Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2023 – 06:18 pm GMT

PDB ID	:	1H0I
Title	:	Complex of a chitinase with the natural product cyclopentapeptide argifin from Gliocladium
Authors	:	Houston, D.R.; Shiomi, K.; Arai, N.; Omura, S.; Peter, M.G.; Turberg, A.; Synstad, B.; Eijsink, V.G.H.; Aalten, D.M.F.
Deposited on	:	2002-06-19
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 (i) 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 (i)) were used in the production of this report:

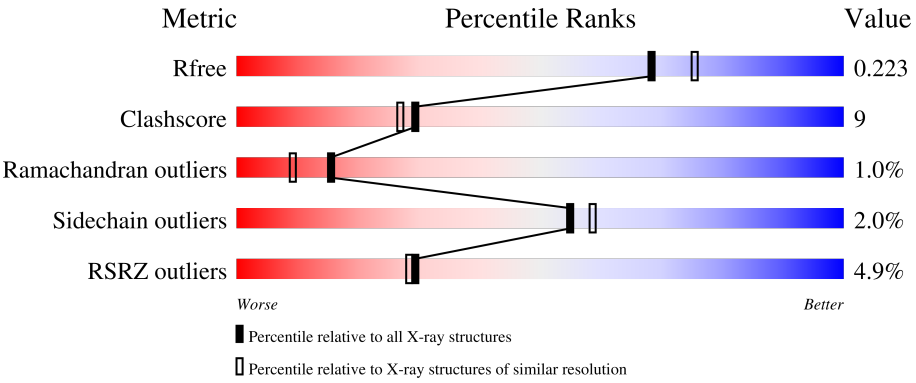
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.00 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))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	499	8%, 83%, 15%
1	B	499	2%, 86%, 13%
2	C	5	40%, 20%, 40%
2	D	5	60%, 40%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9031 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 CHITINASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	3	1
			3912	2501	662	735	14			
1	B	497	Total	C	N	O	S	0	2	0
			3905	2497	657	737	14			

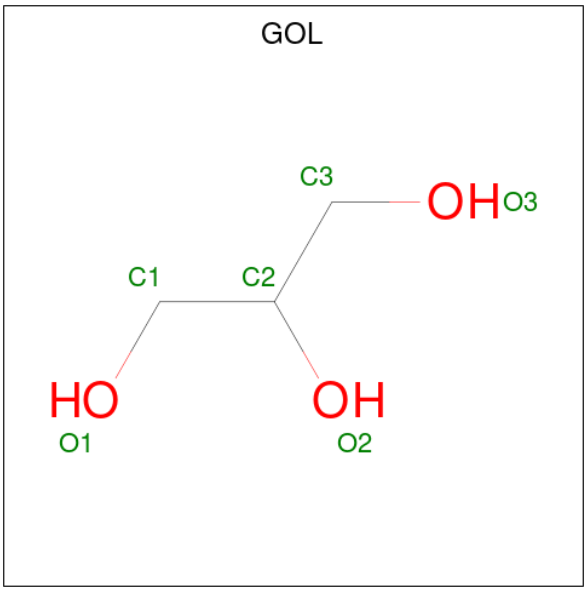
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	SER	ALA	conflict	UNP P11797
A	171	THR	ALA	conflict	UNP P11797
A	223	VAL	ILE	conflict	UNP P11797
A	320	SER	ASN	conflict	UNP P11797
A	321	THR	ALA	conflict	UNP P11797
A	329	GLU	ASP	conflict	UNP P11797
A	498	VAL	LEU	conflict	UNP P11797
B	119	SER	ALA	conflict	UNP P11797
B	171	THR	ALA	conflict	UNP P11797
B	223	VAL	ILE	conflict	UNP P11797
B	320	SER	ASN	conflict	UNP P11797
B	321	THR	ALA	conflict	UNP P11797
B	329	GLU	ASP	conflict	UNP P11797
B	498	VAL	LEU	conflict	UNP P11797

- Molecule 2 is a protein called ARGIFIN.

