



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:21 AM UTC

PDB ID : 1H0I / pdb_00001h0i
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 ⓘ 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

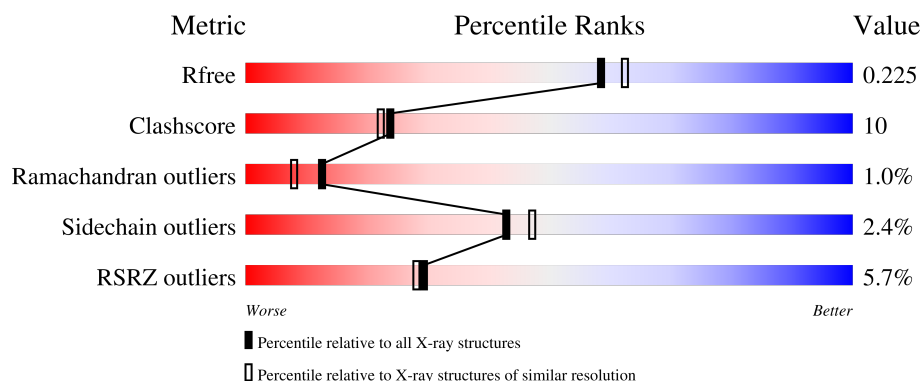
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	9% 80% 16% ..
1	B	499	3% 82% 15% .
2	C	5	40% 20% 40%
2	D	5	60% 40%

2 Entry composition

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 (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is water.

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

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



4 Data and refinement statistics

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) 97.0 (34.71-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.192 , 0.232 0.186 , 0.225	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 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

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: MEA, IAS, SO4, DAL, VR0, GOL

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	0.47	1/4036 (0.0%)	1.29	21/5501 (0.4%)
1	B	0.49	0/4024	0.97	23/5486 (0.4%)
All	All	0.48	1/8060 (0.0%)	1.14	44/10987 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	498	VAL	C-N	-5.66	1.25	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ASP	CA-C-N	44.45	175.41	119.84
1	A	316	ASP	C-N-CA	44.45	175.41	119.84
1	A	316	ASP	C-N-CD	-12.31	74.51	125.00
1	B	115	LYS	N-CA-C	9.40	121.13	111.07
1	B	100	SER	N-CA-C	8.52	123.90	113.17
1	A	100	SER	N-CA-C	8.05	123.29	113.38
1	B	309	SER	N-CA-C	-7.84	100.77	110.41
1	A	52	LEU	N-CA-C	-6.99	100.12	110.46
1	A	207	ASP	N-CA-C	-6.97	103.77	112.90
1	B	218	GLY	CA-C-N	6.96	126.66	119.56
1	B	218	GLY	C-N-CA	6.96	126.66	119.56
1	A	184	ALA	N-CA-C	-6.75	98.22	108.96
1	B	423	ASN	N-CA-C	6.74	123.49	114.12
1	B	63	ASP	N-CA-C	-6.70	99.83	109.48
1	A	45	THR	N-CA-C	-6.68	105.66	113.88
1	A	309	SER	N-CA-C	-6.61	101.81	110.53
1	A	321	THR	N-CA-C	-6.48	103.70	112.26
1	B	151	VAL	N-CA-C	6.46	117.21	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	318	TYR	CA-C-N	6.44	126.06	119.56
1	B	318	TYR	C-N-CA	6.44	126.06	119.56
1	A	317	PRO	CA-N-CD	-6.35	103.11	112.00
1	A	485	ALA	N-CA-C	6.30	118.98	110.29
1	B	207	ASP	N-CA-C	-6.26	103.75	112.45
1	B	45	THR	N-CA-C	-6.24	106.20	113.88
1	A	68	ASP	N-CA-C	5.90	118.47	111.33
1	A	115	LYS	N-CA-C	5.90	117.38	111.07
1	A	480	GLY	N-CA-C	5.79	122.04	112.89
1	B	177	LEU	CA-C-N	5.79	125.80	119.90
1	B	177	LEU	C-N-CA	5.79	125.80	119.90
1	A	189	ALA	N-CA-C	5.63	118.96	111.75
1	A	423	ASN	N-CA-C	5.56	121.85	114.12
1	A	487	GLY	N-CA-C	-5.50	108.15	115.40
1	B	189	ALA	N-CA-C	5.35	118.60	111.75
1	A	413	ASP	N-CA-C	5.34	117.10	111.28
1	B	184	ALA	N-CA-C	-5.34	100.54	109.24
1	B	484	SER	N-CA-C	5.26	119.70	113.28
1	A	457	VAL	N-CA-C	5.21	113.17	107.60
1	B	330	GLU	N-CA-C	-5.20	105.50	111.07
1	B	52	LEU	N-CA-C	-5.17	102.80	110.46
1	B	324	TRP	N-CA-C	5.15	119.55	113.16
1	B	96	GLY	N-CA-C	-5.14	106.20	112.68
1	B	295	ALA	N-CA-C	5.06	118.00	109.95
1	A	151	VAL	N-CA-C	5.06	115.28	110.42
1	B	450	ILE	N-CA-C	-5.03	103.01	109.30

