



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:10 PM UTC

PDB ID : 3T22 / pdb_00003t22
Title : Crystal structure of OxyR mutant from Porphyromonas gingivalis
Authors : Svintradze, D.V.; Wright, H.T.; Lewis, J.P.
Deposited on : 2011-07-22
Resolution : 2.20 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

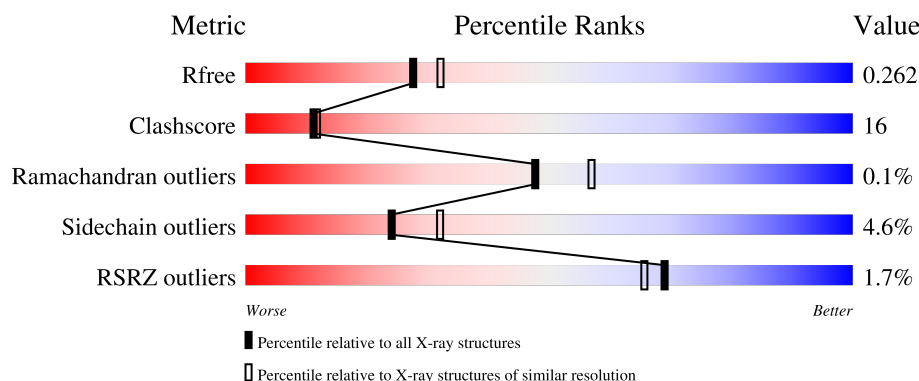
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	223	2% 71% 22% 6%
1	B	223	58% 30% 7%
1	C	223	76% 20%
1	D	223	3% 59% 30% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7103 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 Redox-sensitive transcriptional activator OxyR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1683	1070	296	307	10			
1	B	207	Total	C	N	O	S	0	0	0
			1661	1057	292	303	9			
1	C	214	Total	C	N	O	S	0	0	0
			1711	1088	301	312	10			
1	D	208	Total	C	N	O	S	0	0	0
			1670	1063	291	306	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	SER	CYS	engineered mutation	UNP Q20K61
A	309	HIS	-	expression tag	UNP Q20K61
A	310	HIS	-	expression tag	UNP Q20K61
A	311	HIS	-	expression tag	UNP Q20K61
A	312	HIS	-	expression tag	UNP Q20K61
B	199	SER	CYS	engineered mutation	UNP Q20K61
B	309	HIS	-	expression tag	UNP Q20K61
B	310	HIS	-	expression tag	UNP Q20K61
B	311	HIS	-	expression tag	UNP Q20K61
B	312	HIS	-	expression tag	UNP Q20K61
C	199	SER	CYS	engineered mutation	UNP Q20K61
C	309	HIS	-	expression tag	UNP Q20K61
C	310	HIS	-	expression tag	UNP Q20K61
C	311	HIS	-	expression tag	UNP Q20K61
C	312	HIS	-	expression tag	UNP Q20K61
D	199	SER	CYS	engineered mutation	UNP Q20K61
D	309	HIS	-	expression tag	UNP Q20K61
D	310	HIS	-	expression tag	UNP Q20K61
D	311	HIS	-	expression tag	UNP Q20K61
D	312	HIS	-	expression tag	UNP Q20K61

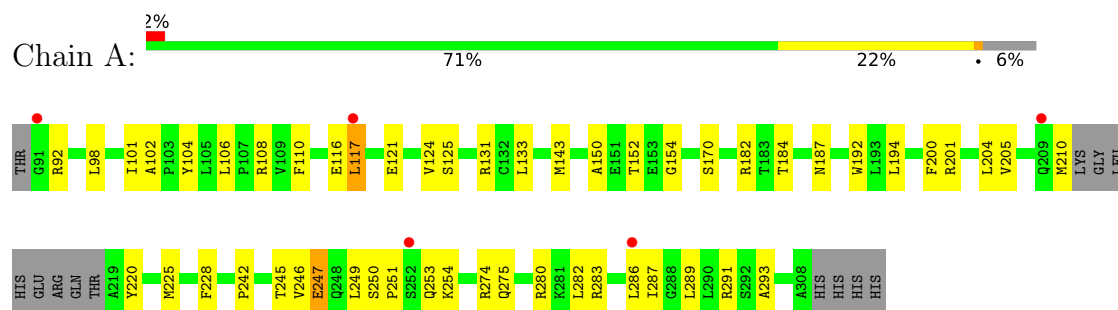
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	106	Total 106	O 106	0	0
2	B	78	Total 78	O 78	0	0
2	C	102	Total 102	O 102	0	0
2	D	92	Total 92	O 92	0	0

