Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:10 PM GMT

PDB ID	:	3T22
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.272
Clashscore		15
Ramachandran outliers		0.1%
Sidechain outliers		4.7%
RSRZ outliers		6.7%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
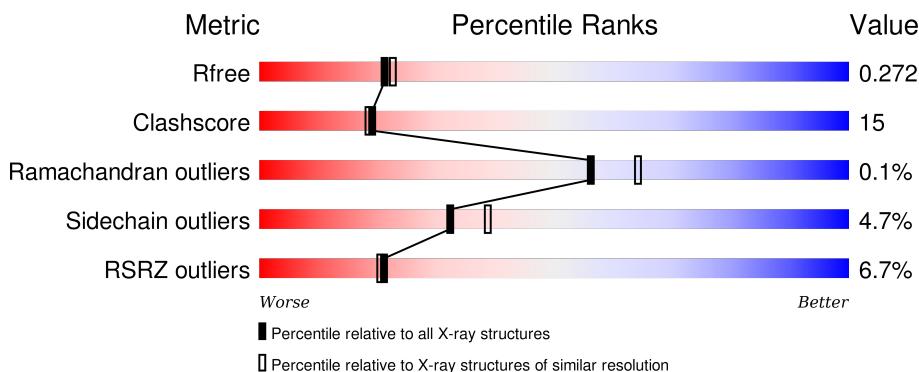
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	6% / 70% 22% • 6%
1	B	223	6% / 60% 29% • 7%
1	C	223	4% / 77% 18% • •
1	D	223	9% / 59% 32% • 7%
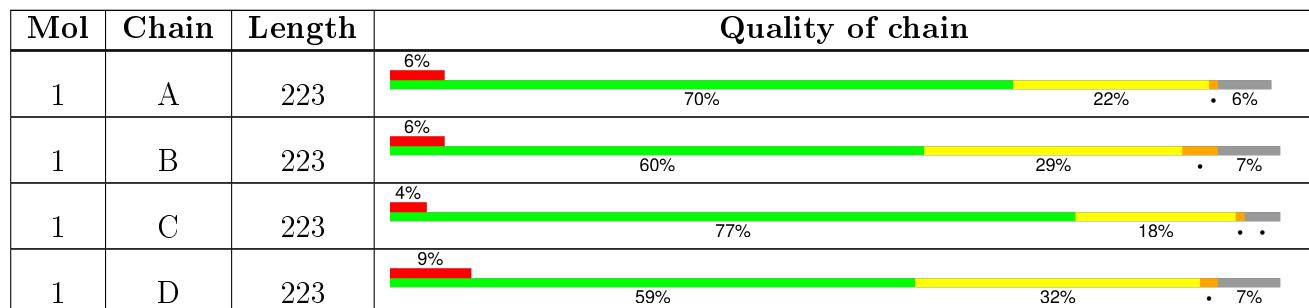
2 Entry composition (i)

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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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
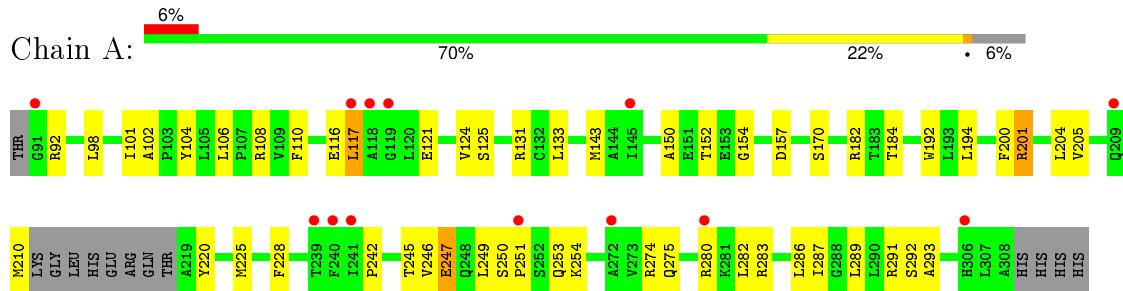
- Molecule 1: Redox-sensitive transcriptional activator OxyR

