



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:29 PM UTC

PDB ID : 2Y8V / pdb_00002y8v
Title : Structure of chitinase, ChiC, from *Aspergillus fumigatus*.
Authors : Rush, C.L.; Schuettelkopf, A.W.; Gay, L.M.; van Aalten, D.M.F.
Deposited on : 2011-02-10
Resolution : 1.99 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
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

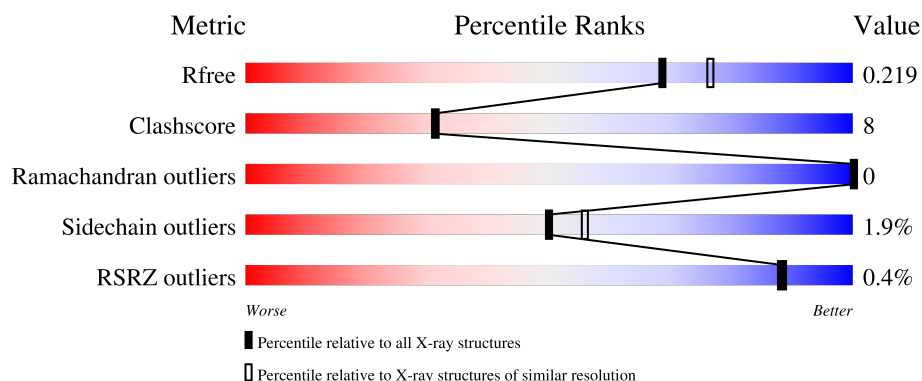
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	290	
1	B	290	
1	C	290	
1	D	290	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9395 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 CLASS III CHITINASE, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2205	1408	385	400	12			
1	B	279	Total	C	N	O	S	0	0	0
			2204	1407	385	400	12			
1	C	281	Total	C	N	O	S	0	0	0
			2212	1411	383	405	13			
1	D	278	Total	C	N	O	S	0	0	0
			2196	1401	382	401	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q4WEQ6
A	0	PRO	-	expression tag	UNP Q4WEQ6
B	-1	GLY	-	expression tag	UNP Q4WEQ6
B	0	PRO	-	expression tag	UNP Q4WEQ6
C	-1	GLY	-	expression tag	UNP Q4WEQ6
C	0	PRO	-	expression tag	UNP Q4WEQ6
D	-1	GLY	-	expression tag	UNP Q4WEQ6
D	0	PRO	-	expression tag	UNP Q4WEQ6

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		

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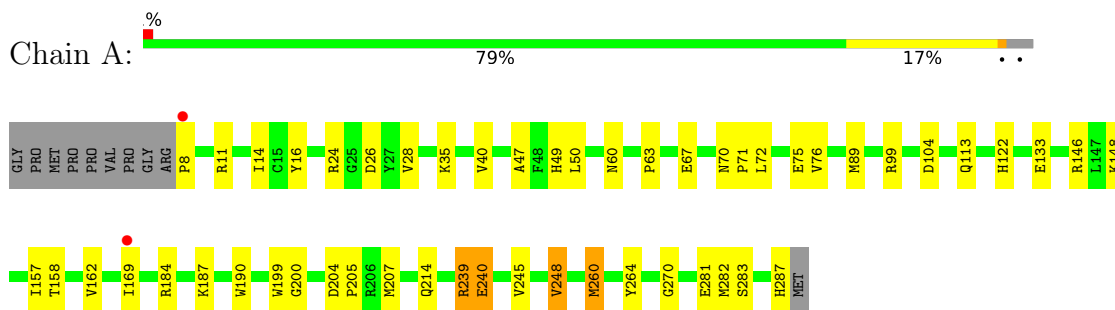
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	162	Total 162	O 162	0	0
3	C	131	Total 131	O 131	0	0
3	D	157	Total 157	O 157	0	0

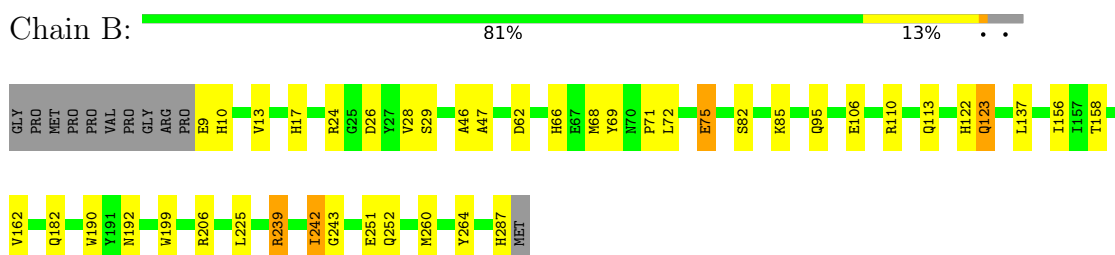
3 Residue-property plots [i](#)