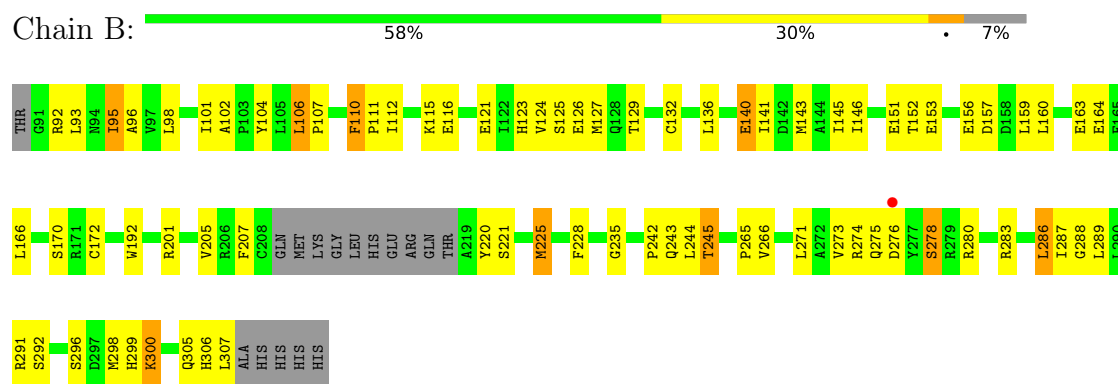
3 Residue-property plots

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.

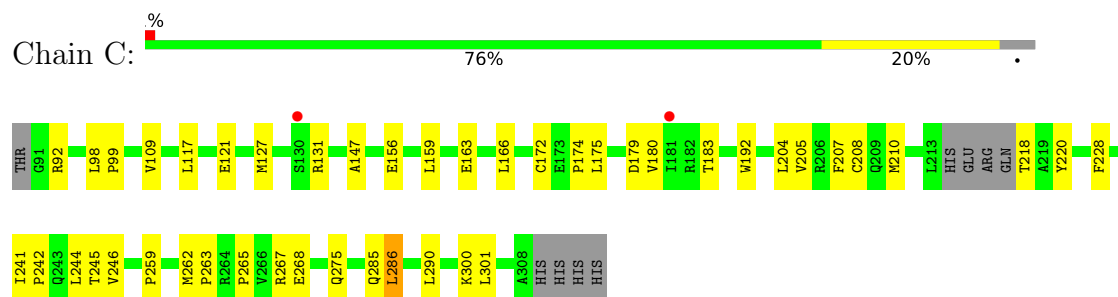
• Molecule 1: Redox-sensitive transcriptional activator OxyR



