



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 03:09 pm GMT

PDB ID : 4C60
Title : Crystal structure of *A. niger* ochratoxinase
Authors : Dobritsch, D.; Wang, H.; Schneider, G.; Yu, S.
Deposited on : 2013-09-17
Resolution : 2.50 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

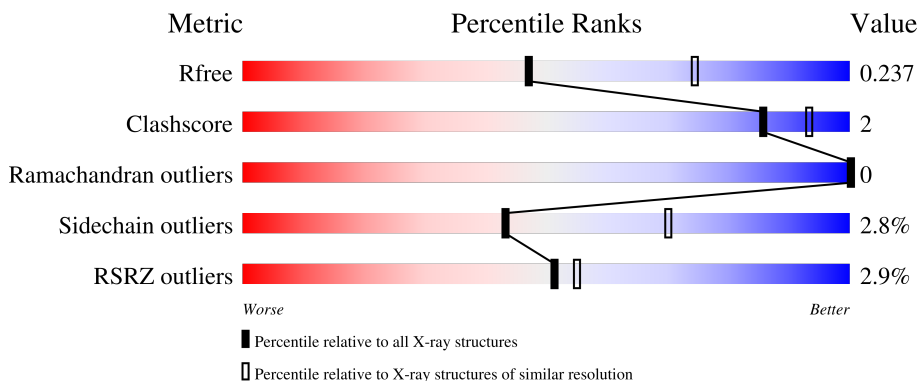
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

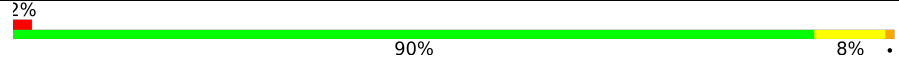
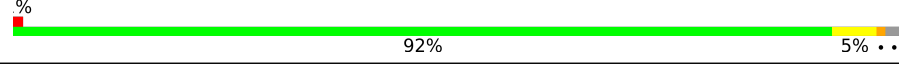
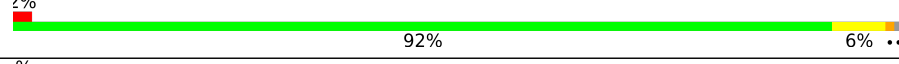
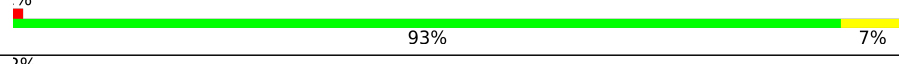
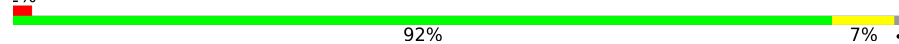
The reported resolution of this entry is 2.50 Å.

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.



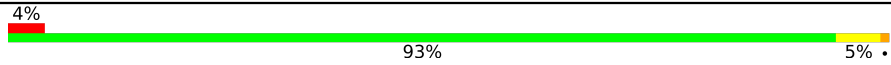
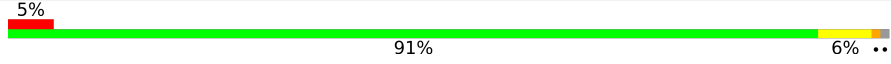
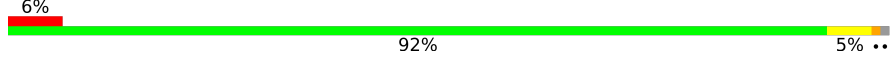
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	438	 2% 90% 8%
1	B	438	 % 92% 5%
1	C	438	 2% 92% 6%
1	D	438	 % 93% 7%
1	E	438	 2% 92% 7%

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Mol	Chain	Length	Quality of chain
1	F	438	 4% 93% 5% •
1	G	438	 5% 91% 6% ••
1	H	438	 6% 92% 5% ••