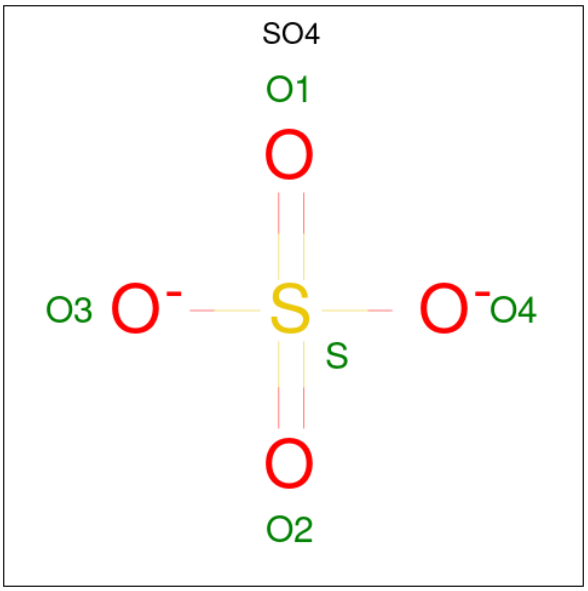
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			48	29	9	10			
2	D	5	Total	C	N	O	0	0	0
			48	29	9	10			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	456	Total O 456 456	0	0
5	B	547	Total O 547 547	0	0

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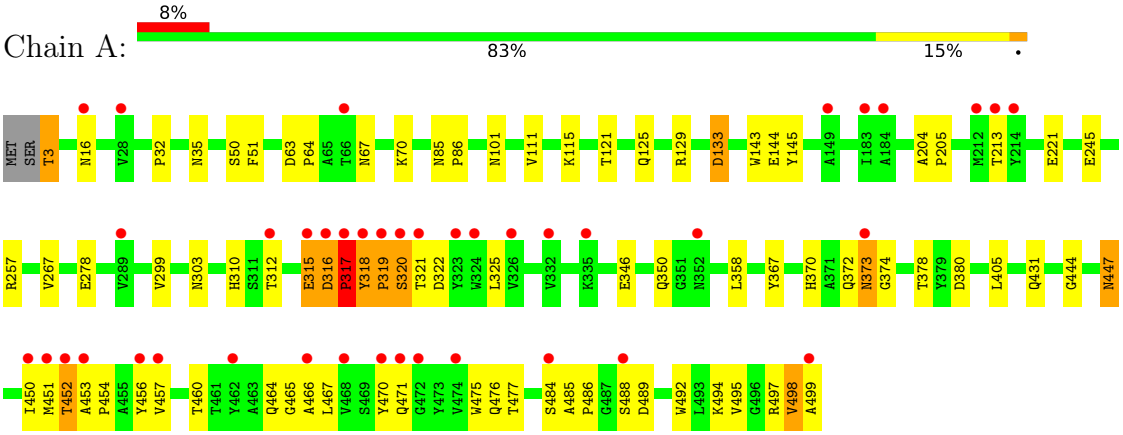
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	4	Total O 4 4	0	0
5	D	19	Total O 19 19	0	0

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 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.

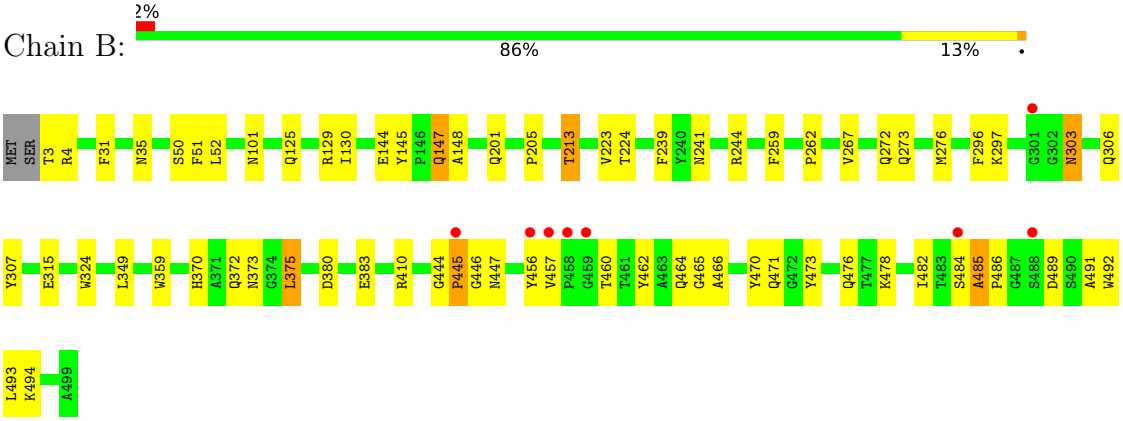
• Molecule 1: CHITINASE B

Chain A:



