Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 09:15 am GMT

PDB ID	:	2YAR
Title	:	X-ray induced reduction of laccase from Thermus thermophilus HB27 (87. 5-100.0 percent dose)
Authors	:	Serrano-Posada, H.; Rudino-Pinera, E.
Deposited on	:	2011-02-24
Resolution	:	1.80 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:

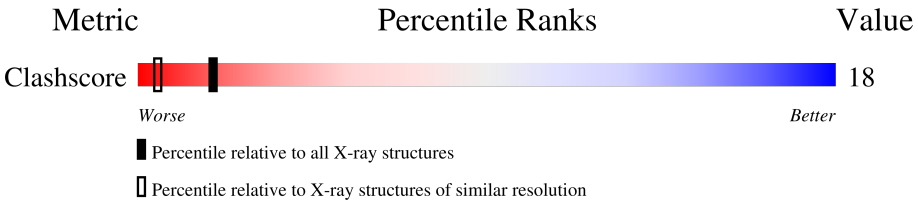
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 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	6793 (1.80-1.80)

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MPD	A	1473	-	-	X	-
3	MPD	A	1474	-	-	X	-
3	MPD	A	1477	-	-	X	-
4	MRD	A	1479	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4380 atoms, of which 1 is hydrogen 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 LACCASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	439	3762	2416	677	653	16	0	38	0

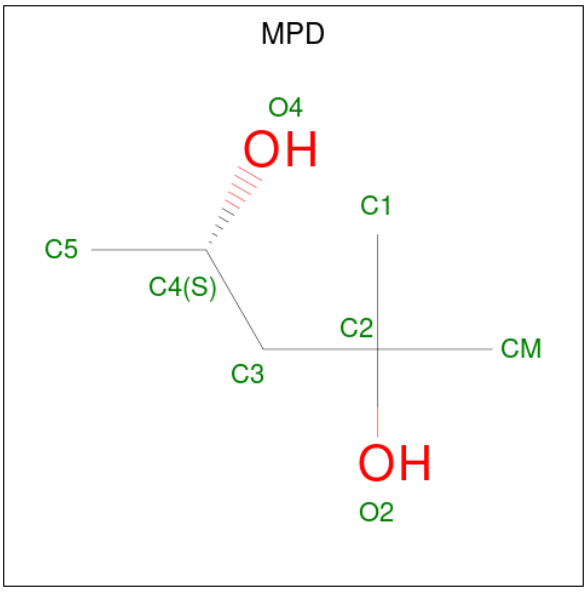
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	LEU	SEE REMARK 999	UNP Q72HW2

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

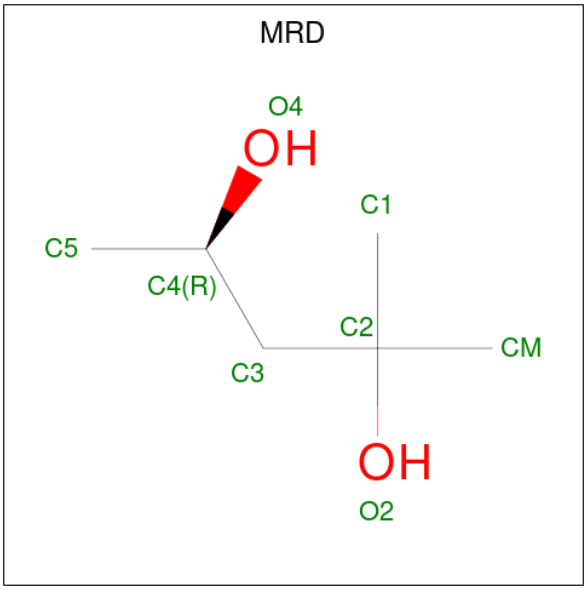
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
2	A	3	3	3	0	0