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26700 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 OCHRATOXINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	436	Total 3269	C 2069	N 568	O 619	S 13	0	0	0
1	B	431	Total 3235	C 2051	N 563	O 608	S 13	0	0	0
1	C	434	Total 3259	C 2064	N 566	O 616	S 13	0	1	0
1	D	436	Total 3269	C 2069	N 568	O 619	S 13	0	0	0
1	E	435	Total 3261	C 2065	N 567	O 616	S 13	0	0	0
1	F	436	Total 3269	C 2069	N 568	O 619	S 13	0	0	0
1	G	433	Total 3248	C 2058	N 565	O 612	S 13	0	0	0
1	H	433	Total 3252	C 2060	N 565	O 614	S 13	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	109	Total 109	O 109	0	0
2	B	85	Total 85	O 85	0	0
2	C	86	Total 86	O 86	0	0
2	D	69	Total 69	O 69	0	0
2	E	96	Total 96	O 96	0	0
2	F	80	Total 80	O 80	0	0

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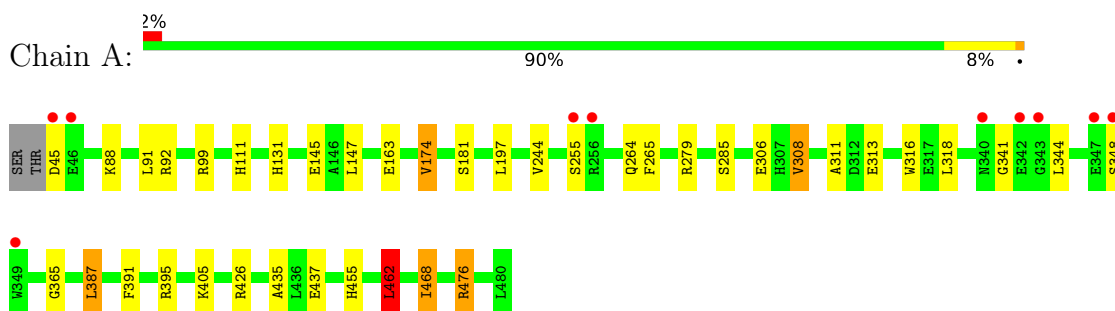
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	65	Total 65	O 65	0	0
2	H	48	Total 48	O 48	0	0

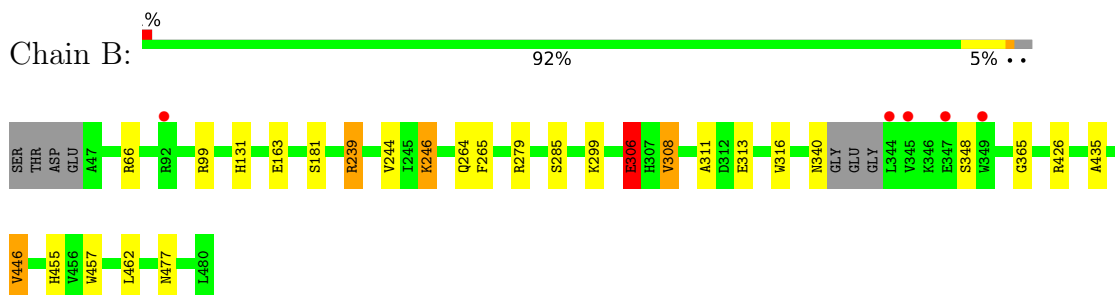
3 Residue-property plots [i](#)

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.

