Full wwPDB X-ray Structure Validation Report (i)

Apr 27, 2016 – 10:35 AM EDT

PDB ID	:	5IR6
Title	:	The structure of bd oxidase from Geobacillus thermodenitrificans
Authors	:	Safarian, S.; Mueller, H.; Rajendran, C.; Preu, J.; Ovchinnikov, S.; Kusumoto, T.; Hirose, T.; Langer, J.; Sakamoto, J.; Michel, H.
Deposited on	:	2016-03-12
Resolution	:	3.80 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
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 (1)) were used in the production of this report:

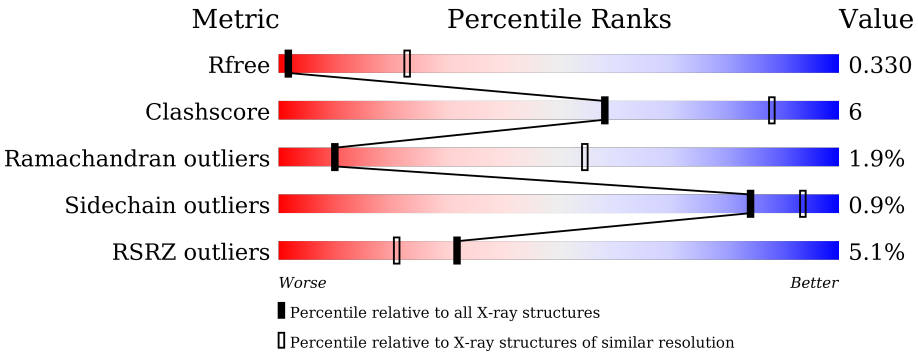
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 3.80 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))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 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	448	4% 78% 18%
2	B	342	6% 90% 6%
3	C	33	3% 88% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6471 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 Bd-type quinol oxidase subunit I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3418	2270	555	574	19			

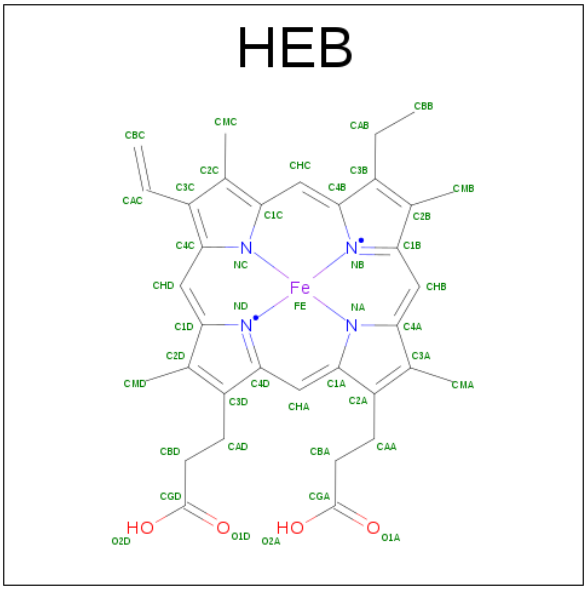
- Molecule 2 is a protein called Bd-type quinol oxidase subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	330	Total	C	N	O	S	0	0	0
			2689	1832	409	442	6			

- Molecule 3 is a protein called Putative membrane protein.

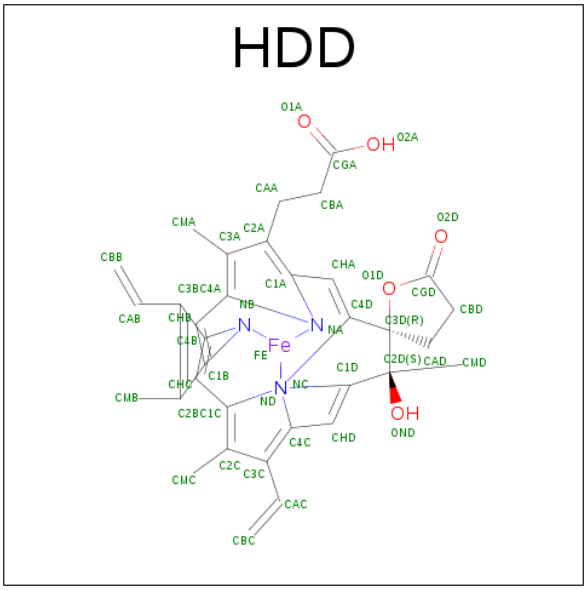
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	30	Total	C	N	O	S	0	0	0
			234	159	35	38	2			

- Molecule 4 is HEME B/C (three-letter code: HEB) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).

