



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:19 AM UTC

PDB ID : 9FBO / pdb_00009fbo
Title : Deletion mutant of chitinase MmChi60
Authors : Malecki, P.H.; Rypniewski, W.
Deposited on : 2024-05-14
Resolution : 2.69 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

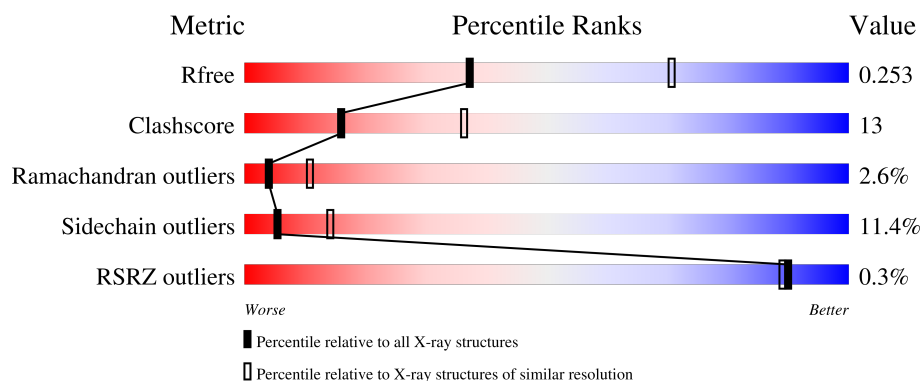
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	446	 64% 31% 5%
1	B	446	 64% 29% 6% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7047 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.

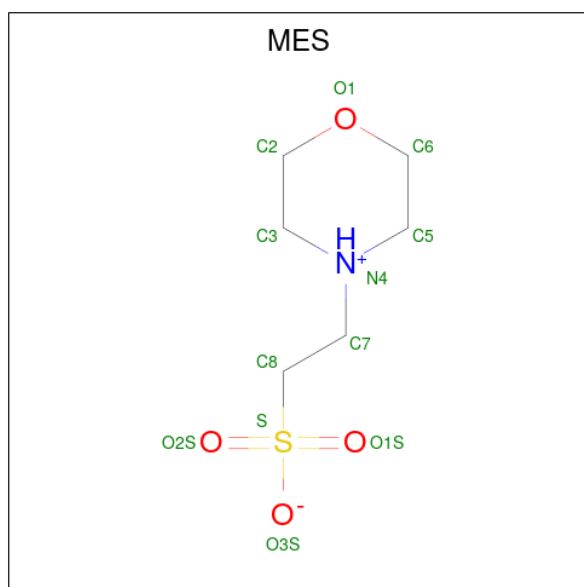
- Molecule 1 is a protein called Chitinase 60.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3513	2226	578	700	9			
1	B	446	Total	C	N	O	S	0	0	0
			3513	2226	578	700	9			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

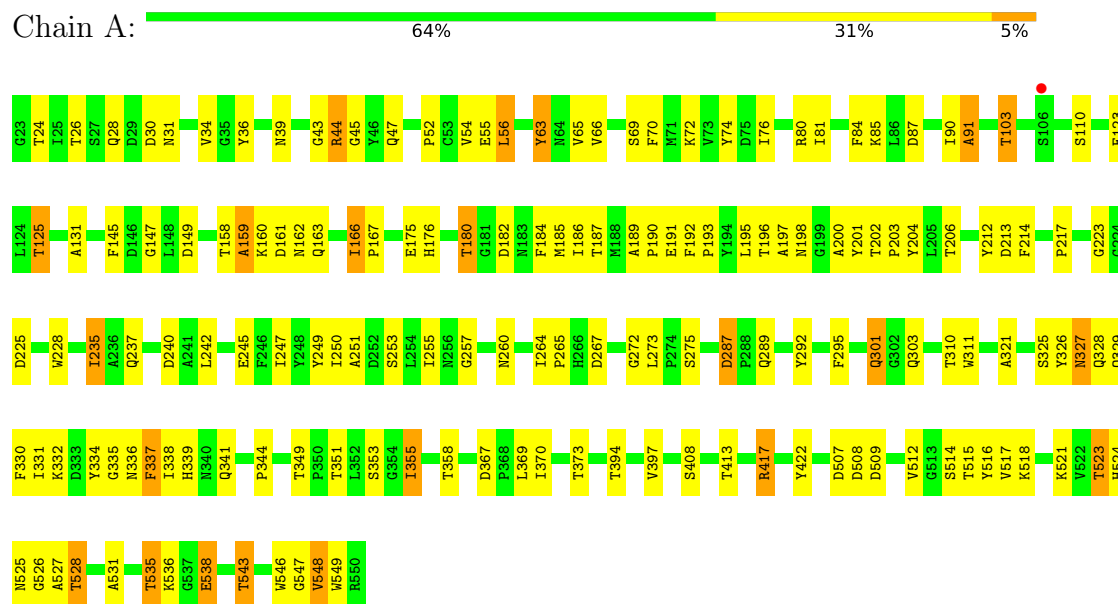
- Molecule 4 is water.