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



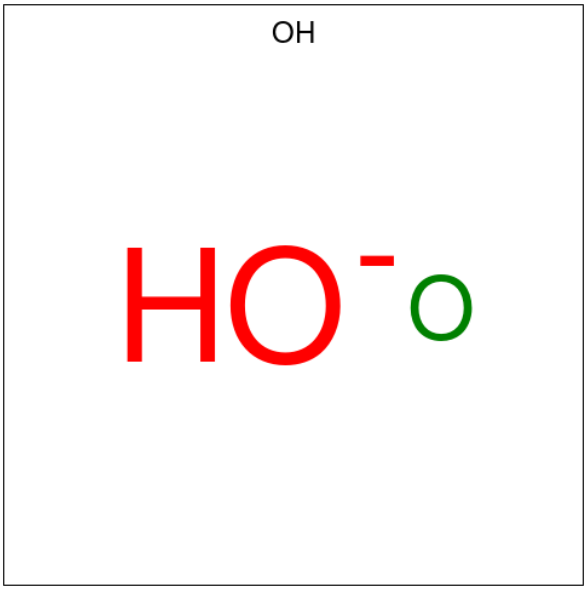
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0

- Molecule 5 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total H O 2 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	501	Total O 501 501	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	93.71Å 110.39Å 96.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.70 – 1.80	Depositor
% Data completeness (in resolution range)	97.3 (28.70-1.80)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 1.79Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.150 , 0.183	Depositor
Wilson B-factor (Å^2)	11.3	Xtriage
Anisotropy	0.036	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4380	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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.

4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, OH, MPD, CU

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	0.43	1/3862 (0.0%)	0.58	1/5256 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	MET	CA-CB	-10.13	1.31	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	301	MET	N-CA-CB	-6.15	99.54	110.60

There are no chirality outliers.

There are no planarity outliers.