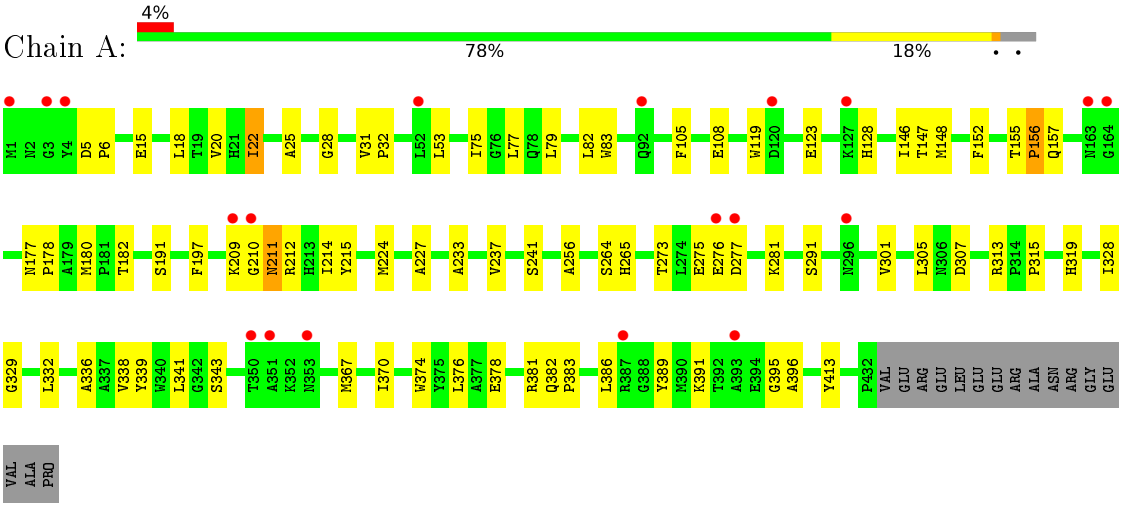


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		

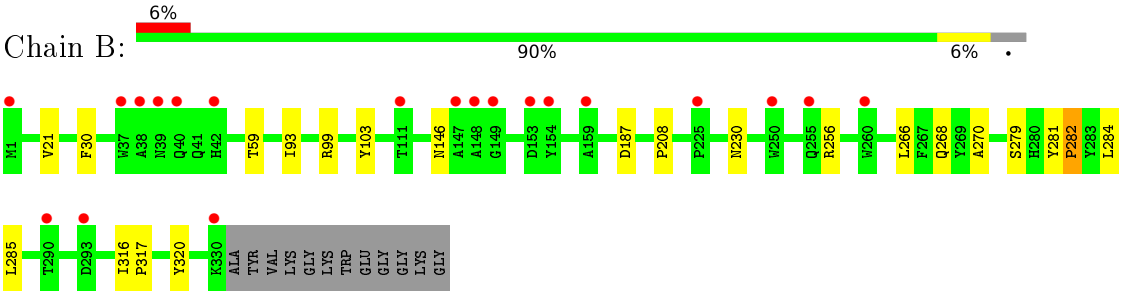
3 Residue-property plots (i)

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.

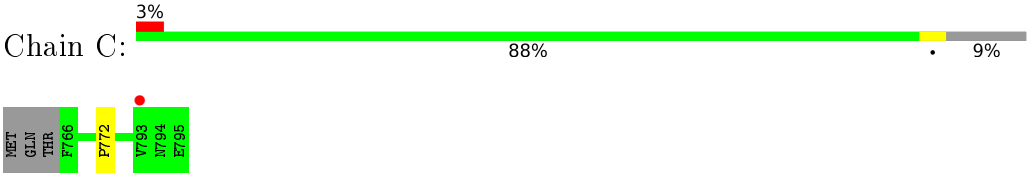
- Molecule 1: Bd-type quinol oxidase subunit I