- Molecule 1: Redox-sensitive transcriptional activator OxyR

- Molecule 1: Redox-sensitive transcriptional activator OxyR

THR GLY ARG L93 N94 I95 A96 V97 L98 A102 L105 L106 F110 P111 K115 G119 L120 E121 I122 H123 V124 M127 C132 L136 I141 D142 M143 A144 I145 I146 A147 S148 K149 A150 E151 T152 E153 G154 L155 L160 E163 E164 F165 L166 G167 Y168 V169 S170 R171

C172 Q178 D179 V180 I181 R182 T183 T184 E185 V186 N187 P188 H189 R190 R201 L204 C208 Q209 M210 LYS GLY LEU HIS GLU ARG GLN T218 A219 Y220 E226 R230 G235 I238 I241 P242 Q243 L244 T245 S250 P251 K254 R258 P263 V266 R267 E268

V269 R270 L271 A272 R279 R280 E284 Q285 L286 I287 G288 L289 L290 R291 S292 T303 H306 L307 ALA HIS HIS HIS HIS
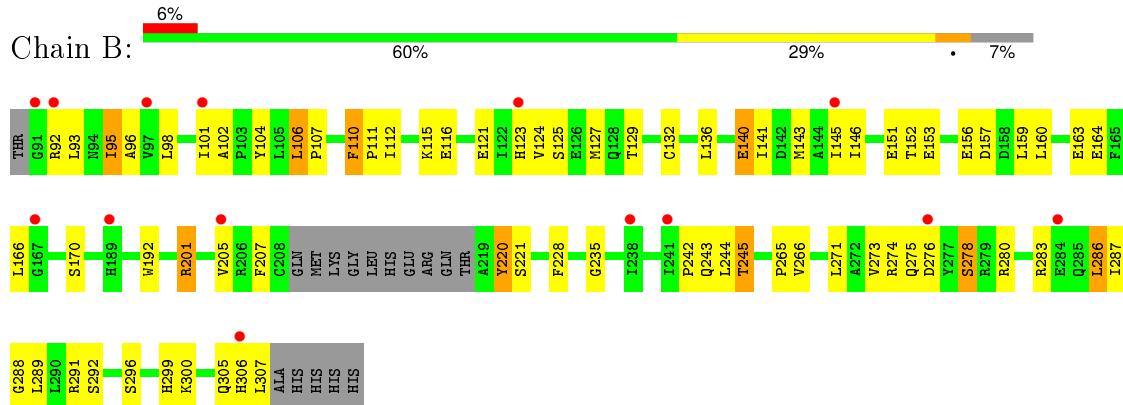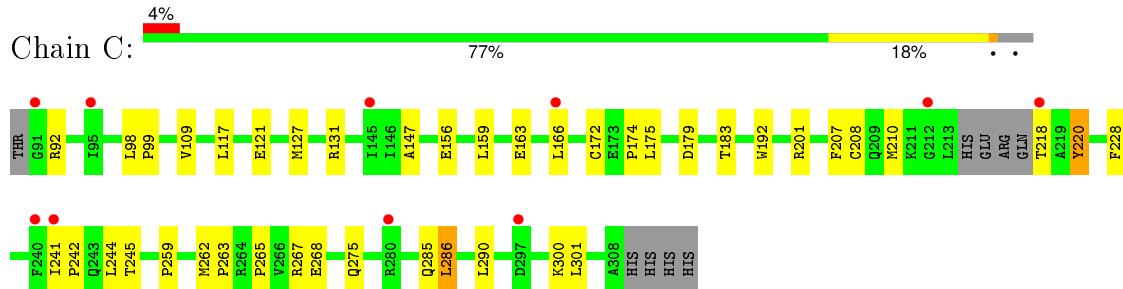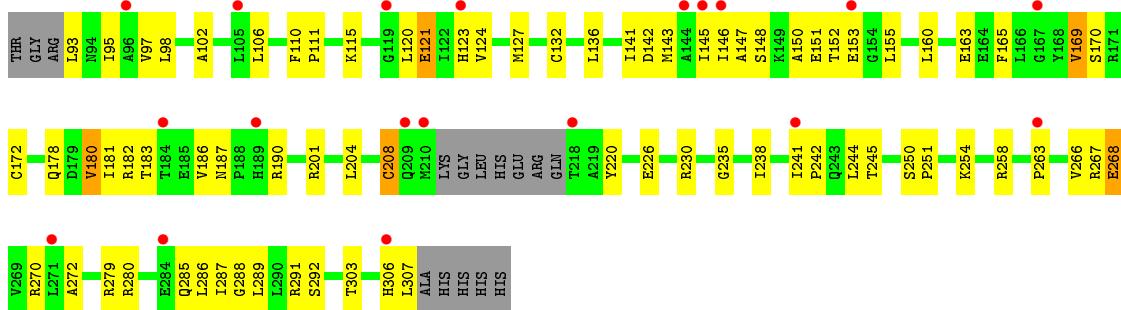
4   Data and refinement statistics (i)

