Full wwPDB X-ray Structure Validation Report (i)

Dec 9, 2023 – 09:45 am GMT

PDB ID	:	1UT8
Title	:	Divalent metal ions (zinc) bound to T5 5'-exonuclease
Authors	:	Ceska, T.A.; Sayers, J.R.; Suck, D.
Deposited on	:	2003-12-04
Resolution	:	2.75 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 (i) 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 (i)) were used in the production of this report:

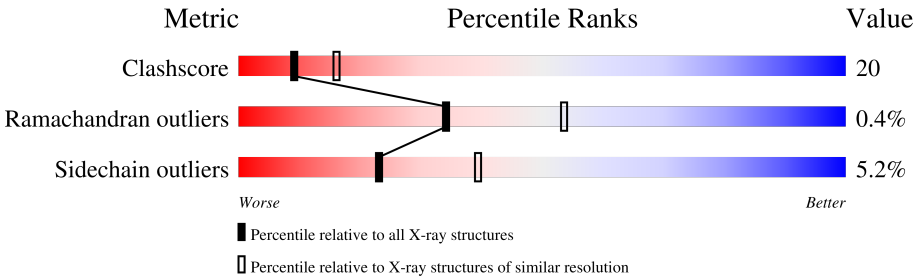
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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))
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	291	55% 37% • 7%
1	B	291	51% 39% • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4624 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 EXODEOXYRIBONUCLEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	1
			2195	1399	372	418	6			
1	B	272	Total	C	N	O	S	0	0	0
			2204	1404	373	421	6			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

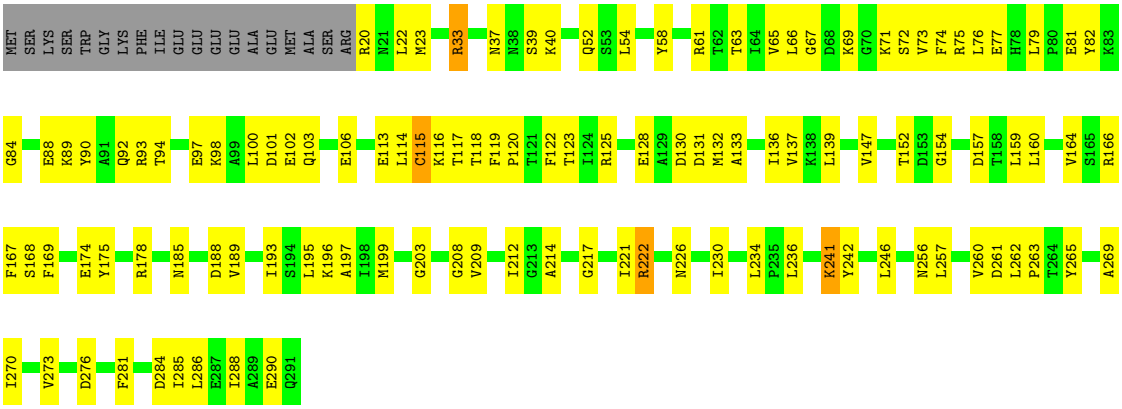
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total	O	0	0
			112	112		
3	B	111	Total	O	0	0
			111	111		

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. 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. 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.

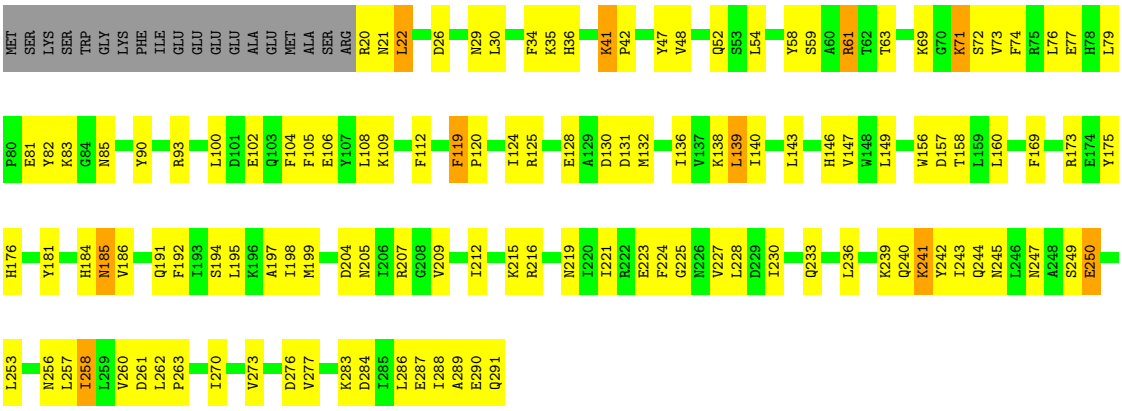
• Molecule 1: EXODEOXYRIBONUCLEASE

Chain A:



• Molecule 1: EXODEOXYRIBONUCLEASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	77.94Å 77.94Å 134.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.75 42.65 – 2.54	Depositor EDS
% Data completeness (in resolution range)	84.5 (25.00-2.75) 77.4 (42.65-2.54)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.54Å)	Xtriage
Refinement program	CNX 2000	Depositor
R, R_{free}	0.235 , 0.313 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 17.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.417 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4624	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN

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	0.46	0/2238	0.60	0/3022
1	B	0.44	0/2247	0.62	0/3032
All	All	0.45	0/4485	0.61	0/6054

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

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	2195	0	2167	88	0
1	B	2204	0	2175	90	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	112	0	0	7	0
3	B	111	0	0	8	0
All	All	4624	0	4342	175	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 20.

All (175) 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:A:20:ARG:HB3	1:A:61:ARG:HB2	1.47	0.96
1:B:242:TYR:HA	1:B:245:ASN:HD22	1.42	0.83
1:A:196:LYS:HA	1:A:196:LYS:HE2	1.62	0.80
1:B:157:ASP:HA	1:B:160:LEU:HG	1.71	0.70
1:A:52:GLN:HE21	1:A:118:THR:HG21	1.54	0.70
1:B:194:SER:HB3	1:B:227:VAL:HG23	1.74	0.68
1:A:94:THR:HG22	1:B:185:ASN:HB2	1.75	0.68
1:A:39:SER:HB3	1:A:100:LEU:HD11	1.76	0.67
1:A:286:LEU:O	1:A:290:GLU:HG2	1.95	0.66
1:A:92:GLN:HB3	1:B:199:MET:CE	2.26	0.65
1:B:106:GLU:HG3	3:B:2045:HOH:O	1.95	0.65
1:B:100:LEU:HD22	3:B:2010:HOH:O	1.96	0.65
1:A:90:TYR:HA	1:A:93:ARG:HG3	1.81	0.63
1:B:22:LEU:HD23	1:B:147:VAL:HG13	1.78	0.63
1:A:199:MET:O	1:A:208:GLY:HA3	1.99	0.63
1:B:233:GLN:HG3	1:B:236:LEU:HD21	1.80	0.63
1:B:284:ASP:O	1:B:287:GLU:HG2	1.99	0.62
1:A:52:GLN:NE2	1:A:118:THR:HG21	2.15	0.61
1:A:270:ILE:O	1:A:273:VAL:HG22	2.01	0.61
1:A:193:ILE:HG23	1:A:260:VAL:HG23	1.83	0.60
1:A:66:LEU:HD23	1:A:122:PHE:HB2	1.84	0.60
1:B:29:ASN:HA	3:B:2003:HOH:O	2.03	0.59
1:A:257:LEU:O	1:A:261:ASP:HB2	2.03	0.59
1:A:128:GLU:HB2	1:A:131:ASP:OD2	2.03	0.59
1:A:67:GLY:HA2	3:A:2020:HOH:O	2.03	0.58
1:A:147:VAL:HB	1:A:164:VAL:HG22	1.85	0.58
1:B:105:PHE:O	1:B:109:LYS:HG3	2.03	0.58
1:B:20:ARG:N	1:B:61:ARG:HB2	2.19	0.58
1:B:140:ILE:HD12	1:B:289:ALA:HB2	1.86	0.57
1:B:30:LEU:HD23	1:B:47:TYR:CE1	2.39	0.57