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	89	0
1	B	3905	0	3719	65	0
2	C	48	0	36	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	48	0	37	1	0
3	A	12	0	16	0	0
3	B	30	0	40	5	0
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	22	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	157	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 10.

All (157) 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:A:317:PRO:O	1:A:318:TYR:C	2.43	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:444:GLY:C	1:B:446:GLY:H	2.07	0.61
1:A:447:ASN:H	1:A:447:ASN:HD22	1.48	0.61
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: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:372:GLN:C	1:A:374:GLY:H	2.13	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:A:310:HIS:CD2	1:A:312:THR:H	2.23	0.56
1:B:372:GLN:C	1:B:373:ASN:HD22	2.14	0.55
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:143:TRP:O	1:A:145:TYR:HA	2.11	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:B:444:GLY:C	1:B:446:GLY:N	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:315:GLU:H	1:B:315:GLU:CD	2.23	0.46
1:B:473:TYR:CD2	1:B:494:LYS:HD3	2.51	0.46
1:A:486:PRO:C	1:A:488:SER:H	2.24	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:390:LYS:NZ	1:A:432:LEU:O	2.47	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:A:316:ASP:CG	2:C:2:MEA:HC3	2.44	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:A:370:HIS:HD1	1:A:372:GLN:C	2.25	0.42
1:B:478:LYS:CE	1:B:493:LEU:HB2	2.48	0.42
1:A:464:GLN:C	5:A:2419:HOH:O	2.61	0.42
1:A:372:GLN:C	1:A:374:GLY:N	2.77	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:470:TYR:CE2	1:B:471:GLN:CD	2.98	0.42
1:B:35:ASN:OD1	1:B:410[A]:ARG:NH1	2.52	0.41
1:A:457:VAL:H	1:A:462:TYR:HH	1.67	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:A:318:TYR:C	1:A:319:PRO:O	2.62	0.41
1:B:273:GLN:HA	1:B:276:MET:HE2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:PHE:CE1	1:B:276:MET:HE1	2.56	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%)	9	4
1	B	497/499 (100%)	486 (98%)	8 (2%)	3 (1%)	21	17
All	All	995/998 (100%)	958 (96%)	27 (3%)	10 (1%)	12	8

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

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Mol	Chain	Res	Type
1	A	319	PRO

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	405/406 (100%)	393 (97%)	12 (3%)	36	38
1	B	402/406 (99%)	395 (98%)	7 (2%)	53	60
All	All	807/812 (99%)	788 (98%)	19 (2%)	43	47

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	133	ASP
1	A	213	THR
1	A	299	VAL
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	A	452	THR
1	A	467	LEU
1	B	129	ARG
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 (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	272	GLN
1	A	303	ASN
1	A	310	HIS
1	A	344	GLN
1	A	347	GLN
1	A	394	GLN
1	A	396	GLN
1	A	447	ASN
1	B	76	ASN
1	B	84	HIS
1	B	147	GLN
1	B	272	GLN
1	B	273	GLN
1	B	303	ASN
1	B	372	GLN
1	B	373	ASN
1	B	394	GLN
1	B	395	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 ⓘ