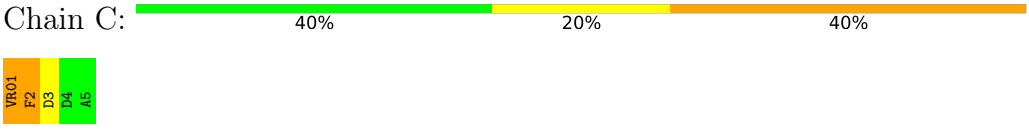
• Molecule 1: CHITINASE B

Chain B:



• Molecule 2: ARGIFIN

Chain C:



• Molecule 2: ARGIFIN

Chain D:


VRO1
F2
A5

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.77Å 103.91Å 186.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.71 – 2.00 34.71 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (34.71-2.00) 96.8 (34.71-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.192 , 0.232 0.185 , 0.223	Depositor DCC
R_{free} test set	722 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9031	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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, 0.333 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: VR0, GOL, IAS, SO4, MEA, DAL

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	0.41	0/4036	0.73	3/5501 (0.1%)
1	B	0.43	0/4024	0.66	0/5486
All	All	0.42	0/8060	0.69	3/10987 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	316	ASP	C-N-CD	-20.95	74.51	120.60
1	A	316	ASP	C-N-CA	12.72	175.41	122.00
1	A	317	PRO	CA-N-CD	-5.99	103.11	111.50

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	3912	0	3741	82	0
1	B	3905	0	3719	63	0
2	C	48	0	36	6	0
2	D	48	0	37	1	0
3	A	12	0	16	0	0
3	B	30	0	40	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	20	0	0	0	0
4	B	25	0	0	0	0
4	D	5	0	0	0	0
5	A	456	0	0	21	0
5	B	547	0	0	9	0
5	C	4	0	0	0	0
5	D	19	0	0	0	0
All	All	9031	0	7589	148	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 9.