- Molecule 2: Bd-type quinol oxidase subunit II



- Molecule 3: Putative membrane protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	110.06Å 120.86Å 122.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.80 19.92 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-3.80) 99.8 (19.92-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	6.22 (at 3.82Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.303 , 0.325 0.301 , 0.330	Depositor DCC
R_{free} test set	807 reflections (5.14%)	DCC
Wilson B-factor (Å^2)	209.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.026 for -h,l,k	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6471	wwPDB-VP
Average B, all atoms (Å^2)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: HDD, HEB

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	0.47	0/3518	0.57	0/4802
2	B	0.40	0/2781	0.50	0/3803
3	C	0.48	0/240	0.52	0/327
All	All	0.44	0/6539	0.54	0/8932

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	3418	0	3485	54	0
2	B	2689	0	2696	11	0
3	C	234	0	241	0	0
4	A	86	0	64	14	0
5	A	44	0	31	17	0
All	All	6471	0	6517	76	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 6.

All (76) 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)
4:A:501:HEB:HHD	4:A:501:HEB:HBC1	1.39	1.02
4:A:502:HEB:HBB1	5:A:503:HDD:HMA2	1.55	0.89
4:A:501:HEB:HBB2	4:A:501:HEB:HHC	1.63	0.80
1:A:147:THR:HA	5:A:503:HDD:O2A	1.95	0.66
1:A:146:ILE:HG13	5:A:503:HDD:O1A	1.98	0.64
1:A:152:PHE:O	1:A:389:TYR:OH	2.18	0.61
4:A:501:HEB:CHD	4:A:501:HEB:HBC1	2.15	0.60
2:B:99:ARG:NH2	2:B:103:TYR:OH	2.39	0.56
1:A:18:LEU:HB3	5:A:503:HDD:HAD2	1.91	0.53
4:A:501:HEB:HHD	4:A:501:HEB:CBC	2.25	0.52
1:A:386:LEU:HA	1:A:391:LYS:HA	1.92	0.51
2:B:316:ILE:HB	2:B:317:PRO:HD3	1.92	0.51
1:A:177:ASN:HB2	1:A:178:PRO:CD	2.41	0.51
1:A:182:THR:HB	1:A:241:SER:HB3	1.93	0.51
2:B:21:VAL:HG23	2:B:59:THR:HG22	1.93	0.51
1:A:374:TRP:CE2	5:A:503:HDD:O2D	2.65	0.50
1:A:275:GLU:O	1:A:277:ASP:N	2.45	0.50
1:A:5:ASP:N	1:A:6:PRO:HD2	2.27	0.50
1:A:374:TRP:CZ2	5:A:503:HDD:O2D	2.64	0.50
1:A:18:LEU:HB3	5:A:503:HDD:CAD	2.42	0.49
5:A:503:HDD:CHA	5:A:503:HDD:CBD	2.90	0.49
1:A:211:ASN:O	1:A:211:ASN:ND2	2.45	0.49
1:A:374:TRP:HA	4:A:501:HEB:HAD2	1.95	0.48
1:A:105:PHE:HA	1:A:108:GLU:HG2	1.95	0.47
1:A:382:GLN:N	1:A:383:PRO:CD	2.77	0.47
1:A:210:GLY:O	1:A:212:ARG:N	2.44	0.47
4:A:501:HEB:CHD	4:A:501:HEB:CBC	2.90	0.47
1:A:338:VAL:O	1:A:339:TYR:C	2.54	0.46
4:A:502:HEB:HMC2	5:A:503:HDD:CBD	2.45	0.46