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: CLASS III CHITINASE, PUTATIVE



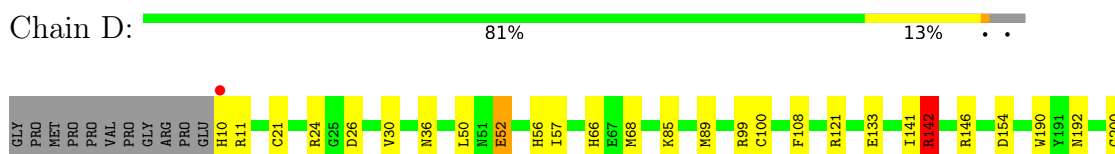
- Molecule 1: CLASS III CHITINASE, PUTATIVE



- Molecule 1: CLASS III CHITINASE, PUTATIVE



- Molecule 1: CLASS III CHITINASE, PUTATIVE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.14Å 145.75Å 82.90Å 90.00° 93.29° 90.00°	Depositor
Resolution (Å)	82.76 – 1.99 82.76 – 1.99	Depositor EDS
% Data completeness (in resolution range)	89.6 (82.76-1.99) 89.6 (82.76-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.59 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.169 , 0.213 0.172 , 0.219	Depositor DCC
R_{free} test set	1507 reflections (1.88%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9395	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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: 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	1.35	6/2265 (0.3%)	1.17	5/3082 (0.2%)
1	B	1.36	3/2264 (0.1%)	1.17	11/3080 (0.4%)
1	C	1.33	4/2273 (0.2%)	1.22	9/3093 (0.3%)
1	D	1.39	3/2255 (0.1%)	1.20	10/3068 (0.3%)
All	All	1.36	16/9057 (0.2%)	1.19	35/12323 (0.3%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	76	VAL	CA-CB	8.70	1.59	1.53
1	A	76	VAL	CA-CB	8.56	1.58	1.54
1	B	9	GLU	CD-OE2	7.79	1.40	1.25
1	A	40	VAL	CA-CB	7.28	1.61	1.54
1	B	28	VAL	CA-CB	6.65	1.62	1.54
1	C	28	VAL	CA-CB	6.62	1.62	1.54
1	A	28	VAL	CA-CB	6.08	1.61	1.54
1	A	248	VAL	CA-CB	5.79	1.61	1.54
1	A	75	GLU	CB-CG	-5.51	1.35	1.52
1	C	239	ARG	CD-NE	-5.32	1.38	1.46
1	D	257	GLY	N-CA	5.26	1.52	1.45
1	B	75	GLU	CB-CG	-5.18	1.36	1.52
1	D	268	ILE	CA-C	5.10	1.58	1.52
1	A	63	PRO	CA-C	5.04	1.54	1.51
1	C	144	ILE	CA-CB	-5.03	1.48	1.54
1	D	52	GLU	CG-CD	5.01	1.64	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	89	MET	CG-SD-CE	-12.60	73.18	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	ARG	NE-CZ-NH1	7.87	129.37	121.50
1	A	8	PRO	N-CA-CB	7.21	110.94	103.00
1	D	142	ARG	NE-CZ-NH2	-7.09	112.82	119.20
1	C	242	ILE	CG1-CB-CG2	-7.07	89.50	110.70
1	D	89	MET	CG-SD-CE	-6.96	85.58	100.90
1	B	137	LEU	CA-C-N	-6.77	111.83	119.28
1	B	137	LEU	C-N-CA	-6.77	111.83	119.28
1	D	36	ASN	CA-C-N	-6.54	113.09	122.77
1	D	36	ASN	C-N-CA	-6.54	113.09	122.77
1	C	264	TYR	N-CA-C	6.54	118.06	111.07
1	C	239	ARG	NE-CZ-NH2	-6.47	113.38	119.20
1	B	264	TYR	N-CA-C	6.39	117.91	111.07
1	D	100	CYS	CA-CB-SG	-6.23	100.06	114.40
1	A	248	VAL	N-CA-CB	6.14	119.80	110.58
1	D	141	ILE	N-CA-C	6.10	116.28	110.42
1	D	264	TYR	N-CA-C	5.77	117.25	111.07
1	A	72	LEU	N-CA-C	-5.47	105.23	111.14
1	A	89	MET	CG-SD-CE	-5.46	88.88	100.90
1	C	120	ARG	NE-CZ-NH1	5.40	126.90	121.50
1	C	76	VAL	N-CA-CB	5.31	113.85	110.50
1	B	123	GLN	CB-CA-C	-5.21	104.48	111.89
1	B	113	GLN	CA-C-N	-5.14	113.63	119.28
1	B	113	GLN	C-N-CA	-5.14	113.63	119.28
1	B	62	ASP	CA-C-N	-5.13	115.92	119.66
1	B	62	ASP	C-N-CA	-5.13	115.92	119.66
1	B	206	ARG	N-CA-C	5.11	116.85	111.28
1	C	137	LEU	CA-C-N	-5.11	113.77	119.19
1	C	137	LEU	C-N-CA	-5.11	113.77	119.19
1	C	98	TYR	CA-CB-CG	-5.11	104.71	113.90
1	D	259	VAL	CG1-CB-CG2	-5.08	99.62	110.80
1	B	95	GLN	N-CA-C	5.07	117.65	110.50
1	A	264	TYR	N-CA-C	5.06	116.49	111.07
1	D	10	HIS	CB-CA-C	5.03	119.66	110.10
1	B	75	GLU	CB-CA-C	-5.01	100.16	110.38