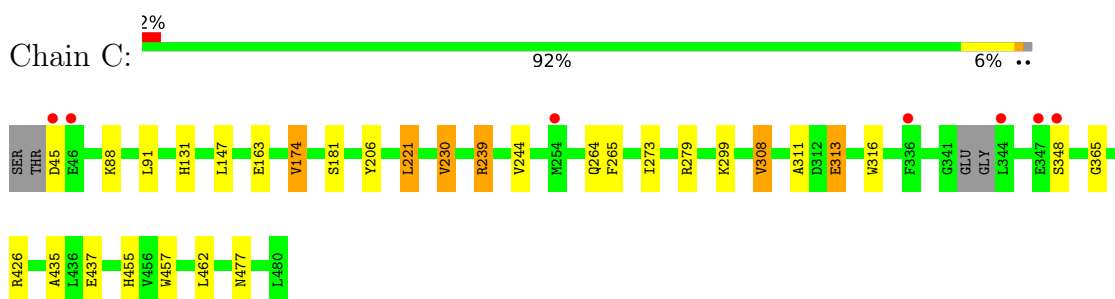
- Molecule 1: OCHRATOXINASE



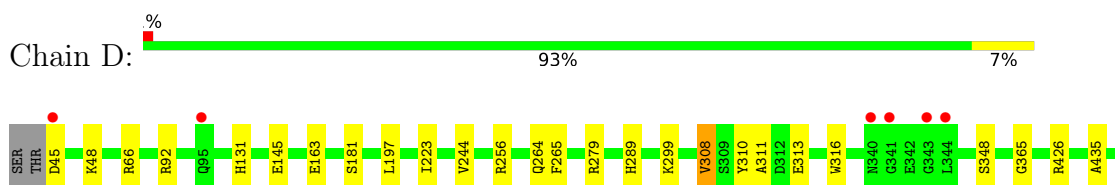
- Molecule 1: OCHRATOXINASE



- Molecule 1: OCHRATOXINASE

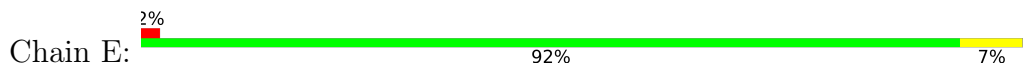


- Molecule 1: OCHRATOXINASE





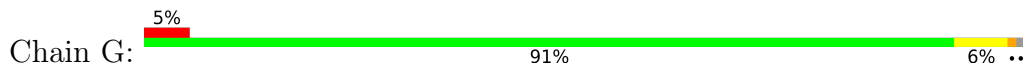
- Molecule 1: OCHRATOXINASE



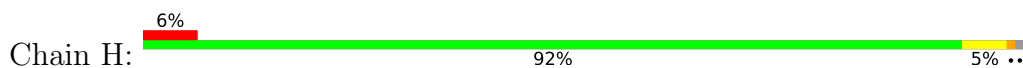
- Molecule 1: OCHRATOXINASE



- Molecule 1: OCHRATOXINASE



- Molecule 1: OCHRATOXINASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.67Å 79.92Å 218.28Å 90.00° 105.25° 90.00°	Depositor
Resolution (Å)	74.47 – 2.50 74.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.5 (74.47-2.50) 90.5 (74.47-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.206 , 0.231 0.211 , 0.237	Depositor DCC
R_{free} test set	5524 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtrriage
Anisotropy	0.319	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.000 for l,-k,h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26700	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.43 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3230e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 i

5.1 Standard geometry i

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	0.53	0/3341	0.81	9/4534 (0.2%)
1	B	0.52	1/3306 (0.0%)	0.71	4/4486 (0.1%)
1	C	0.50	0/3333	0.69	3/4522 (0.1%)
1	D	0.50	0/3341	0.70	3/4534 (0.1%)
1	E	0.49	0/3333	0.67	4/4523 (0.1%)
1	F	0.48	0/3341	0.71	4/4534 (0.1%)
1	G	0.53	3/3319 (0.1%)	0.73	7/4503 (0.2%)
1	H	0.47	0/3323	0.69	4/4509 (0.1%)
All	All	0.50	4/26637 (0.0%)	0.72	38/36145 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	306	GLU	CD-OE2	8.38	1.34	1.25
1	B	306	GLU	CD-OE1	6.27	1.32	1.25
1	G	306	GLU	CG-CD	-5.42	1.43	1.51
1	G	442	GLU	CD-OE2	-5.04	1.20	1.25