1:A:195:LEU:HG	1:A:199:MET:HE3	1.85	0.57
1:B:149:LEU:HD13	1:B:156:TRP:CE3	2.39	0.57
1:B:250:GLU:HB2	3:B:2099:HOH:O	2.04	0.57
1:B:69:LYS:O	1:B:125:ARG:HA	2.06	0.56
1:A:75:ARG:HG2	1:A:75:ARG:HH11	1.69	0.56
1:B:284:ASP:O	1:B:288:ILE:HG13	2.05	0.56
1:B:158:THR:HG22	1:B:192:PHE:CD2	2.41	0.55
1:A:174:GLU:HG2	3:A:2069:HOH:O	2.06	0.55
1:B:71:LYS:HE3	1:B:76:LEU:HD12	1.88	0.55
1:B:244:GLN:HA	1:B:247:ASN:HD22	1.71	0.55
1:A:284:ASP:O	1:A:288:ILE:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ARG:CB	1:A:61:ARG:HB2	2.29	0.55
1:B:149:LEU:HD13	1:B:156:TRP:HE3	1.72	0.55
1:A:133:ALA:O	1:A:137:VAL:HG23	2.07	0.55
1:A:197:ALA:HA	1:A:256:ASN:HB3	1.89	0.55
1:A:84:GLY:O	1:A:88:GLU:HG2	2.07	0.55
1:B:125:ARG:NH1	3:B:2053:HOH:O	2.40	0.54
1:A:281:PHE:O	1:A:285:ILE:HG13	2.07	0.54
1:B:249:SER:O	1:B:253:LEU:HG	2.08	0.53
1:B:194:SER:CB	1:B:227:VAL:HG23	2.36	0.53
1:A:189:VAL:O	1:A:193:ILE:HG13	2.08	0.53
1:B:90:TYR:HA	1:B:93:ARG:HG3	1.91	0.53
1:B:83:LYS:HE2	1:B:204:ASP:OD1	2.08	0.52
1:B:216:ARG:NH1	1:B:242:TYR:CE2	2.77	0.52
1:A:66:LEU:HD11	1:A:136:ILE:CD1	2.39	0.52
1:B:54:LEU:HD11	1:B:169:PHE:CZ	2.45	0.52
1:A:69:LYS:O	1:A:125:ARG:HA	2.09	0.52
1:B:241:LYS:HE3	1:B:241:LYS:HA	1.91	0.52
1:B:54:LEU:HD11	1:B:169:PHE:CE1	2.45	0.52
1:B:61:ARG:HH21	1:B:291:GLN:C	2.13	0.52
1:A:73:VAL:O	1:A:77:GLU:HG3	2.10	0.52
1:A:71:LYS:HB3	1:A:76:LEU:HD11	1.92	0.51
1:B:79:LEU:HD23	1:B:82:TYR:HD1	1.75	0.51
1:B:130:ASP:HB3	1:B:156:TRP:NE1	2.25	0.51
1:A:66:LEU:CD2	1:A:122:PHE:HB2	2.41	0.51
1:A:159:LEU:HD21	1:A:262:LEU:HD23	1.92	0.51
1:B:157:ASP:OD2	1:B:184:HIS:NE2	2.33	0.51
1:A:23:MET:CE	1:A:58:TYR:HB2	2.41	0.51
1:A:199:MET:CE	1:A:214:ALA:HA	2.41	0.51
1:B:52:GLN:HG2	1:B:119:PHE:HZ	1.75	0.51
1:A:199:MET:HE2	1:A:214:ALA:HA	1.92	0.51
1:B:20:ARG:HB2	1:B:59:SER:O	2.12	0.50
1:B:221:ILE:HA	1:B:225:GLY:O	2.12	0.49
1:A:106:GLU:HG3	3:A:2040:HOH:O	2.11	0.49
1:B:41:LYS:HG2	1:B:42:PRO:N	2.26	0.49
1:A:199:MET:HE1	1:A:214:ALA:HB2	1.94	0.49
1:B:197:ALA:HB3	1:B:227:VAL:HG21	1.94	0.49
1:A:154:GLY:O	1:A:157:ASP:HB2	2.13	0.49
1:A:89:LYS:O	1:A:93:ARG:HG2	2.13	0.49
1:B:48:VAL:O	1:B:52:GLN:HG3	2.12	0.49
1:A:90:TYR:HA	1:A:93:ARG:CG	2.43	0.49
1:A:93:ARG:HA	1:A:97:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLN:HG2	1:A:119:PHE:HZ	1.77	0.48
1:A:74:PHE:HB2	1:A:269:ALA:HA	1.94	0.48
1:A:81:GLU:H	1:A:81:GLU:CD	2.17	0.48
1:A:98:LYS:HD2	1:B:215:LYS:HE3	1.96	0.48
1:A:241:LYS:NZ	1:A:241:LYS:HB2	2.28	0.48