• Molecule 1: Redox-sensitive transcriptional activator OxyR

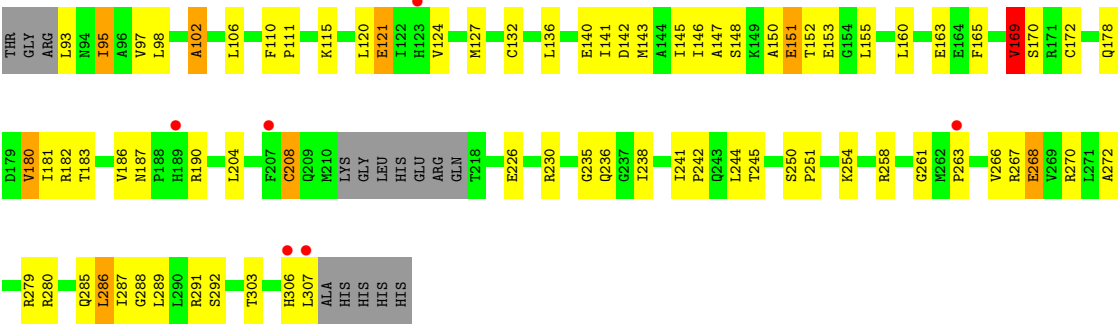


• Molecule 1: Redox-sensitive transcriptional activator OxyR



• Molecule 1: Redox-sensitive transcriptional activator OxyR





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.21Å 64.36Å 81.31Å 111.75° 90.56° 111.24°	Depositor
Resolution (Å)	18.36 – 2.20 18.36 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.6 (18.36-2.20) 91.4 (18.36-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.234 , 0.274 0.230 , 0.262	Depositor DCC
R_{free} test set	3485 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7103	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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

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	0.57	0/1716	0.83	2/2318 (0.1%)
1	B	0.53	0/1694	0.89	0/2289
1	C	0.55	0/1744	0.87	0/2355
1	D	0.56	0/1703	0.93	6/2302 (0.3%)
All	All	0.55	0/6857	0.88	8/9264 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	102	ALA	CA-C-N	-6.41	113.09	119.56
1	D	102	ALA	C-N-CA	-6.41	113.09	119.56
1	D	286	LEU	N-CA-C	-5.92	104.91	111.36
1	A	187	ASN	CA-C-N	5.75	125.61	119.28
1	A	187	ASN	C-N-CA	5.75	125.61	119.28
1	D	169	VAL	N-CA-C	5.71	118.37	108.95
1	D	236	GLN	N-CA-C	5.28	118.30	107.69
1	D	261	GLY	N-CA-C	-5.17	105.14	112.37

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	1683	0	1703	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1661	0	1681	76	0
1	C	1711	0	1737	31	0
1	D	1670	0	1689	69	0
2	A	106	0	0	3	0
2	B	78	0	0	10	0
2	C	102	0	0	5	0
2	D	92	0	0	7	0
All	All	7103	0	6810	221	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 16.