4.2 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	3762	0	3829	120	0
2	A	3	0	0	0	0
3	A	64	0	112	30	0
4	A	48	0	83	21	0
5	A	1	1	0	1	0
6	A	501	0	0	33	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4379	1	4024	146	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (146) 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)
3:A:1477:MPD:H52	3:A:1477:MPD:H11	1.11	1.10
3:A:1477:MPD:H11	3:A:1477:MPD:C5	1.88	1.03
1:A:189:HIS:HB2	4:A:1479:MRD:HMC1	1.43	0.98
3:A:1477:MPD:H52	3:A:1477:MPD:C1	1.95	0.96
1:A:189:HIS:H	4:A:1479:MRD:HMC3	1.32	0.95
1:A:338:THR:O	6:A:2384:HOH:O	1.85	0.94
1:A:67:PHE:HZ	1:A:177[A]:LYS:HD2	1.31	0.93
1:A:111:GLU:HG2	1:A:138:LEU:HD11	1.51	0.92
1:A:345:THR:OG1	3:A:1474:MPD:HM3	1.69	0.90
1:A:331:LYS:HD2	6:A:2375:HOH:O	1.71	0.90
1:A:430[B]:ARG:NH2	6:A:2471:HOH:O	2.06	0.89
1:A:311:ARG:HH11	1:A:311:ARG:HG3	1.41	0.85
1:A:325:LYS:HE2	6:A:2365:HOH:O	1.76	0.85
1:A:189:HIS:H	4:A:1479:MRD:CM	1.90	0.84
1:A:423:LEU:HD21	1:A:429:ALA:HB2	1.61	0.83
1:A:296:MET:HG2	1:A:305[A]:MET:HG3	1.60	0.82
1:A:26[B]:SER:HB2	6:A:2264:HOH:O	1.78	0.82
1:A:43[B]:LYS:HE2	1:A:85:GLU:HB2	1.62	0.80
1:A:257[A]:GLU:OE1	3:A:1473:MPD:H13	1.82	0.80
1:A:311:ARG:HH11	1:A:311:ARG:CG	1.95	0.79
3:A:1477:MPD:HM2	3:A:1477:MPD:H53	1.65	0.79
1:A:189:HIS:N	4:A:1479:MRD:HMC3	1.98	0.78
1:A:67:PHE:CZ	1:A:177[A]:LYS:HD2	2.19	0.77
1:A:26[A]:SER:HB3	6:A:2264:HOH:O	1.84	0.77
1:A:343:VAL:HG23	1:A:344[B]:VAL:HG13	1.69	0.75
3:A:1474:MPD:H12	3:A:1474:MPD:H52	1.69	0.75
1:A:298:MET:HB2	1:A:301:MET:HG3	1.68	0.74
1:A:296:MET:HG2	1:A:305[A]:MET:CG	2.18	0.74
1:A:311:ARG:HG3	1:A:311:ARG:NH1	2.02	0.74
1:A:296:MET:HG2	1:A:305[B]:MET:HG3	1.70	0.73
1:A:298:MET:H	1:A:301:MET:HB2	1.54	0.73
1:A:278:GLU:OE2	1:A:322:LYS:HG3	1.91	0.70
1:A:399[B]:VAL:HG23	1:A:400:HIS:CD2	2.26	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLU:HG2	1:A:138:LEU:CD1	2.22	0.70
1:A:338:THR:HG23	6:A:2383:HOH:O	1.91	0.69
1:A:301:MET:SD	1:A:303:HIS:CE1	2.87	0.68
3:A:1473:MPD:HM3	4:A:1478:MRD:CM	2.26	0.66
1:A:293[A]:MET:HE3	6:A:2403:HOH:O	1.95	0.65
4:A:1479:MRD:H5C3	6:A:2119:HOH:O	1.96	0.65
1:A:301:MET:O	1:A:302:ALA:HB3	1.96	0.65
1:A:137[A]:HIS:HD2	6:A:2486:HOH:O	1.78	0.65
1:A:296:MET:CG	1:A:305[A]:MET:HG3	2.27	0.64
3:A:1473:MPD:H52	3:A:1473:MPD:C1	2.28	0.64
4:A:1469:MRD:H5C1	6:A:2490:HOH:O	1.98	0.63
1:A:53[B]:ILE:CD1	1:A:179:LEU:HD23	2.29	0.62
3:A:1473:MPD:HM3	4:A:1478:MRD:HMC3	1.81	0.62
1:A:43[A]:LYS:HD2	1:A:83:THR:HB	1.81	0.62