1:B:90:TYR:O	1:B:93:ARG:HG3	2.14	0.48
1:B:130:ASP:HB3	1:B:156:TRP:HE1	1.78	0.48
1:A:22:LEU:HD23	1:A:147:VAL:HG13	1.96	0.47
1:B:140:ILE:CD1	1:B:289:ALA:HB2	2.44	0.47
1:B:181:TYR:HA	1:B:186:VAL:O	2.15	0.47
1:A:54:LEU:HD11	1:A:169:PHE:HE2	1.80	0.47
1:A:98:LYS:O	1:A:102:GLU:HG2	2.15	0.47
1:A:209:VAL:HG21	1:A:246:LEU:HD12	1.95	0.47
1:B:191:GLN:HG2	1:B:221:ILE:HG21	1.97	0.47
1:B:128:GLU:O	1:B:131:ASP:HB2	2.15	0.46
1:A:33:ARG:NE	3:A:2006:HOH:O	2.40	0.46
1:B:191:GLN:HG2	1:B:221:ILE:CG2	2.44	0.46
1:A:132:MET:O	1:A:136:ILE:HG13	2.16	0.46
1:B:270:ILE:O	1:B:273:VAL:HG22	2.15	0.45
1:B:139:LEU:CD2	1:B:286:LEU:HD21	2.45	0.45
1:A:166:ARG:CG	1:A:167:PHE:N	2.79	0.45
1:B:242:TYR:HA	1:B:245:ASN:ND2	2.21	0.45
1:A:22:LEU:HD23	1:A:147:VAL:HG22	1.98	0.45
1:A:33:ARG:CZ	1:A:37:ASN:HD21	2.29	0.45
1:B:30:LEU:HG	1:B:34:PHE:HE1	1.82	0.45
1:A:52:GLN:HG2	1:A:119:PHE:CZ	2.52	0.45
1:B:209:VAL:HB	1:B:212:ILE:HD12	1.98	0.45
1:B:73:VAL:HG21	1:B:273:VAL:HG12	1.99	0.45
1:A:65:VAL:HG21	1:A:115:CYS:SG	2.57	0.44
1:A:66:LEU:HD11	1:A:136:ILE:HD12	1.97	0.44
1:A:113:GLU:O	1:A:116:LYS:HB2	2.17	0.44
1:B:52:GLN:HG2	1:B:119:PHE:CZ	2.51	0.44
1:A:157:ASP:HA	1:A:160:LEU:HG	1.99	0.44
1:B:256:ASN:O	1:B:260:VAL:HG13	2.16	0.44
1:A:226:ASN:O	1:A:230:ILE:HG13	2.18	0.44
1:A:230:ILE:O	1:A:234:LEU:HG	2.18	0.44
1:B:125:ARG:O	3:B:2051:HOH:O	2.21	0.44
1:A:139:LEU:HG	1:A:286:LEU:HD21	1.99	0.44
1:A:166:ARG:HG2	1:A:167:PHE:N	2.33	0.44
1:B:207:ARG:HH11	1:B:207:ARG:HB2	1.82	0.44
1:B:230:ILE:HG23	1:B:236:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:THR:O	1:A:120:PRO:HD2	2.18	0.43
1:A:79:LEU:HD23	1:A:82:TYR:HA	1.98	0.43
1:B:250:GLU:HA	1:B:253:LEU:HD12	1.99	0.43
1:B:283:LYS:O	1:B:287:GLU:HB3	2.18	0.43
1:B:108:LEU:HD11	1:B:112:PHE:CZ	2.53	0.43
1:A:236:LEU:HD12	1:A:246:LEU:HD23	2.01	0.43
1:B:244:GLN:HA	1:B:247:ASN:ND2	2.33	0.43
1:B:74:PHE:HE2	1:B:258:ILE:HG23	1.83	0.43
1:B:132:MET:O	1:B:136:ILE:HG13	2.19	0.43
1:B:176:HIS:HA	3:B:2066:HOH:O	2.19	0.43
1:B:239:LYS:O	1:B:239:LYS:HG2	2.18	0.43
1:B:257:LEU:O	1:B:261:ASP:HB2	2.19	0.43
1:A:72:SER:HB2	1:A:128:GLU:HG3	2.01	0.43
1:B:173:ARG:NH1	3:B:2072:HOH:O	2.52	0.42
1:B:124:ILE:HD13	1:B:277:VAL:CG1	2.49	0.42
1:B:240:GLN:O	1:B:244:GLN:HG2	2.19	0.42
1:A:136:ILE:HG12	1:A:285:ILE:HD13	2.01	0.42
1:B:26:ASP:O	1:B:29:ASN:HB3	2.19	0.42
1:B:90:TYR:HA	1:B:93:ARG:CG	2.48	0.42
1:B:160:LEU:HD13	1:B:175:TYR:O	2.20	0.42
1:A:125:ARG:NH1	1:A:125:ARG:HG3	2.35	0.42