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 23.24 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.6 (18.36-2.20) 76.3 (23.24-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.234 , 0.274 0.242 , 0.272	Depositor DCC
R_{free} test set	2296 reflections (5.36%)	DCC
Wilson B-factor (Å²)	36.5	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.37 , 51.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \mid L \mid > = 0.53$, $< L^2 > = 0.37$	Xtriage
Outliers	0 of 69444 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7103	wwPDB-VP
Average B, all atoms (Å²)	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.*

---

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< \mid L \mid >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.44	0/1716	0.56	0/2318
1	B	0.41	0/1694	0.57	0/2289
1	C	0.44	0/1744	0.57	0/2355
1	D	0.45	0/1703	0.59	0/2302
All	All	0.43	0/6857	0.57	0/9264

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1683	0	1703	45	0
1	B	1661	0	1681	65	0
1	C	1711	0	1737	30	0
1	D	1670	0	1689	68	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	6	0
All	All	7103	0	6810	205	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 15.

All (205) 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: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:B:93:LEU:HD21	1:B:143:MET:HE1	1.59	0.84
1:A:204:LEU:HG	1:A:210:MET:HE1	1.59	0.82
1:A:116:GLU:C	1:A:117:LEU:HD12	2.02	0.80
1:D:250:SER:CB	1:D:251:PRO:HD2	2.12	0.80
1:D:181:ILE:HD11	1:D:258:ARG:HB2	1.63	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:B:273:VAL:HG21	1:B:283:ARG:HD2	1.66	0.77
1:A:204:LEU:HG	1:A:210:MET:HE2	1.67	0.76
1:B:95:ILE:HD11	1:B:145:ILE:HG13	1.67	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
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:C:109:VAL:HG11	1:C:290:LEU:HD23	1.77	0.67
1:B:170:SER:OG	1:B:235:GLY:HA2	1.95	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: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:N	1:A:117:LEU:HD12	2.12	0.65
1:A:117:LEU:CD1	1:A:289:LEU:HD11	2.26	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