All (221) 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:250:SER:HB2	1:D:251:PRO:HD2	1.38	1.05
1:A:204:LEU:HG	1:A:210:MET:CE	1.96	0.95
1:C:300:LYS:HE2	2:C:338:HOH:O	1.72	0.90
1:D:242:PRO:O	1:D:245:THR:HG22	1.75	0.86
1:A:116:GLU:C	1:A:117:LEU:HD12	2.02	0.84
1:D:268:GLU:HG2	1:D:307:LEU:HD21	1.59	0.84
1:B:93:LEU:HD21	1:B:143:MET:CE	2.08	0.84
1:A:204:LEU:HG	1:A:210:MET:HE2	1.60	0.83
1:A:143:MET:HE1	1:A:286:LEU:HD12	1.62	0.80
1:D:181:ILE:HD11	1:D:258:ARG:HB2	1.63	0.80
1:D:250:SER:CB	1:D:251:PRO:HD2	2.12	0.80
1:A:242:PRO:O	1:A:245:THR:HG22	1.83	0.78
1:D:150:ALA:O	1:D:152:THR:HG23	1.84	0.78
1:D:115:LYS:HE2	2:D:368:HOH:O	1.82	0.78
1:A:204:LEU:HG	1:A:210:MET:HE1	1.66	0.78
1:B:273:VAL:HG21	1:B:283:ARG:HD2	1.66	0.77
1:B:95:ILE:HD11	1:B:145:ILE:HG13	1.67	0.75
1:B:93:LEU:HD21	1:B:143:MET:HE2	1.65	0.75
1:B:140:GLU:HG3	2:B:331:HOH:O	1.85	0.75
1:D:152:THR:OG1	1:D:155:LEU:HD12	1.86	0.75
1:C:183:THR:HG21	1:C:208:CYS:HB3	1.68	0.74
1:C:242:PRO:O	1:C:245:THR:HG22	1.88	0.74
1:D:170:SER:HB2	1:D:235:GLY:HA2	1.68	0.74
1:B:242:PRO:O	1:B:245:THR:HG23	1.90	0.72
1:C:262:MET:HG3	1:C:263:PRO:HA	1.70	0.72
1:D:250:SER:HB2	1:D:251:PRO:CD	2.18	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:ILE:CD1	1:D:258:ARG:HB2	2.22	0.70
1:A:117:LEU:HD11	1:A:289:LEU:HD11	1.73	0.69
1:D:287:ILE:O	1:D:291:ARG:HG2	1.91	0.69
1:B:156:GLU:HG2	1:B:275:GLN:HA	1.74	0.69
1:B:170:SER:OG	1:B:235:GLY:HA2	1.95	0.67
1:C:109:VAL:HG11	1:C:290:LEU:HD23	1.77	0.67
1:C:241:ILE:HD12	1:C:245:THR:HG21	1.75	0.66
1:B:116:GLU:HB2	1:B:289:LEU:HD11	1.78	0.66
1:B:93:LEU:HD11	1:B:143:MET:HE2	1.78	0.66
1:D:266:VAL:HG23	1:D:307:LEU:CD1	2.25	0.65
1:D:106:LEU:HD21	1:D:124:VAL:HG11	1.79	0.65
1:A:117:LEU:HD12	1:A:117:LEU:N	2.12	0.65
1:A:117:LEU:CD1	1:A:289:LEU:HD11	2.26	0.64
1:A:205:VAL:HA	1:A:210:MET:HE3	1.80	0.64
1:C:92:ARG:HA	1:C:121:GLU:O	1.98	0.63
1:B:140:GLU:CG	2:B:331:HOH:O	2.43	0.63
1:D:181:ILE:CD1	1:D:258:ARG:CB	2.77	0.63
1:D:169:VAL:HB	1:D:238:ILE:HG12	1.81	0.62
1:C:183:THR:OG1	1:C:210:MET:HE2	1.99	0.62
1:D:250:SER:CB	1:D:251:PRO:CD	2.78	0.61
1:A:150:ALA:O	1:A:152:THR:HG23	2.01	0.60
1:B:274:ARG:CD	2:B:355:HOH:O	2.48	0.60
1:A:98:LEU:HB2	1:A:101:ILE:HD12	1.83	0.60
1:D:241:ILE:HD12	1:D:245:THR:CG2	2.31	0.59
1:B:299:HIS:C	1:B:300:LYS:HG2	2.27	0.59
1:B:112:ILE:HG22	1:B:289:LEU:HD13	1.84	0.59
1:B:153:GLU:CD	1:B:153:GLU:H	2.11	0.59
1:B:305:GLN:C	1:B:306:HIS:CG	2.80	0.58
1:B:143:MET:HE1	1:B:286:LEU:HG	1.84	0.58
1:B:110:PHE:HB2	1:B:111:PRO:HD3	1.84	0.58