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

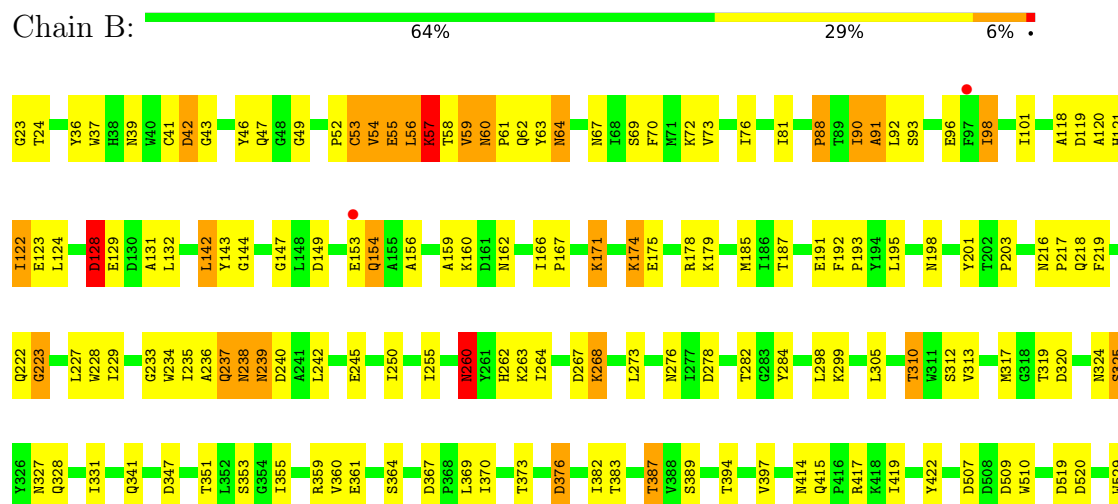
3 Residue-property plots

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 60



• Molecule 1: Chitinase 60



T530	A531	T535	E539	T543	V548	W549	R550
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4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	225.74Å 225.74Å 65.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.17 – 2.69 65.17 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.3 (65.17-2.69) 99.3 (65.17-2.69)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.194 , 0.252 0.202 , 0.253	Depositor DCC
R_{free} test set	1000 reflections (2.92%)	wwPDB-VP
Wilson B-factor (Å ²)	94.0	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7047	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: MES, NA

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	0.63	0/3602	1.27	16/4919 (0.3%)
1	B	0.54	0/3602	1.12	6/4919 (0.1%)
All	All	0.59	0/7204	1.20	22/9838 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	PHE	N-CA-CB	8.03	121.71	110.07
1	A	344	PRO	N-CA-C	-7.22	100.58	111.41
1	A	103	THR	CA-CB-OG1	-6.60	99.70	109.60
1	B	519	ASP	CB-CA-C	6.51	116.27	109.83
1	A	30	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	507	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	413	THR	CA-CB-OG1	-6.03	100.56	109.60
1	A	337	PHE	CA-CB-CG	-5.95	107.85	113.80
1	A	422	TYR	CA-CB-CG	5.89	124.50	113.90
1	A	247	ILE	O-C-N	5.65	127.35	121.87
1	B	128	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	52	PRO	N-CA-C	-5.46	102.69	111.38
1	B	376	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	63	TYR	N-CA-CB	-5.37	102.45	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	THR	CA-CB-OG1	-5.27	101.69	109.60
1	A	247	ILE	CA-C-O	-5.17	115.57	120.95
1	A	31	ASN	N-CA-C	-5.14	103.75	110.53
1	B	88	PRO	N-CA-CB	-5.10	97.89	103.25
1	B	387	THR	CA-CB-OG1	-5.09	101.96	109.60
1	A	249	TYR	CB-CA-C	5.09	119.26	110.86
1	B	520	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	515	THR	CA-CB-OG1	-5.03	102.06	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	417	ARG	Sidechain