All (148) 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:485:ALA:HB1	5:A:2436:HOH:O	1.66	0.94
1:A:444:GLY:H	1:A:447:ASN:HD21	1.07	0.93
1:B:31:PHE:HB3	3:B:1503:GOL:H32	1.57	0.87
1:A:451:MET:O	1:A:452:THR:HG22	1.78	0.83
1:A:444:GLY:H	1:A:447:ASN:ND2	1.76	0.82
1:B:147:GLN:HE21	1:B:148:ALA:H	1.29	0.81
1:A:484:SER:HB3	1:A:489:ASP:HB2	1.65	0.77
1:A:456:TYR:HB3	5:A:2410:HOH:O	1.86	0.74
1:B:3:THR:N	5:B:2005:HOH:O	2.20	0.74
1:A:32:PRO:HD2	1:A:35:ASN:ND2	2.06	0.71
1:B:4:ARG:HB3	3:B:1501:GOL:H11	1.75	0.69
1:A:498:VAL:HG12	1:A:499:ALA:N	2.07	0.69
1:A:319:PRO:O	1:A:320:SER:O	2.11	0.68
1:A:457:VAL:HA	5:A:2411:HOH:O	1.93	0.67
1:A:316:ASP:HB3	2:C:3:IAS:OD1	1.93	0.67
1:A:498:VAL:CG1	1:A:499:ALA:N	2.58	0.67
1:A:32:PRO:HD2	1:A:35:ASN:HD21	1.62	0.65
1:B:147:GLN:HE21	1:B:148:ALA:N	1.96	0.63
1:A:370:HIS:ND1	1:A:372:GLN:O	2.30	0.63
1:A:470:TYR:CZ	1:A:471:GLN:HG3	2.33	0.62
1:A:470:TYR:HD2	1:A:486:PRO:HB2	1.64	0.62
1:B:478:LYS:HE3	1:B:493:LEU:HB2	1.82	0.62
1:B:31:PHE:CB	3:B:1503:GOL:H32	2.28	0.62
1:A:121:THR:O	1:A:125[B]:GLN:HG3	2.00	0.61
1:A:454:PRO:HD3	5:A:2406:HOH:O	2.00	0.61
1:A:447:ASN:H	1:A:447:ASN:HD22	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ALA:HA	5:A:2406:HOH:O	1.99	0.61
1:A:321:THR:HG22	1:A:321:THR:O	2.01	0.60
1:B:273:GLN:HA	1:B:276:MET:HE2	1.83	0.60
1:B:244:ARG:HD3	1:B:259:PHE:O	2.02	0.60
1:B:147:GLN:NE2	1:B:148:ALA:H	1.99	0.59
1:A:470:TYR:CD2	1:A:486:PRO:HB2	2.39	0.58
1:B:373:ASN:HD22	1:B:373:ASN:N	2.01	0.58
3:B:1510:GOL:H31	5:B:2356:HOH:O	2.02	0.58
1:A:310:HIS:HD2	1:A:312:THR:H	1.52	0.58
1:A:372:GLN:HG2	1:A:373:ASN:OD1	2.03	0.57
1:A:470:TYR:CE1	1:A:471:GLN:HG3	2.39	0.57
1:A:317:PRO:O	1:A:318:TYR:C	2.43	0.57
1:A:467:LEU:HA	1:A:475:TRP:O	2.05	0.56
1:A:471:GLN:HA	5:A:2424:HOH:O	2.04	0.56
1:B:370:HIS:HB3	1:B:375:LEU:HB2	1.87	0.56
1:B:244:ARG:HD3	1:B:259:PHE:HB2	1.86	0.56
1:A:460:THR:HG21	5:A:2414:HOH:O	2.04	0.56
1:B:444:GLY:C	1:B:446:GLY:H	2.07	0.56
1:A:310:HIS:CD2	1:A:312:THR:H	2.23	0.56
1:A:464:GLN:HG2	5:A:2419:HOH:O	2.04	0.55
1:A:444:GLY:N	1:A:447:ASN:HD21	1.90	0.55
1:B:125:GLN:HG2	5:B:2031:HOH:O	2.06	0.55
1:A:3:THR:N	5:A:2002:HOH:O	2.40	0.54
1:A:278:GLU:HG2	5:A:2296:HOH:O	2.08	0.54
1:A:466:ALA:O	1:A:476:GLN:HA	2.08	0.54
1:A:451:MET:HE3	5:A:2234:HOH:O	2.08	0.54
1:A:350:GLN:HG3	5:A:2321:HOH:O	2.06	0.54
1:A:492:TRP:HB2	5:A:2437:HOH:O	2.07	0.52
1:B:486:PRO:HG3	1:B:492:TRP:CD2	2.44	0.52
1:A:372:GLN:O	1:A:374:GLY:N	2.42	0.52
1:B:223:VAL:CG1	1:B:307:TYR:HA	2.40	0.51
1:A:372:GLN:C	1:A:374:GLY:H	2.13	0.51
1:A:143:TRP:O	1:A:145:TYR:HA	2.11	0.51
1:B:372:GLN:C	1:B:373:ASN:HD22	2.14	0.51
1:A:316:ASP:OD1	2:C:2:MEA:HC3	2.11	0.50
1:A:129[A]:ARG:NH2	5:A:2173:HOH:O	2.44	0.50
1:A:316:ASP:CB	2:C:3:IAS:HA	2.41	0.50
1:A:451:MET:O	1:A:452:THR:CG2	2.56	0.50
1:B:484:SER:O	1:B:485:ALA:HB3	2.11	0.50
1:A:467:LEU:N	1:A:467:LEU:HD22	2.26	0.49
1:A:475:TRP:CH2	1:A:494:LYS:HE3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:GLN:HA	1:A:477:THR:OG1	2.13	0.49
1:B:129:ARG:NE	5:B:2227:HOH:O	2.39	0.49
1:A:465:GLY:N	1:A:477:THR:OG1	2.45	0.49
1:A:447:ASN:HD22	1:A:447:ASN:N	2.05	0.49
1:A:245:GLU:HG3	1:B:478:LYS:HD3	1.95	0.48
1:A:144:GLU:HA	1:A:145:TYR:CG	2.49	0.48
1:B:457:VAL:HG13	1:B:460:THR:OG1	2.14	0.48
1:B:201:GLN:HG3	5:B:2310:HOH:O	2.13	0.47
1:B:445:PRO:HG3	5:B:2527:HOH:O	2.14	0.47