1:C:241:ILE:HD12	1:C:245:THR:CG2	2.34	0.58
1:A:117:LEU:N	1:A:117:LEU:CD1	2.67	0.57
1:B:274:ARG:HD3	2:B:355:HOH:O	2.03	0.57
1:B:110:PHE:CB	1:B:111:PRO:HD3	2.34	0.57
1:B:201:ARG:O	1:B:205:VAL:HG22	2.04	0.57
1:D:266:VAL:HG23	1:D:307:LEU:HD12	1.85	0.57
1:B:163:GLU:OE2	1:B:244:LEU:HB2	2.04	0.57
1:D:268:GLU:OE1	1:D:270:ARG:NH1	2.38	0.57
1:B:296:SER:HB3	2:B:354:HOH:O	2.03	0.56
1:D:285:GLN:O	1:D:289:LEU:HG	2.05	0.56
1:D:163:GLU:OE2	1:D:244:LEU:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:ILE:HD12	1:D:245:THR:HG23	1.88	0.56
1:C:172:CYS:SG	2:C:326:HOH:O	2.35	0.56
1:D:165:PHE:CD2	1:D:204:LEU:HD13	2.40	0.56
1:A:108:ARG:HD3	1:A:293:ALA:O	2.06	0.56
1:B:244:LEU:HD13	1:B:298:MET:HE1	1.88	0.55
1:B:273:VAL:HG21	1:B:283:ARG:CD	2.36	0.55
1:A:143:MET:HE1	1:A:286:LEU:CD1	2.33	0.55
1:B:92:ARG:HA	1:B:121:GLU:HG3	1.88	0.55
1:B:305:GLN:O	1:B:306:HIS:CD2	2.60	0.54
1:A:249:LEU:HD22	1:A:253:GLN:HB3	1.89	0.54
1:D:187:ASN:HD22	1:D:190:ARG:HD3	1.73	0.53
1:D:160:LEU:O	1:D:291:ARG:HD2	2.07	0.53
1:B:151:GLU:O	1:B:152:THR:HG23	2.08	0.53
1:B:242:PRO:HD2	1:B:245:THR:HG21	1.89	0.53
1:D:263:PRO:HB2	1:D:306:HIS:CE1	2.43	0.53
1:C:147:ALA:HB1	1:C:267:ARG:HD2	1.90	0.53
1:D:127:MET:HG3	1:D:132:CYS:SG	2.49	0.52
1:A:143:MET:CE	1:A:286:LEU:HD12	2.36	0.52
1:B:129:THR:O	1:B:132:CYS:HB2	2.10	0.52
1:C:174:PRO:HA	2:C:349:HOH:O	2.09	0.52
1:D:266:VAL:CG2	1:D:307:LEU:HD12	2.40	0.52
1:A:143:MET:SD	1:A:286:LEU:CD1	2.98	0.52
1:D:266:VAL:HG23	1:D:307:LEU:HD11	1.91	0.52
1:B:102:ALA:O	1:B:106:LEU:HB2	2.10	0.52
1:D:151:GLU:O	1:D:152:THR:CG2	2.58	0.51
1:A:104:TYR:OH	1:A:225:MET:HG2	2.10	0.51
1:B:164:GLU:HG2	1:B:266:VAL:HG12	1.92	0.51
1:A:287:ILE:HG22	1:A:291:ARG:HD2	1.91	0.51
1:C:207:PHE:CE2	1:C:265:PRO:HB3	2.46	0.51
1:D:136:LEU:HD23	1:D:141:ILE:HG13	1.91	0.51
1:B:98:LEU:HD13	1:B:146:ILE:HA	1.91	0.51
1:B:115:LYS:HB2	1:B:115:LYS:HZ3	1.76	0.51
1:C:192:TRP:HB3	1:C:228:PHE:CD1	2.46	0.50
1:D:151:GLU:C	1:D:152:THR:HG23	2.37	0.50
1:A:117:LEU:HD11	1:A:289:LEU:CD1	2.42	0.50
1:B:104:TYR:CD1	1:B:245:THR:HG22	2.46	0.50
1:A:250:SER:HB2	1:A:251:PRO:HD2	1.93	0.50
1:B:274:ARG:NH1	2:B:320:HOH:O	2.41	0.50
1:D:110:PHE:N	1:D:111:PRO:CD	2.74	0.50
1:A:282:LEU:O	1:A:286:LEU:HG	2.12	0.50
1:A:133:LEU:HD13	1:A:152:THR:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:LEU:HB2	2:D:381:HOH:O	2.11	0.49
1:A:194:LEU:O	1:A:201:ARG:NH2	2.42	0.49
1:B:242:PRO:HD2	1:B:245:THR:CG2	2.41	0.49
1:B:291:ARG:NH2	2:B:349:HOH:O	2.44	0.49