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	3513	0	3313	95	0
1	B	3513	0	3313	91	0
2	A	1	0	0	0	0
3	A	12	0	13	5	0
4	A	4	0	0	1	0
4	B	4	0	0	0	0
All	All	7047	0	6639	180	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 13.

All (180) 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:B:535:THR:HB	1:B:548:VAL:HG21	1.64	0.79
1:A:531:ALA:HB2	1:A:549:TRP:CZ3	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:TRP:HB3	1:B:198:ASN:HA	1.67	0.77
1:A:44:ARG:O	3:A:602:MES:H81	1.88	0.74
1:A:44:ARG:NH1	1:A:45:GLY:O	2.20	0.73
1:A:326:TYR:O	1:A:327:ASN:C	2.33	0.72
1:B:56:LEU:O	1:B:58:THR:N	2.24	0.70
1:A:39:ASN:ND2	1:A:84:PHE:HE1	1.90	0.70
1:A:158:THR:HA	1:A:163:GLN:HE21	1.56	0.70
1:A:260:ASN:OD1	1:B:260:ASN:HB3	1.94	0.68
1:B:60:ASN:O	1:B:62:GLN:N	2.28	0.67
1:B:298:LEU:HD13	1:B:305:LEU:HD21	1.76	0.67
1:B:118:ALA:HA	1:B:153:GLU:HG2	1.77	0.66
1:A:166:ILE:HB	1:A:167:PRO:HD3	1.78	0.64
1:A:326:TYR:O	1:A:328:GLN:N	2.30	0.64
1:A:287:ASP:OD2	1:A:289:GLN:HB2	1.97	0.64
1:A:39:ASN:ND2	1:A:84:PHE:CE1	2.67	0.63
1:B:62:GLN:HB2	1:B:331:ILE:HD11	1.81	0.63
1:B:123:GLU:HG3	1:B:159:ALA:HB1	1.80	0.63
1:A:202:THR:N	1:A:203:PRO:HD2	2.15	0.62
1:A:311:TRP:HZ2	3:A:602:MES:H22	1.64	0.62
1:B:23:GLY:HA3	1:B:144:GLY:HA3	1.81	0.62
1:A:161:ASP:HA	4:A:702:HOH:O	1.99	0.61
1:B:59:VAL:O	1:B:60:ASN:C	2.43	0.61
1:B:417:ARG:HD3	1:B:419:ILE:HD11	1.83	0.61
1:A:535:THR:HB	1:A:548:VAL:HG21	1.82	0.60
1:B:236:ALA:HB1	1:B:238:ASN:OD1	2.03	0.59
1:A:235:ILE:HD13	1:A:245:GLU:HB3	1.84	0.58
1:B:219:PHE:C	1:B:237:GLN:HE22	2.10	0.58
1:B:222:GLN:O	1:B:223:GLY:C	2.47	0.58
1:A:514:SER:HB2	1:A:516:TYR:CE1	2.39	0.57
1:A:543:THR:HB	1:A:547:GLY:HA3	1.86	0.57
1:B:123:GLU:CG	1:B:159:ALA:HB1	2.35	0.57
1:B:81:ILE:HD13	1:B:124:LEU:HD22	1.87	0.56
1:A:538:GLU:O	1:A:549:TRP:NE1	2.39	0.56
1:B:229:ILE:O	1:B:233:GLY:N	2.36	0.56
1:A:310:THR:HB	1:A:330:PHE:CZ	2.41	0.56
1:A:180:THR:OG1	1:A:182:ASP:OD1	2.23	0.55
1:A:260:ASN:CG	1:B:260:ASN:HB3	2.31	0.55
1:A:508:ASP:O	1:A:509:ASP:C	2.47	0.55