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ARG	NE-CZ-NH1	19.30	129.95	120.30
1	A	279	ARG	NE-CZ-NH2	-16.73	111.93	120.30
1	G	306	GLU	OE1-CD-OE2	10.30	135.66	123.30
1	A	468	ILE	CA-CB-CG1	-8.17	95.47	111.00
1	D	223	ILE	CG1-CB-CG2	-8.17	93.43	111.40
1	C	279	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	E	223	ILE	CG1-CB-CG2	-7.94	93.94	111.40
1	G	306	GLU	CG-CD-OE1	-7.84	102.61	118.30
1	B	239	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	F	279	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	C	279	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	F	239	ARG	NE-CZ-NH2	-7.22	116.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	279	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	G	279	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	C	239	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	G	279	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	H	279	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	279	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	E	279	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	G	256	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	B	279	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	F	279	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	476	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	D	279	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	D	279	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	F	426	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	E	279	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	405	LYS	CD-CE-NZ	5.91	125.30	111.70
1	A	395	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	G	239	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	G	239	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	468	ILE	CB-CG1-CD1	5.30	128.73	113.90
1	H	462	LEU	CB-CG-CD1	5.17	119.79	111.00
1	H	314	GLU	OE1-CD-OE2	-5.15	117.11	123.30
1	A	468	ILE	CG1-CB-CG2	-5.10	100.17	111.40
1	A	462	LEU	CB-CG-CD1	5.10	119.66	111.00
1	B	239	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	E	119	ASP	CB-CG-OD2	5.06	122.86	118.30

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	3269	0	3242	24	1
1	B	3235	0	3219	16	1
1	C	3259	0	3237	17	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3269	0	3242	13	1
1	E	3261	0	3238	19	0
1	F	3269	0	3242	15	1
1	G	3248	0	3228	18	0
1	H	3252	0	3229	15	1
2	A	109	0	0	0	0
2	B	85	0	0	0	0
2	C	86	0	0	0	0
2	D	69	0	0	0	0
2	E	96	0	0	0	0
2	F	80	0	0	0	0
2	G	65	0	0	0	0
2	H	48	0	0	0	0
All	All	26700	0	25877	116	3

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 2.