1:A:246:VAL:HG22	1:A:247:GLU:OE2	2.13	0.49
1:B:123:HIS:CD2	1:B:124:VAL:N	2.81	0.49
1:A:106:LEU:O	1:A:110:PHE:HD2	1.96	0.49
1:A:154:GLY:O	1:A:275:GLN:HG3	2.12	0.49
1:A:250:SER:HB2	1:A:251:PRO:CD	2.43	0.49
1:B:166:LEU:HD12	1:B:243:GLN:HA	1.95	0.49
1:B:170:SER:OG	1:B:235:GLY:CA	2.60	0.49
1:B:192:TRP:HB3	1:B:228:PHE:CD1	2.48	0.49
1:D:143:MET:SD	1:D:286:LEU:HD12	2.53	0.48
1:B:95:ILE:HD12	1:B:143:MET:O	2.13	0.48
1:B:115:LYS:HG2	1:B:116:GLU:OE1	2.13	0.48
1:B:307:LEU:N	1:B:307:LEU:HD12	2.28	0.48
1:D:169:VAL:HG23	1:D:170:SER:N	2.27	0.48
1:A:182:ARG:NH1	1:A:184:THR:OG1	2.46	0.48
1:B:115:LYS:HB2	1:B:115:LYS:NZ	2.27	0.48
1:D:93:LEU:N	1:D:121:GLU:OE2	2.47	0.48
1:B:286:LEU:C	1:B:288:GLY:N	2.67	0.48
1:C:300:LYS:HG2	1:C:301:LEU:N	2.27	0.48
1:D:250:SER:O	1:D:254:LYS:HG3	2.14	0.48
1:B:220:TYR:HD1	1:B:220:TYR:C	2.22	0.48
1:D:152:THR:O	1:D:153:GLU:C	2.57	0.48
1:D:121:GLU:O	1:D:121:GLU:HG2	2.12	0.47
1:D:148:SER:HB2	2:D:359:HOH:O	2.13	0.47
1:A:131:ARG:HH22	1:C:175:LEU:CD2	2.27	0.47
1:B:93:LEU:HD21	1:B:143:MET:HE1	1.96	0.47
1:D:120:LEU:HD11	2:D:381:HOH:O	2.14	0.47
1:A:283:ARG:O	1:A:287:ILE:HG13	2.15	0.47
1:B:166:LEU:CD1	1:B:243:GLN:HA	2.44	0.47
1:D:181:ILE:CD1	1:D:258:ARG:HB3	2.45	0.47
1:B:160:LEU:O	1:B:291:ARG:HG2	2.15	0.47
1:C:218:THR:HB	2:C:371:HOH:O	2.15	0.47
1:D:178:GLN:NE2	1:D:182:ARG:CZ	2.77	0.47
1:C:286:LEU:HD13	1:C:286:LEU:HA	1.69	0.47
1:A:154:GLY:C	1:A:275:GLN:HG3	2.40	0.47
1:B:220:TYR:C	1:B:220:TYR:CD1	2.92	0.47
1:B:307:LEU:HD12	1:B:307:LEU:H	1.80	0.46
1:B:207:PHE:C	1:B:207:PHE:CD2	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:LEU:HD12	1:D:142:ASP:HB2	1.96	0.46
1:D:151:GLU:C	1:D:152:THR:CG2	2.88	0.46
1:B:278:SER:HA	2:B:333:HOH:O	2.16	0.46
1:A:106:LEU:HD11	1:A:124:VAL:HG11	1.98	0.46
1:D:97:VAL:HG22	1:D:145:ILE:HD12	1.98	0.46
1:D:285:GLN:C	1:D:288:GLY:H	2.24	0.46
1:D:102:ALA:O	1:D:106:LEU:HB2	2.16	0.45
1:A:192:TRP:HB3	1:A:228:PHE:CD1	2.51	0.45
1:B:283:ARG:O	1:B:287:ILE:HG13	2.16	0.45
1:D:183:THR:O	1:D:186:VAL:HG22	2.16	0.45
1:D:151:GLU:O	1:D:152:THR:HG22	2.15	0.45
1:A:106:LEU:O	1:A:110:PHE:CD2	2.69	0.45
1:B:207:PHE:CD1	1:B:265:PRO:HB3	2.52	0.45
1:A:220:TYR:OH	1:B:126:GLU:OE2	2.28	0.45
1:C:220:TYR:HA	1:D:124:VAL:O	2.17	0.45
1:D:226:GLU:O	1:D:230:ARG:HG2	2.17	0.45
1:C:183:THR:OG1	1:C:210:MET:HG2	2.16	0.45
1:A:280:ARG:NH1	2:A:390:HOH:O	2.49	0.44
1:B:151:GLU:O	1:B:152:THR:CG2	2.65	0.44
1:A:102:ALA:O	1:A:106:LEU:HB2	2.18	0.44
1:A:131:ARG:HH22	1:C:175:LEU:HD23	1.81	0.44