1:B:4:ARG:HB3	3:B:1501:GOL:C1	2.44	0.47
1:B:370:HIS:CE1	1:B:372:GLN:HB3	2.50	0.47
1:B:52:LEU:CD2	1:B:130:ILE:HG21	2.45	0.47
1:B:239:PHE:O	1:B:262:PRO:HA	2.15	0.47
1:A:497:ARG:O	1:A:498:VAL:O	2.32	0.47
1:B:444:GLY:C	1:B:446:GLY:N	2.68	0.47
1:B:213:THR:HB	1:B:267:VAL:HG22	1.97	0.46
1:A:101:ASN:HA	1:A:144:GLU:O	2.15	0.46
1:B:473:TYR:CD2	1:B:494:LYS:HD3	2.51	0.46
1:B:297:LYS:HD2	1:B:324:TRP:CE2	2.51	0.45
1:A:318:TYR:OH	1:A:322:ASP:O	2.29	0.45
1:A:457:VAL:HB	5:A:2414:HOH:O	2.16	0.45
1:A:450:ILE:HA	1:A:497:ARG:O	2.16	0.45
1:A:372:GLN:HG2	1:A:373:ASN:N	2.32	0.45
1:B:444:GLY:O	1:B:446:GLY:N	2.50	0.45
1:B:444:GLY:N	1:B:447:ASN:OD1	2.42	0.45
1:A:67:ASN:OD1	1:A:70:LYS:HG2	2.17	0.45
1:B:205:PRO:HB3	5:B:2124:HOH:O	2.17	0.45
1:B:224:THR:HG22	1:B:296:PHE:CD2	2.51	0.45
1:B:272:GLN:O	1:B:276:MET:HG3	2.17	0.45
1:A:431:GLN:HB2	5:A:2383:HOH:O	2.16	0.45
1:A:346:GLU:O	1:A:350:GLN:HG2	2.17	0.44
1:B:373:ASN:N	1:B:373:ASN:ND2	2.66	0.44
1:B:486:PRO:HG3	1:B:492:TRP:CE2	2.53	0.44
1:A:316:ASP:HB3	2:C:3:IAS:HA	1.99	0.44
1:A:475:TRP:CD2	1:A:486:PRO:HB3	2.53	0.44
1:B:470:TYR:CD2	1:B:471:GLN:HG3	2.53	0.44
1:B:223:VAL:HG12	1:B:307:TYR:HA	1.98	0.44
1:B:460:THR:HG23	5:B:2516:HOH:O	2.18	0.43
2:D:1:VR0:HA	2:D:2:MEA:HA	1.67	0.43
1:A:460:THR:HG23	5:A:2417:HOH:O	2.17	0.43
1:B:359:TRP:CH2	1:B:383:GLU:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:VR0:O1	2:C:1:VR0:NH2	2.45	0.43
2:C:1:VR0:HA	2:C:2:MEA:HA	1.58	0.43
1:A:221:GLU:O	1:A:310:HIS:HE1	2.01	0.43
1:A:358:LEU:HB2	1:A:367:TYR:CZ	2.53	0.43
1:A:456:TYR:HE1	5:A:2434:HOH:O	2.01	0.43
1:B:457:VAL:HG12	1:B:462:TYR:OH	2.19	0.43
1:B:50:SER:HA	1:B:51:PHE:HA	1.74	0.43
1:B:485:ALA:HA	1:B:486:PRO:HD3	1.86	0.43
1:B:101:ASN:HA	1:B:144:GLU:O	2.18	0.43
1:A:63:ASP:OD2	1:A:64:PRO:HD2	2.18	0.43
1:B:410[B]:ARG:NH2	5:B:2461:HOH:O	2.45	0.43
1:A:257:ARG:HH12	1:A:495:VAL:HA	1.84	0.42
1:A:315:GLU:N	1:A:315:GLU:OE1	2.53	0.42
1:B:478:LYS:CE	1:B:493:LEU:HB2	2.48	0.42
1:B:456:TYR:CE1	1:B:462:TYR:HE2	2.37	0.42
1:B:464:GLN:HE21	1:B:465:GLY:N	2.18	0.42
1:B:35:ASN:OD1	1:B:410[A]:ARG:NH1	2.52	0.41
1:A:3:THR:CA	5:A:2002:HOH:O	2.68	0.41
1:B:244:ARG:CD	1:B:259:PHE:HB2	2.50	0.41
1:B:315:GLU:H	1:B:315:GLU:CD	2.23	0.41
1:A:486:PRO:C	1:A:488:SER:H	2.24	0.41
1:B:457:VAL:HG13	1:B:457:VAL:O	2.20	0.41
1:B:464:GLN:HE21	1:B:465:GLY:CA	2.34	0.41
1:A:16:ASN:ND2	5:A:2022:HOH:O	2.52	0.41
1:A:204:ALA:HB3	1:A:205:PRO:HD3	2.02	0.41
1:A:50:SER:HA	1:A:51:PHE:HA	1.71	0.41
1:A:456:TYR:CE2	1:A:485:ALA:HB2	2.55	0.41
1:B:303:ASN:HD22	1:B:303:ASN:HA	1.57	0.41
1:B:144:GLU:HA	1:B:145:TYR:CG	2.56	0.40
1:B:241:ASN:O	1:B:244:ARG:HG3	2.21	0.40
1:A:85:ASN:HA	1:A:86:PRO:HD2	1.96	0.40
1:A:111:VAL:O	1:A:115:LYS:HG3	2.21	0.40
1:A:358:LEU:HD22	1:A:358:LEU:N	2.36	0.40
1:B:303:ASN:O	1:B:306:GLN:HB2	2.22	0.40
1:A:213:THR:HB	1:A:267:VAL:HG22	2.03	0.40
1:A:454:PRO:HB2	5:A:2408:HOH:O	2.22	0.40
1:B:466:ALA:O	1:B:476:GLN:HA	2.22	0.40
1:B:482:ILE:HD12	1:B:491:ALA:HB1	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	498/499 (100%)	472 (95%)	19 (4%)	7 (1%)	11 5
1	B	497/499 (100%)	486 (98%)	8 (2%)	3 (1%)	25 19
All	All	995/998 (100%)	958 (96%)	27 (3%)	10 (1%)	15 9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	PRO
1	A	320	SER
1	A	498	VAL
1	A	373	ASN
1	A	452	THR
1	A	318	TYR
1	B	485	ALA
1	B	489	ASP
1	B	445	PRO
1	A	319	PRO