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	2205	0	2136	46	0
1	B	2204	0	2140	35	0
1	C	2212	0	2135	45	0
1	D	2196	0	2133	38	0
2	C	1	0	0	0	0
3	A	127	0	0	9	1
3	B	162	0	0	10	0
3	C	131	0	0	7	0
3	D	157	0	0	12	1
All	All	9395	0	8544	143	1

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 (143) 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:C:121:ARG:HD3	3:C:2064:HOH:O	1.42	1.15
1:A:67:GLU:HG3	3:A:2039:HOH:O	1.58	1.03
1:B:182:GLN:HB3	3:B:2103:HOH:O	1.60	1.00
1:C:178:ARG:HD3	1:C:214:GLN:NE2	1.84	0.92
1:B:252:GLN:HG2	3:B:2149:HOH:O	1.72	0.89
1:A:239:ARG:HH11	1:A:239:ARG:HG3	1.40	0.86
1:D:52:GLU:H	1:D:52:GLU:CD	1.87	0.83
1:B:66:HIS:HD2	1:B:68:MET:H	1.25	0.80
1:D:99:ARG:HD3	3:D:2070:HOH:O	1.83	0.77
1:D:68:MET:HE3	3:D:2012:HOH:O	1.83	0.77
1:A:169:ILE:HG22	1:A:169:ILE:O	1.86	0.76
1:C:169:ILE:CG2	1:C:169:ILE:O	2.33	0.75
1:A:99:ARG:HD3	3:A:2067:HOH:O	1.86	0.75
1:A:239:ARG:HG3	1:A:239:ARG:NH1	1.99	0.74
1:C:169:ILE:O	1:C:169:ILE:HG22	1.88	0.74
1:C:22:PRO:HD2	1:C:28:VAL:HG13	1.69	0.73
1:C:178:ARG:HD3	1:C:214:GLN:HE21	1.54	0.72
1:D:85:LYS:CE	3:D:2031:HOH:O	2.38	0.71
1:A:16:TYR:HE1	1:A:260:MET:HG3	1.55	0.71
1:C:239:ARG:HD2	1:D:281:GLU:OE1	1.91	0.70
1:C:178:ARG:CD	1:C:214:GLN:NE2	2.54	0.69
1:A:104:ASP:OD2	3:A:2049:HOH:O	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:TRP:HE1	1:C:192:ASN:HD21	1.42	0.66
1:B:10:HIS:HD2	3:B:2002:HOH:O	1.78	0.66
1:C:120:ARG:HD3	3:C:2061:HOH:O	1.94	0.66
1:D:56:HIS:HD2	3:D:2025:HOH:O	1.76	0.66
1:A:287:HIS:C	3:A:2127:HOH:O	2.38	0.65
1:D:142:ARG:HD2	3:D:2050:HOH:O	1.95	0.64
1:A:282:MET:CE	1:B:225:LEU:HD12	2.27	0.64
1:C:286:MET:O	1:D:11:ARG:HD2	1.98	0.64
1:A:184:ARG:HD2	1:A:187:LYS:HD2	1.80	0.63
1:A:282:MET:HE1	1:B:225:LEU:CD1	2.29	0.62
1:B:17:HIS:HD2	3:B:2155:HOH:O	1.83	0.61
1:A:239:ARG:HH11	1:A:239:ARG:CG	2.12	0.61
1:C:207:MET:O	1:C:211:ILE:HD13	2.01	0.60
3:A:2003:HOH:O	1:B:287:HIS:HE1	1.85	0.60
1:D:85:LYS:HE2	3:D:2031:HOH:O	2.02	0.60
1:C:47:ALA:H	1:C:60:ASN:ND2	2.00	0.59
1:D:21:CYS:SG	1:D:68:MET:HE2	2.43	0.59
1:A:16:TYR:HE1	1:A:260:MET:CG	2.15	0.59
1:C:176:ASP:HB3	1:C:179:GLN:HG3	1.84	0.58
1:D:190:TRP:HE1	1:D:192:ASN:ND2	2.01	0.58
1:B:106:GLU:HG2	1:B:110:ARG:NH1	2.19	0.58