1:A:34:VAL:HG22	1:A:65:VAL:HB	1.87	0.55
1:B:41:CYS:O	1:B:42:ASP:C	2.49	0.54
1:A:158:THR:HA	1:A:163:GLN:NE2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:THR:HA	1:A:527:ALA:O	2.07	0.54
1:A:192:PHE:CG	1:A:193:PRO:HD3	2.43	0.54
1:B:238:ASN:OD1	1:B:238:ASN:N	2.38	0.54
1:B:81:ILE:HD11	1:B:128:ASP:HB3	1.90	0.53
1:B:238:ASN:HB3	1:B:282:THR:HG21	1.89	0.53
1:A:275:SER:HA	1:A:330:PHE:CD2	2.44	0.53
1:B:192:PHE:N	1:B:193:PRO:CD	2.72	0.53
1:A:90:ILE:O	1:A:91:ALA:HB3	2.09	0.53
1:B:98:ILE:HG23	1:B:143:TYR:O	2.09	0.53
1:B:276:ASN:OD1	1:B:278:ASP:N	2.43	0.52
1:B:147:GLY:HA3	1:B:185:MET:O	2.09	0.52
1:A:202:THR:N	1:A:203:PRO:CD	2.72	0.52
1:A:237:GLN:O	1:A:237:GLN:HG2	2.09	0.52
1:A:147:GLY:HA2	1:A:184:PHE:CE1	2.44	0.52
1:A:521:LYS:HD2	1:A:528:THR:HG22	1.90	0.52
1:A:192:PHE:O	1:A:195:LEU:HB2	2.10	0.52
1:A:255:ILE:HD12	1:A:303:GLN:HB3	1.92	0.52
1:A:200:ALA:O	1:A:203:PRO:HD2	2.10	0.52
1:A:336:ASN:O	1:A:337:PHE:C	2.52	0.51
1:B:73:VAL:HG11	1:B:121:HIS:O	2.10	0.51
1:B:191:GLU:C	1:B:193:PRO:HD2	2.34	0.51
1:A:186:ILE:HB	1:A:212:TYR:HA	1.92	0.51
1:B:217:PRO:HB2	1:B:219:PHE:CE1	2.45	0.51
1:B:219:PHE:HE2	1:B:250:ILE:HG12	1.76	0.51
1:B:90:ILE:C	1:B:92:LEU:N	2.68	0.51
1:A:301:GLN:HA	1:B:422:TYR:CZ	2.46	0.50
1:B:174:LYS:O	1:B:178:ARG:HG3	2.11	0.50
1:A:228:TRP:CZ3	1:B:203:PRO:HG3	2.47	0.50
1:A:198:ASN:HB3	1:B:227:LEU:HB2	1.95	0.49
1:A:538:GLU:O	1:A:549:TRP:CD1	2.66	0.49
1:B:242:LEU:HD22	1:B:245:GLU:OE1	2.12	0.49
1:B:299:LYS:NZ	1:B:341:GLN:OE1	2.36	0.49
1:A:196:THR:O	1:A:197:ALA:C	2.55	0.49
1:A:289:GLN:HA	1:A:292:TYR:CD2	2.48	0.49
1:B:93:SER:O	1:B:96:GLU:N	2.46	0.48
1:A:81:ILE:HD11	1:A:131:ALA:HB3	1.95	0.48
1:A:329:GLN:O	1:A:330:PHE:C	2.56	0.48
1:B:228:TRP:HE3	1:B:234:TRP:HB2	1.79	0.48
1:A:63:TYR:CD2	1:A:331:ILE:HD13	2.48	0.48
1:A:514:SER:HB2	1:A:516:TYR:CZ	2.48	0.48
1:B:55:GLU:O	1:B:56:LEU:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:O	1:A:310:THR:HA	2.13	0.48
1:B:90:ILE:O	1:B:92:LEU:N	2.47	0.48
1:A:189:ALA:N	1:A:190:PRO:CD	2.77	0.47
1:A:201:TYR:HA	1:A:204:TYR:HD2	1.79	0.47