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	405/406 (100%)	395 (98%)	10 (2%)	47 49
1	B	402/406 (99%)	396 (98%)	6 (2%)	65 69
All	All	807/812 (99%)	791 (98%)	16 (2%)	55 58

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	133	ASP
1	A	299	VAL
1	A	303	ASN
1	A	315	GLU
1	A	325	LEU
1	A	378	THR
1	A	380	ASP
1	A	405	LEU
1	A	447	ASN
1	B	147	GLN
1	B	213	THR
1	B	303	ASN
1	B	349	LEU
1	B	375	LEU
1	B	380	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	17	GLN
1	A	35	ASN
1	A	303	ASN
1	A	310	HIS
1	A	347	GLN
1	A	447	ASN
1	B	17	GLN
1	B	76	ASN
1	B	147	GLN
1	B	273	GLN
1	B	303	ASN
1	B	373	ASN
1	B	394	GLN
1	B	464	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are 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	IAS	D	3	2	6,7,8	0.97	0	6,8,10	1.13	0
2	IAS	C	3	2	6,7,8	1.12	0	6,8,10	1.03	0
2	IAS	D	4	2	6,7,8	0.97	0	6,8,10	1.16	0
2	MEA	D	2	2	11,12,13	1.10	0	13,14,16	1.11	1 (7%)
2	VR0	C	1	2	11,14,15	1.03	1 (9%)	10,16,18	1.09	1 (10%)
2	MEA	C	2	2	11,12,13	1.07	0	13,14,16	1.12	1 (7%)
2	VR0	D	1	2	11,14,15	1.15	2 (18%)	10,16,18	0.79	0
2	IAS	C	4	2	6,7,8	1.06	0	6,8,10	1.09	0