1:C:22:PRO:HG2	1:C:28:VAL:HG11	1.84	0.58
1:C:239:ARG:NH2	1:D:285:SER:OG	2.37	0.58
1:D:52:GLU:CD	1:D:52:GLU:N	2.60	0.57
1:A:113:GLN:NE2	1:A:146:ARG:NH2	2.52	0.57
1:C:122:HIS:HD2	3:C:2065:HOH:O	1.86	0.57
1:C:190:TRP:HE1	1:C:192:ASN:ND2	2.02	0.57
1:A:169:ILE:O	1:A:169:ILE:CG2	2.52	0.57
1:C:47:ALA:H	1:C:60:ASN:HD21	1.51	0.57
1:C:66:HIS:ND1	1:C:68:MET:HG2	2.19	0.57
1:A:113:GLN:HE22	1:A:146:ARG:NH2	2.03	0.57
1:D:190:TRP:HE1	1:D:192:ASN:HD21	1.54	0.56
1:A:283:SER:HB3	1:B:13:VAL:HG21	1.87	0.56
1:B:252:GLN:CG	3:B:2149:HOH:O	2.43	0.56
1:B:24:ARG:HD3	1:C:26:ASP:OD2	2.05	0.56
1:D:108:PHE:CD1	1:D:142:ARG:HD3	2.40	0.56
1:A:24:ARG:HD3	1:D:26:ASP:OD2	2.06	0.56
1:D:68:MET:CE	3:D:2012:HOH:O	2.49	0.55
1:A:47:ALA:H	1:A:60:ASN:ND2	2.06	0.54
1:A:200:GLY:HA2	1:A:207:MET:SD	2.48	0.54
1:C:286:MET:HB3	1:D:11:ARG:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:ASP:HB2	3:D:2082:HOH:O	2.09	0.53
1:C:237:VAL:CG1	1:C:242:ILE:HG12	2.38	0.53
1:B:190:TRP:HE1	1:B:192:ASN:ND2	2.06	0.52
1:A:158:THR:HG21	1:A:190:TRP:CE2	2.44	0.52
1:D:50:LEU:HD23	1:D:57:ILE:HD12	1.92	0.52
1:C:178:ARG:HH11	1:C:214:GLN:NE2	2.07	0.52
1:A:282:MET:HE2	1:B:225:LEU:HD12	1.91	0.51
1:A:281:GLU:OE1	1:B:239:ARG:HD2	2.10	0.51
1:B:251:GLU:OE2	3:B:2148:HOH:O	2.18	0.51
1:C:56:HIS:HD2	3:C:2024:HOH:O	1.92	0.51
1:D:121:ARG:HG2	1:D:121:ARG:HH11	1.75	0.51
1:C:56:HIS:HE1	3:C:2026:HOH:O	1.93	0.51
1:B:66:HIS:CD2	1:B:68:MET:H	2.17	0.50
1:D:50:LEU:CD2	1:D:57:ILE:HD12	2.41	0.50
1:A:35:LYS:HG3	3:A:2018:HOH:O	2.11	0.50
1:B:182:GLN:CB	3:B:2103:HOH:O	2.38	0.50
1:A:282:MET:CE	1:B:225:LEU:CD1	2.90	0.49
1:A:205:PRO:HD3	1:A:245:VAL:HG13	1.94	0.49
1:A:113:GLN:HE22	1:A:146:ARG:HH21	1.60	0.49
1:D:99:ARG:HG3	1:D:133:GLU:OE2	2.13	0.49
1:B:26:ASP:OD2	1:C:24:ARG:HD3	2.12	0.49
1:D:56:HIS:HE1	3:D:2027:HOH:O	1.95	0.49
1:A:47:ALA:H	1:A:60:ASN:HD21	1.59	0.48
1:D:146:ARG:HG2	3:D:2077:HOH:O	2.11	0.48
1:C:178:ARG:CD	1:C:214:GLN:HE21	2.19	0.48
1:B:122:HIS:HD2	3:B:2075:HOH:O	1.95	0.48
1:C:282:MET:HE2	1:D:239:ARG:CD	2.43	0.48
1:C:22:PRO:CD	1:C:28:VAL:HG13	2.41	0.48
1:A:204:ASP:HB2	1:C:234:GLN:NE2	2.29	0.47
1:A:239:ARG:NH1	1:A:270:GLY:O	2.47	0.47
1:C:10:HIS:CD2	1:C:255:ASN:HA	2.49	0.47