1:A:18:LEU:HD21	1:A:75:ILE:HG12	1.97	0.46
1:A:197:PHE:CE1	1:A:227:ALA:HB1	2.51	0.46
2:B:281:TYR:HB3	2:B:282:PRO:HA	1.98	0.46
1:A:374:TRP:CZ3	4:A:501:HEB:HBD1	2.51	0.45
5:A:503:HDD:CHA	5:A:503:HDD:HBD1	2.46	0.45
2:B:317:PRO:HA	2:B:320:TYR:HB3	1.97	0.45
1:A:53:LEU:HD21	1:A:215:TYR:HB3	1.98	0.45
1:A:156:PRO:HB3	1:A:157:GLN:HA	1.99	0.45
1:A:329:GLY:CA	4:A:501:HEB:HMC2	2.47	0.45
1:A:31:VAL:N	1:A:32:PRO:HD2	2.31	0.44
4:A:501:HEB:CHC	4:A:501:HEB:HBB2	2.42	0.44
1:A:378:GLU:O	1:A:381:ARG:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:VAL:HG21	1:A:413:TYR:HB3	2.00	0.44
1:A:15:GLU:CD	5:A:503:HDD:HBC1	2.38	0.44
2:B:230:ASN:HB3	2:B:279:SER:HA	1.98	0.44
1:A:224:MET:CE	1:A:336:ALA:HA	2.48	0.44
1:A:256:ALA:O	1:A:319:HIS:ND1	2.48	0.44
1:A:367:MET:O	1:A:370:ILE:HB	2.18	0.44
1:A:18:LEU:HD13	5:A:503:HDD:HAD1	1.99	0.44
1:A:83:TRP:HA	1:A:395:GLY:O	2.18	0.43
1:A:146:ILE:CG1	5:A:503:HDD:O1A	2.66	0.43
1:A:22:ILE:HA	1:A:22:ILE:HD12	1.85	0.43
1:A:177:ASN:HB2	1:A:178:PRO:HD2	2.01	0.43
1:A:77:LEU:CB	2:B:93:ILE:HD11	2.49	0.43
1:A:273:THR:HB	1:A:281:LYS:HB2	2.00	0.43
2:B:284:LEU:O	2:B:285:LEU:HB3	2.18	0.43
1:A:148:MET:HG2	1:A:180:MET:HG3	2.01	0.42
2:B:266:LEU:O	2:B:270:ALA:CB	2.68	0.42
1:A:119:TRP:HA	1:A:128:HIS:NE2	2.34	0.42
4:A:501:HEB:HHC	4:A:501:HEB:CBB	2.42	0.42
1:A:378:GLU:OE2	5:A:503:HDD:NA	2.53	0.42
1:A:328:ILE:O	1:A:332:LEU:HB2	2.20	0.42
1:A:119:TRP:HA	1:A:128:HIS:CE1	2.54	0.42
2:B:266:LEU:O	2:B:270:ALA:HB2	2.19	0.41
4:A:501:HEB:HAC	4:A:501:HEB:HMC1	1.88	0.41
2:B:187:ASP:OD1	2:B:256:ARG:NH2	2.53	0.41
1:A:305:LEU:HD11	1:A:313:ARG:HB2	2.01	0.41
1:A:370:ILE:HG12	4:A:501:HEB:HBC2	2.02	0.41
1:A:264:SER:OG	1:A:265:HIS:N	2.53	0.41
1:A:264:SER:HA	1:A:301:VAL:HA	2.03	0.41
1:A:378:GLU:HG2	5:A:503:HDD:NC	2.35	0.41
1:A:25:ALA:O	1:A:28:GLY:N	2.54	0.41
1:A:233:ALA:O	1:A:237:VAL:HG22	2.20	0.40
1:A:82:LEU:O	1:A:396:ALA:HA	2.21	0.40
1:A:18:LEU:CB	5:A:503:HDD:HMD2	2.52	0.40
1:A:146:ILE:HG23	5:A:503:HDD:O1A	2.21	0.40
1:A:376:LEU:HD23	1:A:376:LEU:C	2.41	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	430/448 (96%)	364 (85%)	56 (13%)	10 (2%)	8 51
2	B	328/342 (96%)	290 (88%)	33 (10%)	5 (2%)	13 59
3	C	28/33 (85%)	20 (71%)	8 (29%)	0	100 100
All	All	786/823 (96%)	674 (86%)	97 (12%)	15 (2%)	10 54

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ILE
1	A	211	ASN
1	A	276	GLU
2	B	30	PHE
1	A	191	SER
1	A	209	LYS
2	B	146	ASN
1	A	79	LEU
1	A	341	LEU
1	A	156	PRO
1	A	291	SER
2	B	268	GLN
2	B	208	PRO
1	A	315	PRO
2	B	282	PRO