1:B:143:LEU:HD12	1:B:289:ALA:HB1	2.02	0.42
1:A:39:SER:HB2	1:A:40:LYS:NZ	2.34	0.42
1:A:188:ASP:HB2	3:A:2080:HOH:O	2.19	0.42
1:A:212:ILE:CG1	1:A:242:TYR:HB2	2.48	0.42
1:A:130:ASP:O	1:A:262:LEU:HD11	2.20	0.42
1:B:74:PHE:CE2	1:B:258:ILE:HG23	2.54	0.42
1:A:261:ASP:HB3	1:A:265:TYR:CD2	2.55	0.42
1:A:152:THR:HA	1:A:168:SER:OG	2.20	0.42
1:B:21:ASN:HB3	1:B:146:HIS:O	2.20	0.42
1:B:195:LEU:O	1:B:199:MET:HB3	2.20	0.42
1:A:130:ASP:HB2	1:A:262:LEU:CD2	2.50	0.41
1:B:158:THR:HG22	1:B:192:PHE:HD2	1.85	0.41
1:B:198:ILE:HD11	1:B:230:ILE:HD12	2.02	0.41
1:B:81:GLU:HB2	1:B:205:ASN:ND2	2.35	0.41
1:B:262:LEU:N	1:B:263:PRO:HD2	2.36	0.41
1:A:114:LEU:O	1:A:117:THR:HG23	2.20	0.41
1:A:90:TYR:O	1:A:93:ARG:HG3	2.21	0.41
1:A:222:ARG:NH1	3:A:2092:HOH:O	2.47	0.41
1:A:39:SER:O	1:A:103:GLN:NE2	2.53	0.41
1:A:175:TYR:CD1	1:A:175:TYR:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:H	1:A:178:ARG:HG2	1.68	0.41
1:A:262:LEU:N	1:A:263:PRO:HD2	2.36	0.41
1:A:203:GLY:HA3	3:A:2031:HOH:O	2.21	0.40
1:B:35:LYS:HD2	1:B:104:PHE:CG	2.57	0.40
1:B:58:TYR:O	1:B:59:SER:C	2.60	0.40
1:B:223:GLU:HG2	1:B:224:PHE:CE1	2.56	0.40
1:B:241:LYS:HE3	1:B:241:LYS:CA	2.49	0.40
1:A:93:ARG:HD3	1:A:101:ASP:OD1	2.20	0.40
1:A:217:GLY:O	1:A:221:ILE:HG13	2.22	0.40
1:B:63:THR:O	1:B:120:PRO:HD2	2.22	0.40
1:B:102:GLU:O	1:B:106:GLU:HG2	2.21	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	270/291 (93%)	252 (93%)	18 (7%)	0	100	100
1	B	270/291 (93%)	251 (93%)	17 (6%)	2 (1%)	22	39
All	All	540/582 (93%)	503 (93%)	35 (6%)	2 (0%)	34	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	71	LYS
1	B	72	SER

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	238/255 (93%)	231 (97%)	7 (3%)	42 62
1	B	239/255 (94%)	221 (92%)	18 (8%)	13 23
All	All	477/510 (94%)	452 (95%)	25 (5%)	23 39

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	115	CYS
1	A	123	THR
1	A	185	ASN
1	A	222	ARG
1	A	241	LYS
1	A	276	ASP
1	B	22	LEU
1	B	36	HIS
1	B	41	LYS
1	B	61	ARG
1	B	77	GLU
1	B	85	ASN
1	B	119	PHE
1	B	138	LYS
1	B	139	LEU
1	B	185	ASN
1	B	219	ASN
1	B	228	LEU
1	B	241	LYS
1	B	243	ILE
1	B	250	GLU
1	B	258	ILE
1	B	276	ASP
1	B	290	GLU

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	52	GLN
1	A	103	GLN
1	A	226	ASN
1	A	275	GLN
1	B	78	HIS
1	B	185	ASN
1	B	244	GLN
1	B	245	ASN
1	B	247	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are 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

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.