All (116) 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:D:289:HIS:O	1:D:310:TYR:HD1	1.68	0.74
1:A:285:SER:OG	1:A:306:GLU:OE1	2.07	0.73
1:F:329:THR:HG21	1:F:378:ASP:HB2	1.74	0.70
1:A:92:ARG:HD3	1:G:451:LYS:HB2	1.74	0.69
1:F:329:THR:CG2	1:F:378:ASP:HB2	2.26	0.66
1:A:88:LYS:HD2	1:G:437:GLU:HG2	1.82	0.62
1:A:92:ARG:HD3	1:G:451:LYS:CB	2.30	0.62
1:G:285:SER:OG	1:G:306:GLU:OE1	2.18	0.61
1:A:285:SER:OG	1:A:306:GLU:CD	2.40	0.59
1:H:339:SER:O	1:H:340:ASN:HB2	2.03	0.59
1:G:339:SER:O	1:G:340:ASN:HB2	2.04	0.57
1:A:285:SER:OG	1:A:306:GLU:OE2	2.26	0.54
1:E:316:TRP:CZ2	1:E:365:GLY:HA3	2.44	0.53
1:F:339:SER:O	1:F:340:ASN:HB2	2.09	0.52
1:C:88:LYS:HD3	1:C:91:LEU:HD12	1.91	0.52
1:H:147:LEU:CD2	1:H:174:VAL:HG13	2.40	0.51
1:G:435:ALA:HB3	1:G:455:HIS:HB2	1.93	0.51
1:C:147:LEU:CD2	1:C:174:VAL:HG13	2.41	0.51
1:B:435:ALA:HB3	1:B:455:HIS:HB2	1.92	0.51
1:B:181:SER:HA	1:B:244:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:ALA:HB3	1:C:455:HIS:HB2	1.93	0.50
1:H:316:TRP:CZ2	1:H:365:GLY:HA3	2.46	0.50
1:A:88:LYS:HD3	1:A:91:LEU:HD12	1.92	0.50
1:A:147:LEU:CD2	1:A:174:VAL:HG13	2.41	0.50
1:E:435:ALA:HB3	1:E:455:HIS:HB2	1.93	0.50
1:A:316:TRP:CZ2	1:A:365:GLY:HA3	2.47	0.50
1:D:316:TRP:CZ2	1:D:365:GLY:HA3	2.47	0.50
1:D:435:ALA:HB3	1:D:455:HIS:HB2	1.92	0.50
1:G:181:SER:HA	1:G:244:VAL:O	2.11	0.50
1:E:88:LYS:HD3	1:E:91:LEU:HD12	1.94	0.50
1:E:181:SER:HA	1:E:244:VAL:O	2.12	0.50
1:E:477:ASN:CG	1:F:145:GLU:HG2	2.32	0.50
1:A:435:ALA:HB3	1:A:455:HIS:HB2	1.94	0.50
1:B:446:VAL:HG23	1:H:88:LYS:HZ1	1.77	0.49
1:C:230:VAL:HG13	1:C:273:ILE:HG13	1.95	0.49
1:H:435:ALA:HB3	1:H:455:HIS:HB2	1.93	0.49
1:A:145:GLU:HG2	1:B:477:ASN:ND2	2.27	0.49
1:F:181:SER:HA	1:F:244:VAL:O	2.12	0.49
1:A:181:SER:HA	1:A:244:VAL:O	2.12	0.49
1:E:145:GLU:HG2	1:F:477:ASN:CG	2.33	0.49
1:G:285:SER:OG	1:G:306:GLU:CD	2.51	0.49
1:C:181:SER:HA	1:C:244:VAL:O	2.12	0.49
1:E:308:VAL:HG12	1:E:311:ALA:HB2	1.95	0.49
1:C:131:HIS:CG	1:D:163:GLU:HG2	2.48	0.49
1:G:316:TRP:CZ2	1:G:365:GLY:HA3	2.48	0.48
1:D:308:VAL:HG12	1:D:311:ALA:HB2	1.95	0.48
1:H:308:VAL:HG12	1:H:311:ALA:HB2	1.96	0.48
1:C:316:TRP:CZ2	1:C:365:GLY:HA3	2.48	0.48
1:E:230:VAL:HG13	1:E:273:ILE:HG13	1.95	0.48
1:C:308:VAL:HG12	1:C:311:ALA:HB2	1.96	0.48
1:F:435:ALA:HB3	1:F:455:HIS:HB2	1.95	0.48
1:G:230:VAL:HG13	1:G:273:ILE:HG13	1.95	0.48
1:B:308:VAL:HG12	1:B:311:ALA:HB2	1.96	0.48
1:A:308:VAL:HG12	1:A:311:ALA:HB2	1.96	0.48
1:A:387:LEU:HD23	1:A:391:PHE:CE2	2.48	0.47
1:F:308:VAL:HG12	1:F:311:ALA:HB2	1.95	0.47
1:F:313:GLU:HA	1:F:316:TRP:CE3	2.49	0.47
1:H:181:SER:HA	1:H:244:VAL:O	2.13	0.47
