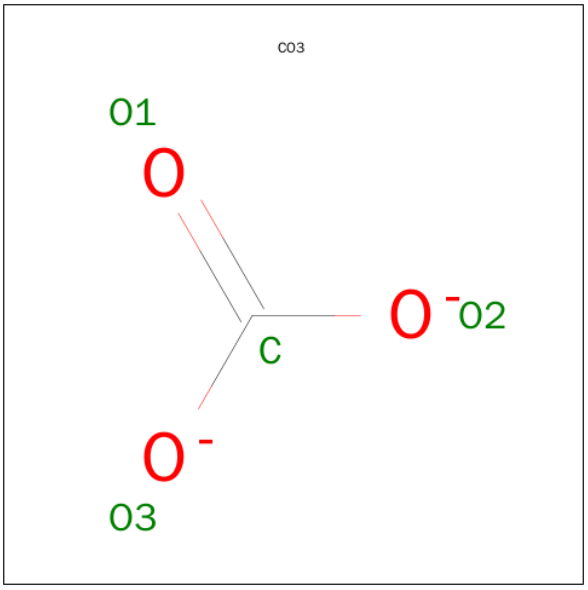
There are 4 unique types of molecules in this entry. The entry contains 6220 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: CO3) (formula: CO_3).



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 (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

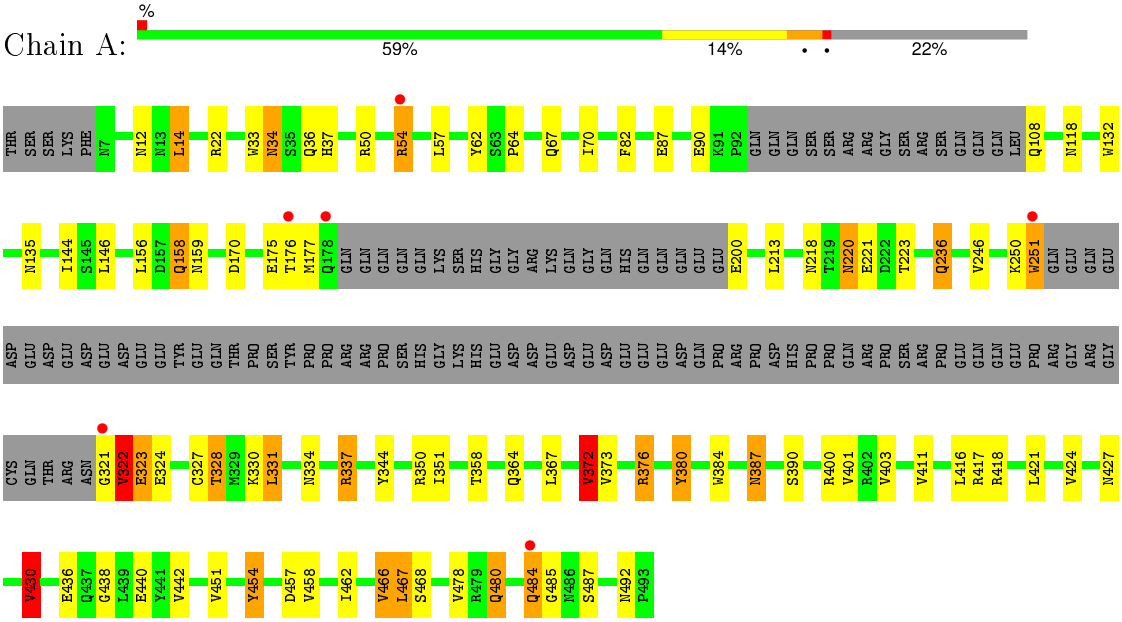
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	102	Total O 102 102	0	0
4	B	112	Total O 112 112	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