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:VAL:HB	1:D:238:ILE:HG12	1.81	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:112:ILE:HG22	1:B:289:LEU:HD13	1.84	0.59
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:D:266:VAL:HG23	1:D:307:LEU:HD12	1.85	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:268:GLU:OE1	1:D:270:ARG:NH1	2.38	0.57
1:B:163:GLU:OE2	1:B:244:LEU:HB2	2.04	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:A:205:VAL:HA	1:A:210:MET:HE3	1.87	0.56
1:D:241:ILE:HD12	1:D:245:THR:HG23	1.88	0.56
1:A:143:MET:CE	1:A:286:LEU:HD12	2.36	0.56
1:D:163:GLU:OE2	1:D:244:LEU:HB2	2.06	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:273:VAL:HG21	1:B:283:ARG:CD	2.36	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:B:153:GLU:H	1:B:153:GLU:CD	2.11	0.54
1:A:249:LEU:HD22	1:A:253:GLN:HB3	1.89	0.54
1:B:299:HIS:C	1:B:300:LYS:HG2	2.27	0.54
1:B:305:GLN:C	1:B:306:HIS:CG	2.80	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:242:PRO:HD2	1:B:245:THR:HG21	1.89	0.53
1:B:151:GLU:O	1:B:152:THR:HG23	2.08	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:VAL:CG2	1:D:307:LEU:HD12	2.40	0.52
1:D:266:VAL:HG23	1:D:307:LEU:HD11	1.91	0.52
1:A:143:MET:SD	1:A:286:LEU:CD1	2.98	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:115:LYS:HB2	1:B:115:LYS:HZ3	1.76	0.51
1:B:98:LEU:HD13	1:B:146:ILE:HA	1.91	0.51
1:C:192:TRP:HB3	1:C:228:PHE:CD1	2.46	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:B:274:ARG:NH1	2:B:320:HOH:O	2.41	0.50
1:A:250:SER:HB2	1:A:251:PRO:HD2	1.93	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:D:169:VAL:HG23	1:D:170:SER:N	2.27	0.49
1:A:133:LEU:HD13	1:A:152:THR:HG21	1.94	0.49
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:250:SER:HB2	1:A:251:PRO:CD	2.43	0.49
1:A:154:GLY:O	1:A:275:GLN:HG3	2.12	0.49
1:B:166:LEU:HD12	1:B:243:GLN:HA	1.95	0.49
1:A:106:LEU:O	1:A:110:PHE:HD2	1.96	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: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:A:182:ARG:NH1	1:A:184:THR:OG1	2.46	0.48
1:D:250:SER:O	1:D:254:LYS:HG3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:LYS:HG2	1:C:301:LEU:N	2.27	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:D:120:LEU:HD11	2:D:381:HOH:O	2.14	0.47
1:A:131:ARG:HH22	1:C:175:LEU:CD2	2.27	0.47
1:D:181:ILE:CD1	1:D:258:ARG:HB3	2.45	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: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:HA	1:C:286:LEU:HD13	1.69	0.47
1:B:286:LEU:C	1:B:288:GLY:N	2.67	0.47
1:B:307:LEU:HD12	1:B:307:LEU:H	1.80	0.46
1:D:93:LEU:HD12	1:D:142:ASP:HB2	1.96	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:A:204:LEU:CG	1:A:210:MET:HE1	2.37	0.46
1:D:151:GLU:C	1:D:152:THR:HG23	2.37	0.46
1:D:102:ALA:O	1:D:106:LEU:HB2	2.16	0.45
1:B:283:ARG:O	1:B:287:ILE:HG13	2.16	0.45
1:A:192:TRP:HB3	1:A:228:PHE:CD1	2.51	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: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:B:151:GLU:O	1:B:152:THR:CG2	2.65	0.44
1:A:280:ARG:NH1	2:A:390:HOH:O	2.49	0.44
1:B:296:SER:CB	2:B:354:HOH:O	2.61	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:C:117:LEU:CD1	1:C:285:GLN:NE2	2.81	0.44
1:B:305:GLN:O	1:B:306:HIS:CG	2.70	0.44
1:D:172:CYS:SG	2:D:321:HOH:O	2.62	0.44
1:A:200:PHE:HA	2:A:5:HOH:O	2.17	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LEU:HD23	1:B:141:ILE:HG13	1.99	0.44
1:D:289:LEU:O	1:D:292:SER:HB3	2.19	0.43
1:D:204:LEU:O	1:D:208:CYS:HB2	2.17	0.43
1:A:92:ARG:HB2	1:A:121:GLU:O	2.18	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:152:THR:O	1:D:153:GLU:C	2.57	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:D:95:ILE:HA	1:D:143:MET:O	2.19	0.42
1:B:157:ASP:HA	1:B:271:LEU:O	2.18	0.42
1:D:146:ILE:HD11	1:D:272:ALA:HB2	2.00	0.42
1:B:220:TYR:C	1:B:220:TYR:HD1	2.22	0.42
1:D:286:LEU:HD23	1:D:286:LEU:HA	1.77	0.42
1:C:98:LEU:HA	1:C:99:PRO:HD3	1.92	0.42
1:D:268:GLU:HG2	1:D:307:LEU:CD2	2.40	0.42
1:D:178:GLN:HG3	1:D:182:ARG:HD2	2.02	0.42
1:B:96:ALA:HA	1:B:125:SER:O	2.19	0.42
1:B:220:TYR:C	1:B:220:TYR:CD1	2.92	0.42
1:C:159:LEU:CD1	1:C:268:GLU:HB2	2.49	0.42
1:D:151:GLU:C	1:D:152:THR:CG2	2.88	0.42
1:D:178:GLN:OE1	1:D:178:GLN:HA	2.20	0.42
1:B:207:PHE:CD2	1:B:207:PHE:C	2.93	0.42
1:B:136:LEU:HA	1:B:136:LEU:HD23	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:B:106:LEU:N	1:B:107:PRO:CD	2.83	0.41
1:A:154:GLY:C	1:A:275:GLN:HG3	2.40	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:D:285:GLN:C	1:D:288:GLY:H	2.24	0.41
1:D:279:ARG:NE	2:D:341:HOH:O	2.54	0.41
1:C:156:GLU:OE2	1:C:275:GLN:HG2	2.21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:HIS:HD2	1:B:124:VAL:N	2.20	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	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%)	34	35
All	All	823/892 (92%)	781 (95%)	41 (5%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	280	ARG