1:B:296:SER:CB	2:B:354:HOH:O	2.61	0.44
1:C:117:LEU:CD1	1:C:285:GLN:NE2	2.81	0.44
1:B:225:MET:HE2	1:B:225:MET:HB2	1.83	0.44
1:B:305:GLN:O	1:B:306:HIS:CG	2.70	0.44
1:A:200:PHE:HA	2:A:5:HOH:O	2.17	0.44
1:D:172:CYS:SG	2:D:321:HOH:O	2.62	0.44
1:B:136:LEU:HD23	1:B:141:ILE:HG13	1.99	0.44
1:C:92:ARG:NH2	2:C:382:HOH:O	2.49	0.44
1:D:93:LEU:HA	1:D:142:ASP:OD2	2.18	0.44
1:D:204:LEU:O	1:D:208:CYS:HB2	2.17	0.43
1:D:289:LEU:O	1:D:292:SER:HB3	2.19	0.43
1:A:92:ARG:HB2	1:A:121:GLU:O	2.18	0.43
1:B:123:HIS:CD2	1:B:123:HIS:C	2.97	0.43
1:B:98:LEU:HB2	1:B:101:ILE:HD12	2.00	0.43
1:C:117:LEU:HD11	1:C:285:GLN:NE2	2.33	0.43
1:C:262:MET:HG3	1:C:263:PRO:CA	2.46	0.43
1:D:180:VAL:HG23	1:D:181:ILE:N	2.33	0.43
1:D:285:GLN:OE1	1:D:285:GLN:N	2.49	0.43
1:B:93:LEU:CD2	1:B:143:MET:HE2	2.43	0.42
1:B:157:ASP:HA	1:B:271:LEU:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:SER:OG	1:B:235:GLY:C	2.62	0.42
1:D:95:ILE:HA	1:D:143:MET:O	2.19	0.42
1:D:146:ILE:HD11	1:D:272:ALA:HB2	2.00	0.42
1:C:98:LEU:HA	1:C:99:PRO:HD3	1.92	0.42
1:D:286:LEU:HA	1:D:286:LEU:HD23	1.77	0.42
1:D:178:GLN:HG3	1:D:182:ARG:HD2	2.02	0.42
1:D:268:GLU:HG2	1:D:307:LEU:CD2	2.40	0.42
1:A:225:MET:HE2	1:A:225:MET:HB2	1.82	0.42
1:B:96:ALA:HA	1:B:125:SER:O	2.19	0.42
1:C:159:LEU:CD1	1:C:268:GLU:HB2	2.49	0.42
1:B:286:LEU:O	1:B:287:ILE:C	2.62	0.42
1:D:178:GLN:HA	1:D:178:GLN:OE1	2.20	0.42
1:B:136:LEU:HD23	1:B:136:LEU:HA	1.85	0.41
1:D:147:ALA:HB1	1:D:267:ARG:HD2	2.02	0.41
1:A:92:ARG:CB	1:A:121:GLU:HG3	2.50	0.41
1:A:220:TYR:C	1:A:220:TYR:CD1	2.97	0.41
1:B:106:LEU:N	1:B:107:PRO:CD	2.83	0.41
1:A:250:SER:O	1:A:254:LYS:HG3	2.21	0.41
1:A:274:ARG:HD3	2:A:319:HOH:O	2.20	0.41
1:C:156:GLU:OE2	1:C:275:GLN:HG2	2.21	0.41
1:D:121:GLU:CD	2:D:358:HOH:O	2.63	0.41
1:D:279:ARG:NE	2:D:341:HOH:O	2.54	0.41
1:B:280:ARG:NH2	2:B:333:HOH:O	2.51	0.41
1:C:127:MET:HB2	1:C:131:ARG:HD3	2.02	0.41
1:A:117:LEU:CD1	1:A:289:LEU:CD1	2.95	0.41
1:C:166:LEU:HD23	1:C:259:PRO:HA	2.03	0.41
1:B:159:LEU:HD12	1:B:160:LEU:N	2.36	0.40
1:A:92:ARG:HB3	1:A:121:GLU:HG3	2.02	0.40
1:C:163:GLU:OE2	1:C:244:LEU:HB2	2.22	0.40
1:B:123:HIS:HD2	1:B:124:VAL:N	2.20	0.40
1:B:151:GLU:C	1:B:152:THR:HG23	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	206/223 (92%)	199 (97%)	7 (3%)	0	100	100
1	B	203/223 (91%)	192 (95%)	11 (5%)	0	100	100
1	C	210/223 (94%)	204 (97%)	6 (3%)	0	100	100
1	D	204/223 (92%)	186 (91%)	17 (8%)	1 (0%)	24	27
All	All	823/892 (92%)	781 (95%)	41 (5%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	280	ARG