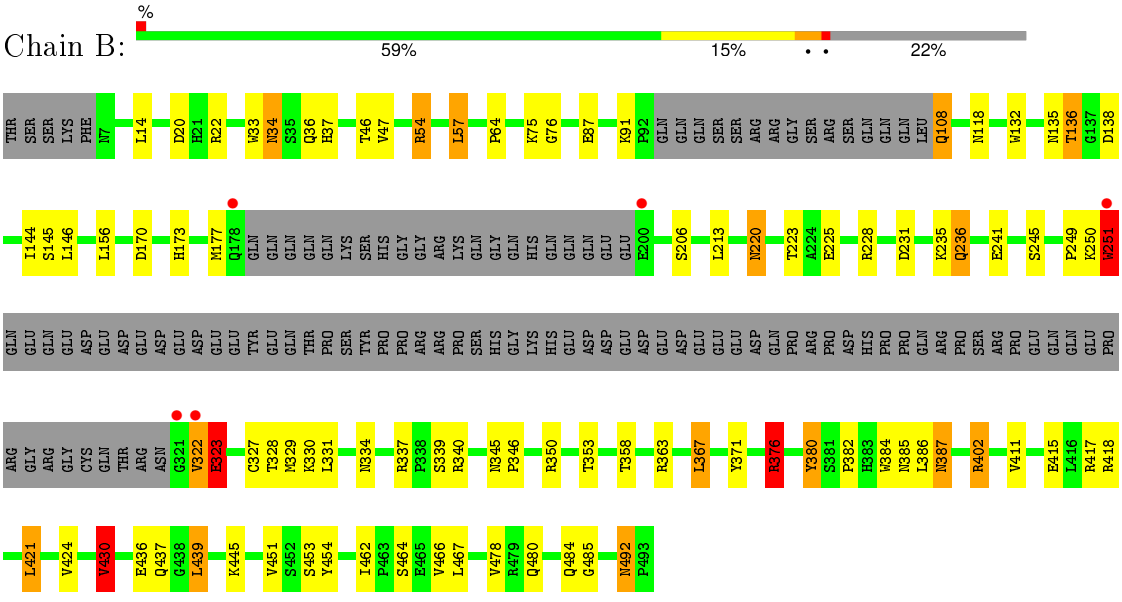
- Molecule 1: GLYCININ

Chain A:



- Molecule 1: GLYCININ

Chain B:



4 Data and refinement statistics (i)

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 9.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.3 (10.00-2.10) 88.4 (9.98-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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%)	DCC
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 71.5	EDS
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 48190 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.82	1/3067 (0.0%)	1.48	32/4168 (0.8%)
1	B	0.83	0/3067	1.46	37/4168 (0.9%)
All	All	0.82	1/6134 (0.0%)	1.47	69/8336 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	VAL	CA-CB	5.19	1.65	1.54