1:A:251:ALA:O	1:A:255:ILE:HG23	2.12	0.47
1:B:56:LEU:O	1:B:57:LYS:C	2.55	0.47
1:B:359:ARG:HB3	1:B:422:TYR:CD2	2.49	0.47
1:A:255:ILE:HD12	1:A:303:GLN:CB	2.44	0.47
1:A:329:GLN:O	1:A:332:LYS:N	2.46	0.47
1:A:367:ASP:HB3	1:A:370:ILE:HD12	1.97	0.47
1:B:531:ALA:HB2	1:B:549:TRP:CZ3	2.50	0.47
1:B:91:ALA:O	1:B:92:LEU:C	2.58	0.47
1:B:367:ASP:HB3	1:B:370:ILE:CD1	2.45	0.47
1:A:123:GLU:HB3	1:A:160:LYS:HE2	1.95	0.47
1:B:535:THR:CB	1:B:548:VAL:HG21	2.40	0.47
1:B:324:ASN:O	1:B:325:SER:C	2.57	0.46
1:B:166:ILE:HB	1:B:167:PRO:HD3	1.97	0.46
1:A:311:TRP:CZ2	3:A:602:MES:H22	2.47	0.46
1:B:312:SER:O	1:B:313:VAL:C	2.58	0.46
1:B:60:ASN:C	1:B:62:GLN:H	2.23	0.46
1:A:192:PHE:N	1:A:193:PRO:CD	2.78	0.46
1:B:160:LYS:HD2	1:B:160:LYS:HA	1.79	0.46
1:B:510:TRP:CZ2	1:B:539:GLU:HA	2.50	0.46
1:B:376:ASP:HB3	1:B:382:ILE:HD13	1.98	0.46
1:A:26:THR:O	1:A:110:SER:OG	2.34	0.45
1:B:327:ASN:O	1:B:328:GLN:C	2.59	0.45
1:A:147:GLY:HA3	1:A:185:MET:O	2.16	0.45
1:B:228:TRP:CE3	1:B:234:TRP:HB2	2.50	0.45
1:B:298:LEU:HD13	1:B:305:LEU:CD2	2.44	0.45
1:A:125:THR:HA	1:A:161:ASP:OD2	2.16	0.45
1:A:311:TRP:HE1	3:A:602:MES:H21	1.82	0.45
1:A:147:GLY:HA2	1:A:184:PHE:CZ	2.52	0.45
1:A:158:THR:HG22	1:A:163:GLN:NE2	2.31	0.45
1:A:87:ASP:OD1	1:A:87:ASP:C	2.59	0.45
1:A:335:GLY:O	1:A:339:HIS:CD2	2.70	0.44
1:A:149:ASP:OD1	1:A:187:THR:OG1	2.23	0.44
1:A:192:PHE:CD1	1:A:193:PRO:HD3	2.52	0.44
1:B:64:ASN:H	1:B:64:ASN:HD22	1.65	0.44
1:B:373:THR:HA	1:B:383:THR:HG23	1.99	0.44
1:A:327:ASN:O	1:A:328:GLN:C	2.60	0.44
1:B:153:GLU:O	1:B:154:GLN:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ASP:HB3	1:B:370:ILE:HD12	2.00	0.44
1:B:122:ILE:O	1:B:162:ASN:ND2	2.51	0.43
1:B:276:ASN:HA	1:B:284:TYR:CZ	2.53	0.43
1:A:253:SER:O	1:A:257:GLY:N	2.51	0.43
1:B:46:TYR:O	1:B:47:GLN:NE2	2.47	0.43
1:B:239:ASN:ND2	1:B:242:LEU:HB2	2.33	0.43
1:B:361:GLU:O	1:B:364:SER:OG	2.28	0.43
1:B:156:ALA:O	1:B:162:ASN:OD1	2.36	0.43
1:B:195:LEU:O	1:B:262:HIS:HB2	2.19	0.43
1:A:213:ASP:O	1:A:214:PHE:HB3	2.18	0.43
1:A:242:LEU:HA	1:A:245:GLU:OE1	2.19	0.43