1:A:278:GLU:HG2	1:A:322:LYS:HA	1.81	0.62
1:A:53[B]:ILE:HD11	1:A:179:LEU:HD23	1.83	0.60
3:A:1476:MPD:C5	3:A:1476:MPD:O2	2.48	0.60
1:A:331:LYS:HD2	1:A:331:LYS:H	1.66	0.60
1:A:405:LEU:HD11	1:A:432[A]:LEU:HG	1.84	0.60
1:A:189:HIS:HB2	4:A:1479:MRD:CM	2.27	0.59
1:A:90:GLU:HB2	1:A:91:PRO:HD2	1.83	0.59
1:A:296:MET:CG	1:A:305[B]:MET:HG3	2.32	0.58
1:A:56[A]:GLN:NE2	6:A:2061:HOH:O	2.37	0.58
3:A:1476:MPD:O2	3:A:1476:MPD:H52	2.04	0.58
1:A:331:LYS:HD2	1:A:331:LYS:N	2.20	0.56
1:A:423:LEU:HD21	1:A:429:ALA:CB	2.33	0.56
1:A:144:PRO:HG3	4:A:1479:MRD:H4	1.87	0.56
3:A:1477:MPD:C5	3:A:1477:MPD:C1	2.61	0.56
1:A:189:HIS:CB	4:A:1479:MRD:HMC1	2.26	0.56
1:A:27:PHE:HZ	1:A:174[A]:LEU:CD2	2.18	0.55
3:A:1473:MPD:H52	3:A:1473:MPD:H11	1.86	0.55
1:A:257[A]:GLU:CD	3:A:1473:MPD:H13	2.26	0.55
1:A:84:LEU:HD22	1:A:94:LEU:HG	1.89	0.55
4:A:1479:MRD:HMC3	6:A:2238:HOH:O	2.07	0.55
4:A:1478:MRD:O2	4:A:1478:MRD:H5C3	2.07	0.54
1:A:338:THR:CB	6:A:2383:HOH:O	2.55	0.54
1:A:263[B]:LEU:HD23	3:A:1466:MPD:CM	2.38	0.54
1:A:223[A]:ARG:NH2	6:A:2273:HOH:O	2.32	0.53
1:A:43[A]:LYS:CD	1:A:83:THR:HB	2.38	0.53
1:A:144:PRO:CG	4:A:1479:MRD:H4	2.38	0.52
1:A:111:GLU:CG	1:A:138:LEU:HD11	2.32	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:MET:O	1:A:302:ALA:CB	2.57	0.52
1:A:151[B]:LEU:HD22	1:A:151[B]:LEU:C	2.31	0.51
1:A:257[B]:GLU:O	1:A:257[B]:GLU:HG3	2.10	0.51
1:A:423:LEU:CD2	1:A:429:ALA:HB2	2.38	0.50
1:A:91:PRO:HB2	1:A:138:LEU:HD21	1.93	0.50
1:A:424[A]:LYS:HE2	6:A:2465:HOH:O	2.11	0.50
1:A:177[A]:LYS:HD3	1:A:178:ASP:O	2.12	0.50
1:A:339:LEU:HD12	1:A:432[B]:LEU:HD23	1.92	0.50
1:A:430[C]:ARG:NH1	6:A:2470:HOH:O	2.43	0.50
1:A:189:HIS:ND1	4:A:1479:MRD:CM	2.75	0.50
1:A:311:ARG:HH11	1:A:311:ARG:CB	2.24	0.50
1:A:72:LEU:HB2	1:A:154[B]:LEU:HD13	1.93	0.50
1:A:96:TRP:HB3	1:A:99[A]:LEU:HD12	1.92	0.50
1:A:424[B]:LYS:HE3	6:A:2464:HOH:O	2.11	0.49
1:A:27:PHE:CZ	1:A:174[A]:LEU:CD2	2.94	0.49
1:A:296:MET:SD	1:A:305[B]:MET:HG3	2.53	0.49
1:A:130:GLY:HA2	6:A:2312:HOH:O	2.11	0.49
3:A:1473:MPD:HM1	4:A:1478:MRD:H1C3	1.95	0.49
1:A:223[B]:ARG:NH1	1:A:270:GLU:OE2	2.45	0.49
1:A:296:MET:SD	1:A:305[A]:MET:HG3	2.53	0.48
1:A:311:ARG:CG	1:A:311:ARG:NH1	2.63	0.48
1:A:278:GLU:CG	1:A:322:LYS:HA	2.43	0.48
1:A:344[B]:VAL:HG22	1:A:381:GLU:HG2	1.95	0.48
1:A:364:GLN:HG3	3:A:1475:MPD:H13	1.96	0.48
1:A:263[A]:LEU:HD12	3:A:1466:MPD:CM	2.43	0.48
1:A:213:LEU:HB3	1:A:318[B]:LEU:HD22	1.96	0.48
1:A:348[B]:LEU:HD12	1:A:348[B]:LEU:N	2.29	0.47