1:A:145:GLU:HG2	1:B:477:ASN:CG	2.34	0.47
1:F:316:TRP:CZ2	1:F:365:GLY:HA3	2.50	0.47
1:G:308:VAL:HG12	1:G:311:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:TRP:CZ2	1:B:365:GLY:HA3	2.49	0.47
1:H:264:GLN:O	1:H:265:PHE:HB2	2.16	0.46
1:E:264:GLN:O	1:E:265:PHE:HB2	2.14	0.46
1:G:264:GLN:O	1:G:265:PHE:HB2	2.14	0.46
1:A:264:GLN:O	1:A:265:PHE:HB2	2.15	0.46
1:F:264:GLN:O	1:F:265:PHE:HB2	2.15	0.46
1:D:181:SER:HA	1:D:244:VAL:O	2.15	0.46
1:A:92:ARG:HG2	1:G:451:LYS:HD3	1.96	0.46
1:A:313:GLU:HA	1:A:316:TRP:CE3	2.51	0.46
1:B:264:GLN:O	1:B:265:PHE:HB2	2.16	0.46
1:C:313:GLU:HA	1:C:316:TRP:CE3	2.50	0.46
1:C:457:TRP:CE2	1:C:462:LEU:HD13	2.51	0.46
1:D:264:GLN:O	1:D:265:PHE:HB2	2.15	0.46
1:H:313:GLU:HA	1:H:316:TRP:CE3	2.51	0.46
1:A:462:LEU:HD13	1:A:468:ILE:CD1	2.46	0.46
1:E:145:GLU:HG2	1:F:477:ASN:ND2	2.32	0.45
1:A:131:HIS:CG	1:B:163:GLU:HG2	2.51	0.45
1:G:111:HIS:CE1	1:G:306:GLU:HG2	2.52	0.45
1:C:230:VAL:CG1	1:C:273:ILE:HG13	2.47	0.45
1:E:230:VAL:CG1	1:E:273:ILE:HG13	2.46	0.45
1:E:457:TRP:CE2	1:E:462:LEU:HD13	2.51	0.45
1:C:264:GLN:O	1:C:265:PHE:HB2	2.16	0.44
1:D:313:GLU:HA	1:D:316:TRP:CE3	2.53	0.44
1:G:313:GLU:HA	1:G:316:TRP:CE3	2.52	0.44
1:B:285:SER:OG	1:B:306:GLU:OE1	2.35	0.44
1:B:313:GLU:HA	1:B:316:TRP:CE3	2.53	0.44
1:G:457:TRP:CE2	1:G:462:LEU:HD13	2.52	0.44
1:A:163:GLU:HG2	1:B:131:HIS:CG	2.53	0.43
1:G:230:VAL:CG1	1:G:273:ILE:HG13	2.48	0.43
1:A:341:GLY:HA2	1:A:344:LEU:HD12	2.00	0.43
1:C:477:ASN:ND2	1:D:145:GLU:HG2	2.34	0.43
1:C:147:LEU:HD23	1:C:174:VAL:HG13	2.01	0.43
1:E:313:GLU:HA	1:E:316:TRP:CE3	2.54	0.42
1:E:316:TRP:CH2	1:E:365:GLY:HA3	2.54	0.42
1:G:163:GLU:HG2	1:H:131:HIS:CG	2.54	0.42
1:C:477:ASN:CG	1:D:145:GLU:HG2	2.40	0.42
1:D:457:TRP:CE2	1:D:462:LEU:HD13	2.55	0.42
1:C:163:GLU:HG2	1:D:131:HIS:CG	2.54	0.42
1:E:480:LEU:HD23	1:F:384:PRO:HB3	2.02	0.42
1:H:147:LEU:HD23	1:H:174:VAL:HG13	2.01	0.42
1:C:206:TYR:CE2	1:C:221:LEU:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:HIS:CE1	1:A:306:GLU:HG2	2.55	0.41
1:B:246:LYS:NZ	1:B:306:GLU:OE2	2.53	0.41
1:B:446:VAL:HG23	1:H:88:LYS:NZ	2.34	0.41
1:E:163:GLU:HG2	1:F:131:HIS:CG	2.56	0.41
1:D:316:TRP:CH2	1:D:365:GLY:HA3	2.56	0.41
1:H:163:GLU:O	1:H:166:LYS:HG3	2.21	0.41
1:B:285:SER:HG	1:B:306:GLU:CD	2.24	0.41
1:B:457:TRP:CE2	1:B:462:LEU:HD13	2.55	0.41
1:E:53:TYR:HB2	1:E:99:ARG:HG3	2.02	0.41
1:E:477:ASN:ND2	1:F:145:GLU:HG2	2.35	0.41
1:H:333:ILE:HA	1:H:336:PHE:CE2	2.55	0.41
1:A:147:LEU:HD23	1:A:174:VAL:HG13	2.02	0.40
1:E:209:MET:HG2	1:E:210:ASN:OD1	2.21	0.40
1:H:316:TRP:CH2	1:H:365:GLY:HA3	2.56	0.40