3:B:2015:HOH:O	1:C:28:VAL:HG12	2.14	0.47
1:C:81:ARG:HD3	3:C:2043:HOH:O	2.14	0.47
1:B:162:VAL:HB	1:B:199:TRP:HB3	1.96	0.47
1:C:282:MET:HB3	1:D:259:VAL:HG11	1.97	0.47
1:B:199:TRP:HD1	3:B:2108:HOH:O	1.97	0.46
1:B:85:LYS:HE2	1:B:156:ILE:HD11	1.98	0.46
1:C:11:ARG:HD2	1:D:286:MET:HB3	1.97	0.46
1:D:108:PHE:CE1	1:D:142:ARG:HD3	2.51	0.46
1:A:204:ASP:HB2	1:C:234:GLN:HE22	1.81	0.46
1:B:29:SER:OG	1:B:75:GLU:OE2	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:TRP:HE1	1:B:192:ASN:HD21	1.64	0.46
1:A:16:TYR:CE1	1:A:260:MET:CG	2.98	0.45
1:C:286:MET:HE2	1:C:286:MET:N	2.31	0.45
1:A:148:LYS:HE2	1:A:157:ILE:HG12	1.99	0.45
1:B:242:ILE:HD13	1:B:242:ILE:HA	1.88	0.45
1:C:178:ARG:HD3	1:C:214:GLN:HE22	1.73	0.45
1:C:40:VAL:O	1:C:40:VAL:HG13	2.15	0.45
1:B:71:PRO:O	1:B:75:GLU:HG3	2.16	0.45
1:A:240:GLU:H	1:A:240:GLU:CD	2.24	0.44
1:A:240:GLU:HG3	1:A:270:GLY:C	2.43	0.44
1:A:49:HIS:HE1	3:A:2043:HOH:O	2.01	0.44
1:D:85:LYS:HE3	3:D:2031:HOH:O	2.12	0.44
1:D:21:CYS:SG	1:D:68:MET:CE	3.05	0.44
1:C:10:HIS:HB2	1:C:256:PHE:O	2.17	0.43
1:D:224:GLY:HA2	1:D:260:MET:HG3	2.01	0.43
1:A:99:ARG:HG3	1:A:133:GLU:OE2	2.19	0.42
1:B:162:VAL:HB	1:B:199:TRP:CB	2.48	0.42
1:A:214:GLN:HE21	1:A:214:GLN:HB3	1.73	0.42
1:D:66:HIS:ND1	1:D:68:MET:HG2	2.34	0.42
1:C:239:ARG:HG2	1:D:282:MET:HE2	2.01	0.42
1:B:46:ALA:HA	1:B:47:ALA:HA	1.88	0.42
1:C:49:HIS:HE1	3:C:2044:HOH:O	2.02	0.42
1:A:14:ILE:HB	1:A:260:MET:HB2	2.01	0.41
1:A:169:ILE:HD13	1:A:169:ILE:HG21	1.72	0.41
1:A:11:ARG:NH1	1:B:287:HIS:CD2	2.89	0.41
1:D:241:ARG:O	1:D:244:PRO:HD2	2.21	0.41
1:A:199:TRP:HD1	3:A:2095:HOH:O	2.03	0.41
1:B:242:ILE:HD12	1:B:242:ILE:HG23	1.46	0.41
1:A:162:VAL:HB	1:A:199:TRP:CB	2.50	0.41
1:A:26:ASP:OD2	1:D:24:ARG:HD3	2.20	0.41
1:B:239:ARG:NH2	1:B:243:GLY:HA3	2.36	0.41
1:D:200:GLY:HA2	1:D:207:MET:SD	2.61	0.41
1:A:70:ASN:HB2	1:A:71:PRO:HD3	2.03	0.41
1:A:122:HIS:HD2	3:A:2062:HOH:O	2.04	0.40
1:D:242:ILE:HG21	3:D:2124:HOH:O	2.20	0.40
1:C:63:PRO:HA	1:C:64:PRO:HD3	1.99	0.40
1:C:46:ALA:HA	1:C:47:ALA:HA	1.91	0.40
1:B:69:TYR:O	1:B:72:LEU:HB3	2.22	0.40
1:B:158:THR:HG21	1:B:190:TRP:CE2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2090:HOH:O	3:D:2072:HOH:O[2_656]	2.07	0.13