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	4	2	6,7,8	0.98	0	3,8,10	1.26	0
2	VR0	D	1	2	11,14,15	0.92	1 (9%)	10,16,18	0.75	0
2	VR0	C	1	2	11,14,15	0.88	1 (9%)	10,16,18	1.03	0
2	IAS	D	3	2	6,7,8	0.97	0	3,8,10	1.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IAS	C	3	2	6,7,8	1.12	0	3,8,10	0.96	0
2	IAS	C	4	2	6,7,8	1.05	0	3,8,10	1.15	0
2	MEA	D	2	2	11,12,13	1.22	0	13,14,16	1.13	1 (7%)
2	MEA	C	2	2	11,12,13	1.18	0	13,14,16	1.15	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
2	IAS	D	4	2	-	1/7/7/8	-
2	VR0	D	1	2	-	1/14/15/17	-
2	VR0	C	1	2	-	1/14/15/17	-
2	IAS	D	3	2	-	2/7/7/8	-
2	IAS	C	3	2	-	2/7/7/8	-
2	IAS	C	4	2	-	1/7/7/8	-
2	MEA	D	2	2	-	0/5/8/10	0/1/1/1
2	MEA	C	2	2	-	0/5/8/10	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	VR0	C6-NH1	-2.30	1.34	1.39
2	D	1	VR0	C6-NH1	-2.08	1.34	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	MEA	C1-N-CA	3.15	123.11	113.70
2	D	2	MEA	C1-N-CA	2.95	122.52	113.70

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	C	3	IAS	OXT-C-CA-N
2	C	3	IAS	O-C-CA-N
2	D	3	IAS	O-C-CA-N
2	D	3	IAS	OXT-C-CA-N

There are no ring outliers.

5 monomers are involved in 8 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
4	SO4	B	1509	-	4,4,4	0.39	0	6,6,6	0.06	0
3	GOL	A	1502	-	5,5,5	0.47	0	5,5,5	0.16	0
4	SO4	A	1504	-	4,4,4	0.38	0	6,6,6	0.11	0
4	SO4	A	1505	-	4,4,4	0.39	0	6,6,6	0.10	0
4	SO4	D	1007	-	4,4,4	0.39	0	6,6,6	0.09	0
4	SO4	B	1507	-	4,4,4	0.36	0	6,6,6	0.08	0
4	SO4	B	1508	-	4,4,4	0.39	0	6,6,6	0.11	0
3	GOL	B	1510	-	5,5,5	0.25	0	5,5,5	0.35	0
3	GOL	B	1503	-	5,5,5	0.42	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	1505	-	4,4,4	0.28	0	6,6,6	0.09	0
3	GOL	B	1502	-	5,5,5	0.42	0	5,5,5	0.17	0
4	SO4	A	1506	-	4,4,4	0.36	0	6,6,6	0.06	0
4	SO4	A	1507	-	4,4,4	0.37	0	6,6,6	0.15	0
4	SO4	B	1506	-	4,4,4	0.40	0	6,6,6	0.07	0
3	GOL	A	1503	-	5,5,5	0.44	0	5,5,5	0.12	0
3	GOL	B	1504	-	5,5,5	0.51	0	5,5,5	0.14	0
3	GOL	B	1501	-	5,5,5	0.32	0	5,5,5	0.21	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	A	1502	-	-	0/4/4/4	-
3	GOL	B	1510	-	-	0/4/4/4	-
3	GOL	B	1503	-	-	0/4/4/4	-
3	GOL	B	1502	-	-	0/4/4/4	-
3	GOL	A	1503	-	-	0/4/4/4	-
3	GOL	B	1504	-	-	0/4/4/4	-
3	GOL	B	1501	-	-	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	1510	GOL	1	0
3	B	1503	GOL	2	0
3	B	1501	GOL	2	0