1:A:524:HIS:O	1:A:526:GLY:N	2.51	0.43
1:A:74:TYR:CZ	1:A:85:LYS:HG2	2.54	0.42
1:A:355:ILE:CG2	1:A:417:ARG:HB2	2.49	0.42
1:B:228:TRP:HB2	1:B:234:TRP:HD1	1.84	0.42
1:A:36:TYR:HB3	1:A:311:TRP:CZ3	2.55	0.42
1:A:80:ARG:HH11	1:A:80:ARG:HG3	1.84	0.42
1:A:159:ALA:O	1:A:160:LYS:C	2.61	0.42
1:B:191:GLU:OE2	1:B:218:GLN:HB2	2.19	0.42
1:A:69:SER:HA	1:A:70:PHE:HA	1.87	0.42
1:A:217:PRO:O	1:A:272:GLY:HA3	2.20	0.42
1:A:161:ASP:O	1:A:162:ASN:C	2.61	0.42
1:A:334:TYR:O	1:A:338:ILE:HG12	2.20	0.42
1:B:149:ASP:HB2	1:B:187:THR:OG1	2.20	0.42
1:A:325:SER:C	1:A:327:ASN:H	2.27	0.42
1:B:273:LEU:O	1:B:310:THR:HA	2.20	0.42
1:A:47:GLN:O	1:A:321:ALA:HB2	2.20	0.41
1:B:36:TYR:OH	1:B:149:ASP:OD2	2.25	0.41
1:B:509:ASP:O	1:B:510:TRP:C	2.61	0.41
1:A:43:GLY:HA3	3:A:602:MES:H61	2.02	0.41
1:A:267:ASP:OD1	1:A:267:ASP:N	2.52	0.41
1:B:242:LEU:HD23	1:B:242:LEU:HA	1.94	0.41
1:B:267:ASP:OD2	1:B:268:LYS:HD3	2.20	0.41
1:B:238:ASN:O	1:B:240:ASP:N	2.54	0.41
1:B:90:ILE:O	1:B:91:ALA:C	2.62	0.41
1:A:202:THR:O	1:A:206:THR:OG1	2.29	0.41
1:B:53:CYS:HB2	1:B:90:ILE:HG12	2.03	0.41
1:B:60:ASN:HD22	1:B:60:ASN:HA	1.73	0.41
1:B:255:ILE:HA	1:B:264:ILE:O	2.20	0.41
1:A:192:PHE:HA	1:A:195:LEU:HD12	2.02	0.41
1:B:37:TRP:CZ3	1:B:39:ASN:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:O	1:A:56:LEU:C	2.64	0.40
1:A:264:ILE:O	1:A:265:PRO:C	2.62	0.40
1:A:85:LYS:HB3	1:A:85:LYS:HE2	1.88	0.40
1:A:175:GLU:O	1:A:176:HIS:C	2.63	0.40
1:B:37:TRP:N	1:B:67:ASN:O	2.54	0.40
1:B:41:CYS:O	1:B:43:GLY:N	2.54	0.40
1:B:81:ILE:HG13	1:B:131:ALA:HB1	2.02	0.40
1:B:171:LYS:O	1:B:175:GLU:HG2	2.20	0.40
1:A:158:THR:O	1:A:159:ALA:C	2.63	0.40
1:B:123:GLU:HG2	1:B:160:LYS:HB2	2.04	0.40
1:B:52:PRO:C	1:B:54:VAL:H	2.30	0.40
1:A:39:ASN:HD22	1:A:84:PHE:HE1	1.63	0.40
1:B:49:GLY:HA2	1:B:320:ASP:C	2.47	0.40
1:B:355:ILE:HD13	1:B:415:GLN:HB3	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	444/446 (100%)	385 (87%)	51 (12%)	8 (2%)	6	18
1	B	444/446 (100%)	370 (83%)	59 (13%)	15 (3%)	3	7
All	All	888/892 (100%)	755 (85%)	110 (12%)	23 (3%)	4	11