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	IAS	D	3	2	-	0/7/7/8	-
2	IAS	C	3	2	-	0/7/7/8	-
2	IAS	D	4	2	-	1/7/7/8	-
2	MEA	D	2	2	-	0/5/8/10	0/1/1/1
2	VR0	C	1	2	-	1/14/15/17	-
2	MEA	C	2	2	-	0/5/8/10	0/1/1/1
2	VR0	D	1	2	-	1/14/15/17	-
2	IAS	C	4	2	-	1/7/7/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	VR0	C6-NH1	-2.46	1.34	1.39
2	D	1	VR0	C6-NH1	-2.24	1.34	1.39
2	D	1	VR0	CZ-NH2	2.05	1.35	1.29

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	MEA	C1-N-CA	3.04	123.11	113.64
2	D	2	MEA	C1-N-CA	2.85	122.52	113.64
2	C	1	VR0	CZ-NH1-C6	-2.02	121.96	125.42

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	VR0	CG-CD-NE-CZ
2	C	4	IAS	CA-CB-CG-OD1
2	D	4	IAS	CA-CB-CG-OD1
2	D	1	VR0	CG-CD-NE-CZ

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	IAS	3	0
2	D	2	MEA	1	0
2	C	1	VR0	2	0
2	C	2	MEA	2	0
2	D	1	VR0	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

17 ligands are 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	$\#\|Z\|>2$
3	GOL	B	1504	-	5,5,5	0.49	0	5,5,5	0.14	0
4	SO4	B	1505	-	4,4,4	0.16	0	6,6,6	0.07	0
3	GOL	B	1502	-	5,5,5	0.40	0	5,5,5	0.15	0
4	SO4	A	1505	-	4,4,4	0.28	0	6,6,6	0.09	0
4	SO4	A	1507	-	4,4,4	0.26	0	6,6,6	0.13	0
4	SO4	A	1504	-	4,4,4	0.28	0	6,6,6	0.11	0
3	GOL	B	1503	-	5,5,5	0.40	0	5,5,5	0.23	0
3	GOL	A	1502	-	5,5,5	0.45	0	5,5,5	0.15	0
3	GOL	B	1501	-	5,5,5	0.31	0	5,5,5	0.19	0
4	SO4	A	1506	-	4,4,4	0.25	0	6,6,6	0.05	0
4	SO4	B	1506	-	4,4,4	0.30	0	6,6,6	0.07	0
4	SO4	B	1507	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	B	1508	-	4,4,4	0.28	0	6,6,6	0.09	0
4	SO4	D	1007	-	4,4,4	0.28	0	6,6,6	0.10	0
3	GOL	A	1503	-	5,5,5	0.42	0	5,5,5	0.11	0
4	SO4	B	1509	-	4,4,4	0.28	0	6,6,6	0.05	0
3	GOL	B	1510	-	5,5,5	0.24	0	5,5,5	0.32	0

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
3	GOL	B	1504	-	-	0/4/4/4	-
3	GOL	B	1502	-	-	0/4/4/4	-
3	GOL	B	1503	-	-	0/4/4/4	-
3	GOL	A	1502	-	-	0/4/4/4	-
3	GOL	B	1501	-	-	0/4/4/4	-
3	GOL	A	1503	-	-	0/4/4/4	-
3	GOL	B	1510	-	-	0/4/4/4	-

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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1503	GOL	2	0
3	B	1501	GOL	2	0
3	B	1510	GOL	1	0