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

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	497/499 (99%)	0.28	44 (8%) 15 14	14, 29, 59, 86	3 (0%)
1	B	497/499 (99%)	-0.19	13 (2%) 57 56	15, 24, 47, 60	2 (0%)
2	C	0/5	-	-	-	-
2	D	0/5	-	-	-	-
All	All	994/1008 (98%)	0.05	57 (5%) 29 28	14, 27, 56, 86	5 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	499	ALA	6.8
1	A	456	TYR	5.3
1	A	484	SER	5.1
1	A	452	THR	4.9
1	A	498	VAL	4.9
1	A	457	VAL	4.8
1	A	470	TYR	4.7
1	A	319	PRO	4.3
1	B	457	VAL	4.2
1	A	318	TYR	4.1
1	A	317	PRO	4.0
1	A	474	VAL	3.8
1	A	466	ALA	3.7
1	A	320	SER	3.4
1	B	445	PRO	3.4
1	A	321	THR	3.3
1	B	456	TYR	3.3
1	A	314	GLY	3.2
1	A	483	THR	3.1
1	A	468	VAL	3.1
1	A	463	ALA	3.0
1	A	488	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	352	ASN	2.8
1	A	471	GLN	2.8
1	A	316	ASP	2.8
1	A	462	TYR	2.8
1	A	454	PRO	2.8
1	A	485	ALA	2.7
1	A	455	ALA	2.6
1	A	469	SER	2.6
1	A	351	GLY	2.6
1	A	487	GLY	2.6
1	A	465	GLY	2.6
1	B	485	ALA	2.6
1	A	461	THR	2.5
1	A	313	PRO	2.5
1	B	455	ALA	2.5
1	B	484	SER	2.5
1	B	470	TYR	2.4
1	A	467	LEU	2.4
1	B	458	PRO	2.4
1	A	486	PRO	2.3
1	A	323	TYR	2.3
1	B	488	SER	2.2
1	A	353	TYR	2.2
1	B	489	ASP	2.2
1	A	312	THR	2.2
1	A	460	THR	2.2
1	B	461	THR	2.2
1	A	326	VAL	2.1
1	A	371	ALA	2.1
1	A	16	ASN	2.1
1	B	481	TYR	2.1
1	A	458	PRO	2.1
1	A	481	TYR	2.1
1	A	453	ALA	2.0
1	B	459	GLY	2.0

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

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	IAS	C	4	8/9	0.75	0.14	46,48,51,52	0
2	IAS	C	3	8/9	0.88	0.09	43,44,46,46	0
2	MEA	C	2	12/13	0.90	0.11	34,38,42,43	0
2	IAS	D	4	8/9	0.91	0.09	27,29,35,38	0
2	VR0	C	1	15/16	0.92	0.09	21,33,40,41	0
2	IAS	D	3	8/9	0.93	0.07	26,28,29,30	0
2	DAL	C	5	5/6	0.93	0.08	43,43,45,46	0
2	VR0	D	1	15/16	0.94	0.07	19,23,25,28	0
2	DAL	D	5	5/6	0.95	0.06	25,26,27,28	0
2	MEA	D	2	12/13	0.96	0.06	22,26,27,27	0

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
4	SO4	A	1504	5/5	0.78	0.13	73,73,73,74	0
4	SO4	B	1508	5/5	0.80	0.15	67,69,69,69	0
3	GOL	B	1504	6/6	0.82	0.14	42,46,46,47	0
4	SO4	A	1506	5/5	0.83	0.14	85,85,86,86	0
3	GOL	B	1503	6/6	0.83	0.16	40,47,48,49	0
4	SO4	B	1509	5/5	0.83	0.11	86,86,86,86	0
4	SO4	A	1507	5/5	0.84	0.11	69,69,69,70	0
3	GOL	A	1503	6/6	0.84	0.13	45,47,48,49	0
3	GOL	B	1510	6/6	0.84	0.13	43,46,46,48	0
4	SO4	A	1505	5/5	0.87	0.10	68,68,70,70	0
4	SO4	D	1007	5/5	0.87	0.11	57,60,60,60	0
3	GOL	B	1501	6/6	0.90	0.12	30,41,42,45	0
4	SO4	B	1507	5/5	0.91	0.10	58,60,60,61	0
4	SO4	B	1506	5/5	0.92	0.09	59,60,60,60	0
3	GOL	A	1502	6/6	0.93	0.09	32,37,38,41	0
4	SO4	B	1505	5/5	0.95	0.21	24,25,26,26	0
3	GOL	B	1502	6/6	0.96	0.07	36,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.