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ASN
1	A	525	ASN
1	A	543	THR
1	B	42	ASP

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Mol	Chain	Res	Type
1	B	56	LEU
1	B	57	LYS
1	B	91	ALA
1	B	239	ASN
1	A	159	ALA
1	A	223	GLY
1	B	61	PRO
1	B	120	ALA
1	B	142	LEU
1	B	223	GLY
1	B	325	SER
1	B	63	TYR
1	B	507	ASP
1	A	145	PHE
1	B	119	ASP
1	B	154	GLN
1	A	341	GLN
1	A	91	ALA
1	B	260	ASN

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	374/374 (100%)	336 (90%)	38 (10%)	7	18
1	B	374/374 (100%)	327 (87%)	47 (13%)	4	11
All	All	748/748 (100%)	663 (89%)	85 (11%)	5	14

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	28	GLN
1	A	44	ARG
1	A	54	VAL

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Mol	Chain	Res	Type
1	A	56	LEU
1	A	66	VAL
1	A	72	LYS
1	A	76	ILE
1	A	103	THR
1	A	125	THR
1	A	166	ILE
1	A	180	THR
1	A	191	GLU
1	A	225	ASP
1	A	235	ILE
1	A	240	ASP
1	A	250	ILE
1	A	287	ASP
1	A	301	GLN
1	A	349	THR
1	A	351	THR
1	A	353	SER
1	A	355	ILE
1	A	358	THR
1	A	369	LEU
1	A	394	THR
1	A	397	VAL
1	A	408	SER
1	A	512	VAL
1	A	517	VAL
1	A	518	LYS
1	A	523	THR
1	A	528	THR
1	A	535	THR
1	A	536	LYS
1	A	538	GLU
1	A	546	TRP
1	A	548	VAL
1	B	24	THR
1	B	53	CYS
1	B	54	VAL
1	B	55	GLU
1	B	57	LYS
1	B	59	VAL
1	B	60	ASN
1	B	64	ASN

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Mol	Chain	Res	Type
1	B	69	SER
1	B	70	PHE
1	B	72	LYS
1	B	76	ILE
1	B	88	PRO
1	B	90	ILE
1	B	98	ILE
1	B	101	ILE
1	B	122	ILE
1	B	128	ASP
1	B	129	GLU
1	B	132	LEU
1	B	142	LEU
1	B	171	LYS
1	B	174	LYS
1	B	179	LYS
1	B	201	TYR
1	B	216	ASN
1	B	235	ILE
1	B	237	GLN
1	B	238	ASN
1	B	260	ASN
1	B	263	LYS
1	B	268	LYS
1	B	310	THR
1	B	317	MET
1	B	319	THR
1	B	347	ASP
1	B	351	THR
1	B	353	SER
1	B	360	VAL
1	B	369	LEU
1	B	387	THR
1	B	389	SER
1	B	394	THR
1	B	397	VAL
1	B	414	ASN
1	B	529	TRP
1	B	543	THR

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	31	ASN
1	A	105	ASN
1	A	163	GLN
1	A	222	GLN
1	A	378	GLN
1	A	395	ASN
1	A	524	HIS
1	B	39	ASN
1	B	60	ASN
1	B	62	GLN
1	B	64	ASN
1	B	67	ASN
1	B	107	GLN
1	B	162	ASN
1	B	218	GLN
1	B	239	ASN
1	B	286	GLN
1	B	336	ASN
1	B	380	ASN
1	B	396	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MES	A	602	-	12,12,12	0.58	0	15,16,16	0.95	1 (6%)

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	MES	A	602	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	602	MES	C2-C3-N4	-2.64	106.10	110.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	MES	5	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 [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	446/446 (100%)	-0.33	1 (0%) 91 90	56, 91, 140, 167	1 (0%)
1	B	446/446 (100%)	-0.32	2 (0%) 88 87	63, 133, 207, 267	0
All	All	892/892 (100%)	-0.32	3 (0%) 90 89	56, 108, 194, 267	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	GLU	3.6
1	A	106	SER	3.3
1	B	97	PHE	2.3

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(Å ²)	Q<0.9
3	MES	A	602	12/12	0.85	0.11	92,113,152,192	0
2	NA	A	601	1/1	0.98	0.04	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.