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	497/499 (99%)	0.27	41 (8%) 11 11	14, 29, 59, 86	0
1	B	497/499 (99%)	-0.20	8 (1%) 72 70	15, 24, 47, 60	0
2	C	0/5	-	-	-	-
2	D	0/5	-	-	-	-
All	All	994/1008 (98%)	0.03	49 (4%) 29 28	14, 27, 56, 86	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	320	SER	7.0
1	A	499	ALA	6.8
1	A	456	TYR	5.9
1	A	470	TYR	5.7
1	B	457	VAL	5.5
1	A	319	PRO	5.4
1	A	323	TYR	5.3
1	A	318	TYR	5.2
1	A	317	PRO	5.1
1	A	321	THR	4.8
1	A	457	VAL	4.6
1	A	452	THR	4.4
1	A	472	GLY	3.9
1	A	450	ILE	3.9
1	A	471	GLN	3.9
1	A	466	ALA	3.7
1	A	453	ALA	3.5
1	B	445	PRO	3.3
1	B	456	TYR	3.3
1	A	316	ASP	3.1
1	A	484	SER	3.0
1	A	332	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	352	ASN	2.8
1	A	468	VAL	2.6
1	A	315	GLU	2.6
1	B	484	SER	2.6
1	A	373	ASN	2.6
1	A	474	VAL	2.6
1	A	451	MET	2.5
1	B	301	GLY	2.5
1	A	289	VAL	2.4
1	A	66	THR	2.4
1	A	16	ASN	2.4
1	A	213	THR	2.4
1	A	488	SER	2.4
1	A	149	ALA	2.3
1	A	184	ALA	2.2
1	A	212	MET	2.2
1	B	459	GLY	2.2
1	B	488	SER	2.2
1	A	335	LYS	2.1
1	A	462	TYR	2.1
1	A	214	TYR	2.1
1	A	183	ILE	2.0
1	B	458	PRO	2.0
1	A	326	VAL	2.0
1	A	312	THR	2.0
1	A	324	TRP	2.0
1	A	28	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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	B-factors(Å^2)	Q<0.9
2	IAS	C	4	8/9	0.82	0.27	46,48,51,52	0
2	DAL	C	5	5/6	0.91	0.12	43,43,45,46	0
2	MEA	C	2	12/13	0.92	0.16	34,38,42,43	0
2	IAS	C	3	8/9	0.92	0.11	43,44,46,46	0
2	IAS	D	4	8/9	0.94	0.13	27,29,35,38	0
2	VR0	C	1	15/16	0.94	0.22	21,33,40,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	VR0	D	1	15/16	0.95	0.15	19,23,25,28	0
2	IAS	D	3	8/9	0.96	0.10	26,28,29,30	0
2	DAL	D	5	5/6	0.96	0.08	25,26,27,28	0
2	MEA	D	2	12/13	0.97	0.10	22,26,27,27	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
3	GOL	B	1504	6/6	0.84	0.17	42,46,46,47	0
3	GOL	A	1503	6/6	0.86	0.19	45,47,48,49	0
3	GOL	B	1503	6/6	0.87	0.25	40,47,48,49	0
3	GOL	B	1510	6/6	0.89	0.26	43,46,46,48	0
4	SO4	B	1508	5/5	0.90	0.20	67,69,69,69	0
4	SO4	A	1505	5/5	0.91	0.18	68,68,70,70	0
3	GOL	B	1501	6/6	0.91	0.17	30,41,42,45	0
3	GOL	A	1502	6/6	0.92	0.14	32,37,38,41	0
4	SO4	A	1504	5/5	0.92	0.21	73,73,73,74	0
4	SO4	D	1007	5/5	0.92	0.15	57,60,60,60	0
4	SO4	B	1509	5/5	0.93	0.13	86,86,86,86	0
4	SO4	A	1506	5/5	0.93	0.14	85,85,86,86	0
4	SO4	A	1507	5/5	0.94	0.14	69,69,69,70	0
3	GOL	B	1502	6/6	0.96	0.11	36,38,38,38	0
4	SO4	B	1506	5/5	0.97	0.15	59,60,60,60	0
4	SO4	B	1505	5/5	0.97	0.24	24,25,26,26	0
4	SO4	B	1507	5/5	0.98	0.15	58,60,60,61	0

6.5 Other polymers (i)

There are no such residues in this entry.