1:A:278:GLU:CD	1:A:322:LYS:HG3	2.35	0.47
1:A:338:THR:OG1	6:A:2383:HOH:O	2.20	0.47
3:A:1473:MPD:HM3	4:A:1478:MRD:HMC2	1.97	0.47
1:A:345:THR:OG1	3:A:1474:MPD:CM	2.54	0.47
1:A:28:PRO:HB3	3:A:1477:MPD:H51	1.98	0.46
4:A:1471:MRD:H1C3	4:A:1471:MRD:H4	1.66	0.46
3:A:1474:MPD:H52	3:A:1474:MPD:C1	2.43	0.46
1:A:221[B]:ARG:HD3	6:A:2272:HOH:O	2.15	0.46
1:A:298:MET:H	1:A:301:MET:CB	2.26	0.46
1:A:398:HIS:O	1:A:399[B]:VAL:HG22	2.16	0.45
3:A:1477:MPD:C5	3:A:1477:MPD:HM2	2.43	0.45
1:A:311:ARG:HH11	1:A:311:ARG:HB2	1.82	0.45
1:A:129:ALA:HB2	4:A:1472:MRD:H1C2	1.98	0.45
1:A:95:HIS:CD2	5:A:1480:OH:O	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:THR:HG1	3:A:1474:MPD:HM3	1.79	0.45
3:A:1473:MPD:H12	6:A:2299:HOH:O	2.18	0.44
1:A:189:HIS:CB	4:A:1479:MRD:CM	2.93	0.44
1:A:91:PRO:HB2	1:A:138:LEU:CD2	2.48	0.44
1:A:438:LYS:HG3	6:A:2482:HOH:O	2.18	0.44
1:A:143:ALA:HB3	1:A:144:PRO:HD3	2.00	0.43
3:A:1474:MPD:H12	3:A:1474:MPD:C5	2.38	0.43
1:A:73:ARG:NE	1:A:157:GLU:OE2	2.42	0.43
1:A:53[B]:ILE:HD12	1:A:179:LEU:HD23	2.01	0.43
3:A:1477:MPD:H51	6:A:2004:HOH:O	2.18	0.43
1:A:384:GLU:HG2	1:A:430[D]:ARG:HG2	1.99	0.43
1:A:47[A]:THR:HG22	6:A:2075:HOH:O	2.18	0.43
1:A:72:LEU:O	1:A:154[B]:LEU:HD12	2.19	0.43
1:A:296:MET:HG2	1:A:305[B]:MET:CG	2.36	0.43
1:A:346:ARG:HD2	1:A:373:LEU:HD13	2.01	0.43
1:A:424[B]:LYS:HE3	1:A:424[B]:LYS:HB3	1.85	0.43
1:A:221[B]:ARG:CD	6:A:2272:HOH:O	2.66	0.43
1:A:398:HIS:C	1:A:399[B]:VAL:HG22	2.39	0.42
1:A:331:LYS:HE2	6:A:2374:HOH:O	2.18	0.42
1:A:349:VAL:HG11	6:A:2441:HOH:O	2.19	0.42
1:A:257[A]:GLU:CD	3:A:1473:MPD:C1	2.88	0.42
4:A:1479:MRD:CM	6:A:2238:HOH:O	2.66	0.42
1:A:338:THR:CG2	6:A:2383:HOH:O	2.55	0.41
1:A:331:LYS:HE3	6:A:2370:HOH:O	2.19	0.41
1:A:174[A]:LEU:HD12	1:A:224:LEU:CD2	2.51	0.41
1:A:382:VAL:HG22	1:A:432[A]:LEU:HD23	2.02	0.41
3:A:1470:MPD:H11	3:A:1470:MPD:H4	1.87	0.41
1:A:253:GLU:HA	1:A:334[B]:SER:O	2.21	0.41
1:A:324:PRO:O	1:A:325:LYS:HD2	2.21	0.41
1:A:223[B]:ARG:HD2	6:A:2221:HOH:O	2.20	0.40
1:A:424[A]:LYS:HD2	6:A:2327:HOH:O	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2192:HOH:O	6:A:2192:HOH:O[3_555]	1.11	1.09

4.3 Torsion angles

4.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

4.3.3 RNA

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 18 ligands modelled in this entry, 3 are monoatomic and 1 is modelled with single atom - leaving 14 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.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.