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	185/197 (94%)	181 (98%)	4 (2%)	45	61
1	B	183/197 (93%)	169 (92%)	14 (8%)	12	13
1	C	188/197 (95%)	182 (97%)	6 (3%)	34	47
1	D	185/197 (94%)	175 (95%)	10 (5%)	20	25
All	All	741/788 (94%)	707 (95%)	34 (5%)	24	32

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	125	SER
1	A	170	SER
1	A	247	GLU
1	B	95	ILE
1	B	106	LEU
1	B	110	PHE

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Mol	Chain	Res	Type
1	B	127	MET
1	B	140	GLU
1	B	172	CYS
1	B	221	SER
1	B	225	MET
1	B	245	THR
1	B	276	ASP
1	B	278	SER
1	B	286	LEU
1	B	292	SER
1	B	300	LYS
1	C	179	ASP
1	C	180	VAL
1	C	204	LEU
1	C	205	VAL
1	C	246	VAL
1	C	286	LEU
1	D	95	ILE
1	D	98	LEU
1	D	121	GLU
1	D	140	GLU
1	D	151	GLU
1	D	169	VAL
1	D	180	VAL
1	D	208	CYS
1	D	268	GLU
1	D	303	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	HIS
1	B	94	ASN
1	B	275	GLN
1	B	302	GLN
1	B	306	HIS
1	C	198	HIS
1	C	248	GLN
1	D	209	GLN
1	D	306	HIS

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 oligosaccharides 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 [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	210/223 (94%)	0.10	5 (2%) 59 56	24, 36, 53, 62	0
1	B	207/223 (92%)	0.25	1 (0%) 87 85	25, 38, 54, 63	0
1	C	214/223 (95%)	0.13	2 (0%) 81 79	21, 37, 54, 63	0
1	D	208/223 (93%)	0.28	6 (2%) 53 50	22, 40, 56, 68	0
All	All	839/892 (94%)	0.19	14 (1%) 69 66	21, 38, 55, 68	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	306	HIS	3.7
1	D	307	LEU	3.3
1	A	117	LEU	3.3
1	C	130	SER	2.8
1	D	263	PRO	2.7
1	D	189	HIS	2.6
1	B	276	ASP	2.6
1	D	123	HIS	2.4
1	A	91	GLY	2.3
1	D	207	PHE	2.2
1	A	209	GLN	2.2
1	A	286	LEU	2.1
1	A	252	SER	2.0
1	C	181	ILE	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 oligosaccharides 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.