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	251	TRP	CD1-CG-CD2	9.20	113.66	106.30
1	B	132	TRP	CD1-CG-CD2	9.16	113.63	106.30
1	A	322	VAL	CA-C-N	8.89	136.75	117.20
1	A	322	VAL	O-C-N	-8.76	108.69	122.70
1	A	485	GLY	CA-C-N	8.57	136.06	117.20
1	A	350	ARG	NE-CZ-NH2	8.54	124.57	120.30
1	A	485	GLY	O-C-N	-8.53	109.06	122.70
1	A	132	TRP	CD1-CG-CD2	8.32	112.95	106.30
1	B	323	GLU	CA-C-N	-8.07	99.43	117.20
1	B	418	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	B	132	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	A	430	VAL	CB-CA-C	-7.67	96.82	111.40
1	A	33	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	A	322	VAL	CG1-CB-CG2	-7.56	98.81	110.90
1	B	421	LEU	CA-CB-CG	7.54	132.65	115.30
1	A	384	TRP	CD1-CG-CD2	7.50	112.30	106.30
1	A	384	TRP	CE2-CD2-CG	-7.38	101.39	107.30
1	A	33	TRP	CE2-CD2-CG	-7.36	101.41	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	384	TRP	CD1-CG-CD2	7.36	112.19	106.30
1	A	132	TRP	CE2-CD2-CG	-7.32	101.45	107.30
1	A	421	LEU	CA-CB-CG	7.21	131.89	115.30
1	A	221	GLU	CA-CB-CG	-7.20	97.56	113.40
1	B	33	TRP	CD1-CG-CD2	7.18	112.05	106.30
1	B	380	TYR	N-CA-C	-7.14	91.72	111.00
1	A	350	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	A	251	TRP	CD1-CG-CD2	7.02	111.92	106.30
1	B	402	ARG	NE-CZ-NH2	6.99	123.79	120.30
1	B	251	TRP	CE2-CD2-CG	-6.86	101.81	107.30
1	B	33	TRP	CE2-CD2-CG	-6.86	101.81	107.30
1	A	251	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	B	371	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	B	46	THR	CA-CB-CG2	6.61	121.66	112.40
1	B	340	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	B	367	LEU	CA-CB-CG	6.37	129.94	115.30
1	B	430	VAL	CB-CA-C	-6.31	99.42	111.40
1	B	363	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	A	380	TYR	N-CA-C	-6.19	94.29	111.00
1	B	251	TRP	CG-CD1-NE1	-6.12	103.98	110.10
1	B	384	TRP	CE2-CD2-CG	-6.10	102.42	107.30
1	A	337	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	132	TRP	CG-CD1-NE1	-5.93	104.17	110.10
1	A	400	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	54	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	33	TRP	CB-CG-CD1	-5.79	119.47	127.00
1	B	33	TRP	CB-CG-CD1	-5.68	119.61	127.00
1	B	132	TRP	CG-CD2-CE3	5.58	138.92	133.90
1	B	376	ARG	CB-CG-CD	5.58	126.09	111.60
1	B	145	SER	N-CA-CB	-5.55	102.18	110.50
1	B	33	TRP	CG-CD2-CE3	5.54	138.88	133.90
1	B	146	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	14	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	146	LEU	CA-CB-CG	5.39	127.70	115.30
1	B	132	TRP	CB-CG-CD1	-5.34	120.06	127.00
1	B	350	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	B	54	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	B	177	MET	CG-SD-CE	-5.24	91.81	100.20
1	A	454	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	A	54	ARG	CA-CB-CG	5.23	124.91	113.40
1	B	57	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	22	ARG	NE-CZ-NH2	5.21	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	33	TRP	CG-CD2-CE3	5.19	138.57	133.90
1	A	485	GLY	C-N-CA	5.18	134.66	121.70
1	B	329	MET	CA-CB-CG	5.16	122.07	113.30
1	B	485	GLY	O-C-N	-5.14	114.47	122.70
1	B	437	GLN	CA-CB-CG	5.11	124.65	113.40
1	B	22	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	54	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	62	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	B	439	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:236:GLN:H	1:A:236:GLN:HE21	1.42	0.68
1:A:34:ASN:HD22	1:A:36:GLN:H	1.41	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:H	1:B:376:ARG:HE	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:B:387:ASN:H	1:B:387:ASN:HD22	1.53	0.57
1:A:467:LEU:HD23	1:A:478:VAL:HG13	1.86	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
1:A:322:VAL:HG12	1:A:324:GLU:HG3	1.86	0.56
1:A:387:ASN:H	1:A:387:ASN:HD22	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:323:GLU:HB2	1:A:327:CYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASN:ND2	1:A:36:GLN:H	2.08	0.51
1:A:220:ASN:HD22	1:A:223:THR:H	1.59	0.50
1:A:321:GLY:N	1:B:454:TYR:HH	2.09	0.50
1:B:462:ILE:CG2	1:B:466:VAL:HG22	2.42	0.50
1:B:385:ASN:HD21	1:B:445:LYS:NZ	2.11	0.49
1:A:387:ASN:ND2	1:A:451:VAL:H	2.11	0.49
1:A:50:ARG:HH12	1:A:67:GLN:NE2	2.11	0.49
1:A:376:ARG:H	1:A:376:ARG:NE	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:N	1:B:376:ARG:HE	2.12	0.47
1:B:376:ARG:NE	1:B:376:ARG:H	2.12	0.46
1:B:387:ASN:HD22	1:B:387:ASN:N	2.13	0.46
1:B:225:GLU:O	1:B:228:ARG:HG2	2.15	0.46
1:A:351:ILE:HG12	1:A:372:VAL:HB	1.97	0.46
1:B:334:ASN:ND2	1:B:337:ARG:HB2	2.31	0.45
1:B:20:ASP:OD1	1:B:37:HIS:HE1	1.99	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
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:424:VAL:HG11	1:B:430:VAL:HG22	2.00	0.43
1:B:345:ASN:HD21	1:B:492:ASN:ND2	2.17	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:H	1:B:492:ASN:ND2	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:B:334:ASN:HD21	1:B:337:ARG:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:VAL:HG22	1:A:430:VAL:HG13	2.01	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%)	34	30
1	B	374/492 (76%)	351 (94%)	21 (6%)	2 (0%)	34	30
All	All	748/984 (76%)	703 (94%)	41 (6%)	4 (0%)	34	30