All (3) 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)
1:B:239:ARG:NH2	1:D:197:LEU:O[2_555]	1.96	0.24
1:F:239:ARG:NH2	1:H:197:LEU:O[2_554]	2.02	0.18
1:A:197:LEU:O	1:C:239:ARG:NH2[2_555]	2.03	0.17

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	434/438 (99%)	417 (96%)	17 (4%)	0	100 100
1	B	427/438 (98%)	411 (96%)	16 (4%)	0	100 100
1	C	431/438 (98%)	414 (96%)	17 (4%)	0	100 100
1	D	434/438 (99%)	419 (96%)	15 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	433/438 (99%)	415 (96%)	18 (4%)	0	100	100
1	F	434/438 (99%)	418 (96%)	16 (4%)	0	100	100
1	G	429/438 (98%)	413 (96%)	16 (4%)	0	100	100
1	H	429/438 (98%)	413 (96%)	16 (4%)	0	100	100
All	All	3451/3504 (98%)	3320 (96%)	131 (4%)	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	331/333 (99%)	319 (96%)	12 (4%)	35	61
1	B	328/333 (98%)	318 (97%)	10 (3%)	41	68
1	C	331/333 (99%)	321 (97%)	10 (3%)	41	68
1	D	331/333 (99%)	321 (97%)	10 (3%)	41	68
1	E	330/333 (99%)	323 (98%)	7 (2%)	53	78
1	F	331/333 (99%)	322 (97%)	9 (3%)	44	71
1	G	329/333 (99%)	319 (97%)	10 (3%)	41	68
1	H	330/333 (99%)	323 (98%)	7 (2%)	53	78
All	All	2641/2664 (99%)	2566 (97%)	75 (3%)	43	70

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASP
1	A	99	ARG
1	A	174	VAL
1	A	255	SER
1	A	308	VAL
1	A	318	LEU

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Mol	Chain	Res	Type
1	A	348	SER
1	A	387	LEU
1	A	426	ARG
1	A	437	GLU
1	A	462	LEU
1	A	476	ARG
1	B	66	ARG
1	B	99	ARG
1	B	246	LYS
1	B	299	LYS
1	B	306	GLU
1	B	308	VAL
1	B	340	ASN
1	B	348	SER
1	B	426	ARG
1	B	446	VAL
1	C	45	ASP
1	C	174	VAL
1	C	221	LEU
1	C	230	VAL
1	C	299	LYS
1	C	308	VAL
1	C	313	GLU
1	C	348	SER
1	C	426	ARG
1	C	437	GLU
1	D	45	ASP
1	D	48	LYS
1	D	66	ARG
1	D	92	ARG
1	D	256	ARG
1	D	299	LYS
1	D	308	VAL
1	D	348	SER
1	D	426	ARG
1	D	476	ARG
1	E	66	ARG
1	E	76	ILE
1	E	99	ARG
1	E	308	VAL
1	E	340	ASN
1	E	348	SER