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	278/290 (96%)	272 (98%)	6 (2%)	0	100	100
1	B	277/290 (96%)	271 (98%)	6 (2%)	0	100	100
1	C	279/290 (96%)	272 (98%)	7 (2%)	0	100	100
1	D	276/290 (95%)	273 (99%)	3 (1%)	0	100	100
All	All	1110/1160 (96%)	1088 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	230/242 (95%)	225 (98%)	5 (2%)	45	50
1	B	231/242 (96%)	226 (98%)	5 (2%)	45	50
1	C	232/242 (96%)	227 (98%)	5 (2%)	45	50
1	D	231/242 (96%)	228 (99%)	3 (1%)	61	68
All	All	924/968 (96%)	906 (98%)	18 (2%)	50	56

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	239	ARG
1	A	240	GLU
1	A	248	VAL
1	A	260	MET
1	B	82	SER
1	B	123	GLN
1	B	239	ARG
1	B	242	ILE
1	B	260	MET
1	C	67	GLU
1	C	89	MET
1	C	149	LEU
1	C	239	ARG
1	C	260	MET
1	D	30	VAL
1	D	142	ARG
1	D	260	MET

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

Mol	Chain	Res	Type
1	A	18	GLN
1	A	49	HIS
1	A	56	HIS
1	A	60	ASN
1	A	105	GLN
1	A	113	GLN
1	A	122	HIS
1	A	179	GLN
1	A	214	GLN
1	B	10	HIS
1	B	17	HIS
1	B	49	HIS
1	B	51	ASN
1	B	66	HIS
1	B	122	HIS
1	B	123	GLN
1	B	192	ASN
1	B	272	GLN
1	B	287	HIS
1	C	36	ASN
1	C	49	HIS

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Mol	Chain	Res	Type
1	C	56	HIS
1	C	60	ASN
1	C	105	GLN
1	C	122	HIS
1	C	192	ASN
1	C	214	GLN
1	C	234	GLN
1	C	252	GLN
1	D	18	GLN
1	D	56	HIS
1	D	113	GLN
1	D	123	GLN
1	D	192	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	280/290 (96%)	-0.30	2 (0%) 84 84	13, 21, 33, 39	0
1	B	279/290 (96%)	-0.42	0 100 100	10, 18, 31, 36	0
1	C	281/290 (96%)	-0.45	1 (0%) 88 88	10, 18, 31, 42	0
1	D	278/290 (95%)	-0.58	1 (0%) 88 88	8, 16, 28, 35	0
All	All	1118/1160 (96%)	-0.44	4 (0%) 88 88	8, 18, 31, 42	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	PRO	2.9
1	C	8	PRO	2.9
1	A	169	ILE	2.7
1	D	10	HIS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	C	1291	1/1	0.91	0.31	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.