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 (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	332/435 (76%)	294 (89%)	38 (11%)	7 4
1	B	332/435 (76%)	299 (90%)	33 (10%)	10 6
All	All	664/870 (76%)	593 (89%)	71 (11%)	8 4

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	34	ASN
1	A	54	ARG
1	A	57	LEU
1	A	87	GLU
1	A	108	GLN
1	A	118	ASN
1	A	135	ASN
1	A	144	ILE
1	A	158	GLN
1	A	177	MET
1	A	213	LEU
1	A	218	ASN
1	A	220	ASN
1	A	236	GLN
1	A	322	VAL
1	A	323	GLU
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	380	TYR
1	A	387	ASN
1	A	390	SER
1	A	417	ARG
1	A	418	ARG
1	A	427	ASN
1	A	430	VAL
1	A	458	VAL
1	A	466	VAL
1	A	467	LEU

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Mol	Chain	Res	Type
1	A	468	SER
1	A	480	GLN
1	A	484	GLN
1	A	487	SER
1	A	492	ASN
1	B	34	ASN
1	B	54	ARG
1	B	57	LEU
1	B	87	GLU
1	B	108	GLN
1	B	118	ASN
1	B	135	ASN
1	B	136	THR
1	B	138	ASP
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
1	B	367	LEU
1	B	376	ARG
1	B	380	TYR
1	B	382	PRO
1	B	387	ASN
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	480	GLN
1	B	492	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	67	GLN
1	A	135	ASN
1	A	159	ASN
1	A	168	ASN
1	A	220	ASN
1	A	236	GLN
1	A	325	ASN
1	A	334	ASN
1	A	385	ASN
1	A	387	ASN
1	A	484	GLN
1	A	492	ASN
1	B	34	ASN
1	B	37	HIS
1	B	53	ASN
1	B	55	ASN
1	B	135	ASN
1	B	168	ASN
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	449	ASN
1	B	480	GLN
1	B	484	GLN
1	B	492	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (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	-	0,3,3	0.00	-	0,3,3	0.00	-
2	CO3	B	497	-	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CO3	A	496	-	-	0/0/0/0	0/0/0/0
2	CO3	B	497	-	-	0/0/0/0	0/0/0/0

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

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, 95^{th} 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%)	-0.35	6 (1%) 74 79	8, 20, 41, 60	0
1	B	382/492 (77%)	-0.37	5 (1%) 79 84	7, 19, 41, 58	0
All	All	764/984 (77%)	-0.36	11 (1%) 78 82	7, 20, 41, 60	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	178	GLN	4.1
1	B	321	GLY	4.1
1	B	322	VAL	4.1
1	A	251	TRP	3.5
1	A	178	GLN	3.5
1	B	251	TRP	3.1
1	A	176	THR	2.9
1	A	484	GLN	2.6
1	A	321	GLY	2.4
1	A	54	ARG	2.3
1	B	200	GLU	2.2

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	CO3	B	497	4/4	0.91	0.09	2.29	25,25,30,33	0
3	MG	B	499	1/1	1.00	0.07	-0.40	10,10,10,10	0
3	MG	A	498	1/1	0.98	0.05	-1.46	6,6,6,6	0
2	CO3	A	496	4/4	0.97	0.07	-1.50	20,22,25,31	0

6.5 Other polymers

There are no such residues in this entry.