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Mol	Chain	Res	Type
1	E	426	ARG
1	F	45	ASP
1	F	88	LYS
1	F	99	ARG
1	F	256	ARG
1	F	308	VAL
1	F	329	THR
1	F	348	SER
1	F	426	ARG
1	F	462	LEU
1	G	65	LEU
1	G	230	VAL
1	G	256	ARG
1	G	308	VAL
1	G	344	LEU
1	G	347	GLU
1	G	348	SER
1	G	368	LYS
1	G	426	ARG
1	G	437	GLU
1	H	48	LYS
1	H	166	LYS
1	H	174	VAL
1	H	308	VAL
1	H	348	SER
1	H	437	GLU
1	H	462	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	280	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	436/438 (99%)	0.02	10 (2%) 60 63	16, 24, 51, 93	0
1	B	431/438 (98%)	0.04	5 (1%) 79 80	16, 28, 53, 82	0
1	C	434/438 (99%)	0.18	7 (1%) 72 74	16, 27, 59, 88	0
1	D	436/438 (99%)	0.12	6 (1%) 75 77	16, 29, 58, 89	0
1	E	435/438 (99%)	0.02	8 (1%) 68 71	20, 29, 56, 96	0
1	F	436/438 (99%)	0.18	18 (4%) 37 40	21, 31, 59, 95	0
1	G	433/438 (98%)	0.30	21 (4%) 30 32	21, 35, 71, 97	0
1	H	433/438 (98%)	0.43	26 (6%) 21 22	21, 36, 74, 107	0
All	All	3474/3504 (99%)	0.16	101 (2%) 51 55	16, 30, 63, 107	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	347	GLU	5.2
1	F	341	GLY	5.1
1	H	347	GLU	4.7
1	F	347	GLU	4.6
1	A	347	GLU	4.4
1	G	343	GLY	4.3
1	F	342	GLU	4.2
1	G	344	LEU	4.2
1	A	343	GLY	4.1
1	A	256	ARG	4.0
1	E	342	GLU	3.9
1	F	336	PHE	3.9
1	C	45	ASP	3.8
1	G	345	VAL	3.8
1	D	45	ASP	3.7
1	F	256	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	344	LEU	3.7
1	E	341	GLY	3.7
1	F	343	GLY	3.6
1	F	344	LEU	3.6
1	E	344	LEU	3.5
1	A	340	ASN	3.4
1	E	343	GLY	3.3
1	A	45	ASP	3.2
1	A	342	GLU	3.2
1	F	346	LYS	3.2
1	H	93	SER	3.1
1	E	95	GLN	3.1
1	H	91	LEU	3.1
1	H	350	ALA	3.1
1	G	442	GLU	3.0
1	H	46	GLU	3.0
1	H	256	ARG	3.0
1	H	255	SER	3.0
1	G	348	SER	2.9
1	B	92	ARG	2.9
1	A	46	GLU	2.9
1	F	46	GLU	2.9
1	A	348	SER	2.8
1	C	254	MET	2.8
1	G	92	ARG	2.8
1	G	476	ARG	2.8
1	H	344	LEU	2.8
1	H	254	MET	2.8
1	H	438	GLU	2.8
1	G	336	PHE	2.7
1	C	344	LEU	2.7
1	F	348	SER	2.7
1	B	349	TRP	2.7
1	D	343	GLY	2.7
1	F	350	ALA	2.6
1	G	335	ILE	2.6
1	H	54	ALA	2.5
1	D	341	GLY	2.5
1	H	452	ALA	2.5
1	F	45	ASP	2.5
1	G	339	SER	2.5
1	G	349	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	476	ARG	2.5
1	F	92	ARG	2.5
1	H	96	SER	2.4
1	H	92	ARG	2.4
1	G	88	LYS	2.4
1	F	354	ALA	2.4
1	H	45	ASP	2.4
1	B	345	VAL	2.4
1	B	347	GLU	2.4
1	C	348	SER	2.4
1	H	475	ALA	2.3
1	D	95	GLN	2.3
1	E	46	GLU	2.3
1	G	347	GLU	2.3
1	H	86	ILE	2.3
1	H	84	ALA	2.3
1	H	450	PRO	2.2
1	F	476	ARG	2.2
1	G	453	VAL	2.2
1	H	94	THR	2.2
1	E	339	SER	2.2
1	G	87	PRO	2.2
1	F	349	TRP	2.2
1	C	46	GLU	2.2
1	A	349	TRP	2.2
1	H	53	TYR	2.2
1	F	65	LEU	2.2
1	H	55	GLY	2.1
1	A	255	SER	2.1
1	G	85	ASP	2.1
1	H	98	HIS	2.1
1	G	80	VAL	2.1
1	D	344	LEU	2.1
1	G	346	LYS	2.1
1	C	336	PHE	2.1
1	F	339	SER	2.1
1	H	460	GLY	2.1
1	H	339	SER	2.0
1	G	340	ASN	2.0
1	G	368	LYS	2.0
1	D	340	ASN	2.0
1	G	480	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	89	LYS	2.0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.