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	185/197 (94%)	177 (96%)	8 (4%)	35	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	183/197 (93%)	170 (93%)	13 (7%)	18	19
1	C	188/197 (95%)	184 (98%)	4 (2%)	61	74
1	D	185/197 (94%)	175 (95%)	10 (5%)	27	31
All	All	741/788 (94%)	706 (95%)	35 (5%)	32	39

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	125	SER
1	A	157	ASP
1	A	170	SER
1	A	201	ARG
1	A	220	TYR
1	A	247	GLU
1	A	292	SER
1	B	95	ILE
1	B	106	LEU
1	B	110	PHE
1	B	127	MET
1	B	140	GLU
1	B	201	ARG
1	B	220	TYR
1	B	221	SER
1	B	245	THR
1	B	276	ASP
1	B	278	SER
1	B	286	LEU
1	B	292	SER
1	C	179	ASP
1	C	201	ARG
1	C	220	TYR
1	C	286	LEU
1	D	98	LEU
1	D	121	GLU
1	D	123	HIS
1	D	169	VAL
1	D	180	VAL
1	D	201	ARG
1	D	208	CYS
1	D	220	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	268	GLU
1	D	303	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	94	ASN
1	B	275	GLN
1	B	302	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 carbohydrates 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	13 (6%)	24	23	24, 36, 53, 62	0
1	B	207/223 (92%)	0.27	14 (6%)	20	20	25, 38, 54, 63	0
1	C	214/223 (95%)	0.05	10 (4%)	35	34	21, 37, 54, 63	0
1	D	208/223 (93%)	0.30	19 (9%)	11	11	22, 40, 56, 68	0
All	All	839/892 (94%)	0.18	56 (6%)	21	20	21, 38, 55, 68	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	145	ILE	4.1
1	A	209	GLN	3.8
1	B	145	ILE	3.7
1	D	123	HIS	3.7
1	D	306	HIS	3.7
1	D	184	THR	3.4
1	B	205	VAL	3.4
1	C	145	ILE	3.3
1	C	240	PHE	3.3
1	C	241	ILE	3.3
1	C	166	LEU	3.3
1	B	91	GLY	3.0
1	B	101	ILE	2.7
1	A	119	GLY	2.7
1	A	306	HIS	2.7
1	A	91	GLY	2.6
1	D	189	HIS	2.6
1	D	271	LEU	2.6
1	D	263	PRO	2.6
1	C	218	THR	2.6
1	B	167	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	280	ARG	2.5
1	D	241	ILE	2.5
1	B	123	HIS	2.5
1	A	117	LEU	2.5
1	A	239	THR	2.5
1	B	276	ASP	2.5
1	B	189	HIS	2.5
1	B	306	HIS	2.5
1	C	280	ARG	2.5
1	B	241	ILE	2.4
1	A	240	PHE	2.4
1	A	118	ALA	2.4
1	D	144	ALA	2.4
1	D	284	GLU	2.4
1	C	95	ILE	2.3
1	D	218	THR	2.3
1	A	241	ILE	2.3
1	C	297	ASP	2.3
1	D	119	GLY	2.3
1	D	210	MET	2.2
1	A	272	ALA	2.2
1	D	153	GLU	2.2
1	B	238	ILE	2.1
1	D	146	ILE	2.1
1	B	97	VAL	2.1
1	A	145	ILE	2.1
1	B	92	ARG	2.1
1	C	212	GLY	2.1
1	A	251	PRO	2.1
1	D	209	GLN	2.1
1	D	105	LEU	2.0
1	B	284	GLU	2.0
1	C	91	GLY	2.0
1	D	167	GLY	2.0
1	D	96	ALA	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 carbohydrates 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.