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	357/370 (96%)	352 (99%)	5 (1%)	74 90
2	B	276/283 (98%)	276 (100%)	0	100 100
3	C	25/28 (89%)	24 (96%)	1 (4%)	38 75
All	All	658/681 (97%)	652 (99%)	6 (1%)	84 93

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	123	GLU
1	A	155	THR
1	A	307	ASP
1	A	343	SER
3	C	772	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	HEB	A	501	1	29,50,50	3.95	11 (37%)	20,82,82	6.25	11 (55%)
4	HEB	A	502	1	29,50,50	4.05	11 (37%)	20,82,82	6.09	14 (70%)
5	HDD	A	503	1	32,52,52	2.32	12 (37%)	22,89,89	3.01	11 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEB	A	501	1	-	0/8/94/94	0/0/8/8
4	HEB	A	502	1	-	0/8/94/94	0/0/8/8
5	HDD	A	503	1	-	1/3/89/89	0/1/9/9

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	HEB	C3C-C2C	-13.93	1.22	1.40
4	A	501	HEB	C3C-C2C	-13.61	1.23	1.40
4	A	502	HEB	C1C-C2C	-11.47	1.22	1.38
4	A	501	HEB	C1C-C2C	-10.58	1.23	1.38
4	A	501	HEB	CHD-C4C	-5.45	1.36	1.51
4	A	502	HEB	CHD-C4C	-5.28	1.37	1.51
4	A	501	HEB	C1A-C2A	-5.03	1.31	1.38
4	A	501	HEB	C1D-ND	-4.99	1.42	1.49
4	A	502	HEB	C1D-ND	-4.68	1.43	1.49
4	A	502	HEB	C1A-C2A	-4.53	1.31	1.38
4	A	501	HEB	C2A-C3A	-4.39	1.24	1.37
4	A	502	HEB	C2A-C3A	-4.39	1.24	1.37
5	A	503	HDD	O1D-C3D	-4.37	1.40	1.46
4	A	502	HEB	CHC-C4B	-4.28	1.45	1.53
5	A	503	HDD	C4D-ND	-3.97	1.31	1.38
5	A	503	HDD	CHD-C1D	-3.68	1.31	1.36
4	A	501	HEB	CHC-C4B	-3.27	1.47	1.53
5	A	503	HDD	FE-ND	-2.61	1.85	1.95
4	A	501	HEB	CHB-C1B	-2.60	1.48	1.53
5	A	503	HDD	C1D-ND	-2.57	1.33	1.38
5	A	503	HDD	CHA-C4D	-2.49	1.32	1.36
4	A	501	HEB	CHA-C1A	-2.37	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	HDD	CAA-C2A	-2.30	1.48	1.52
4	A	501	HEB	CHD-C1D	-2.25	1.49	1.53
4	A	502	HEB	CHB-C1B	-2.18	1.49	1.53
4	A	502	HEB	CHD-C1D	-2.14	1.49	1.53
4	A	502	HEB	C3C-CAC	2.09	1.52	1.47
5	A	503	HDD	C4A-CHB	2.41	1.46	1.40
5	A	503	HDD	C2A-C3A	2.42	1.44	1.37
4	A	501	HEB	CBC-CAC	3.01	1.51	1.28
4	A	502	HEB	CBC-CAC	3.13	1.52	1.28
5	A	503	HDD	C3C-C2C	3.23	1.44	1.40
5	A	503	HDD	O1D-CGD	4.89	1.43	1.35
5	A	503	HDD	C3B-C2B	5.42	1.47	1.40

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	HEB	CAA-C2A-C1A	-9.10	117.29	127.20
4	A	501	HEB	CMC-C2C-C1C	-8.31	118.64	127.13
4	A	502	HEB	CAA-C2A-C1A	-7.56	118.97	127.20
5	A	503	HDD	C4D-ND-C1D	-7.35	103.00	107.37
4	A	502	HEB	CMC-C2C-C1C	-6.91	120.08	127.13
4	A	501	HEB	CMA-C3A-C4A	-6.60	120.40	127.13
4	A	501	HEB	C3C-CAC-CBC	-6.35	113.64	126.40
4	A	502	HEB	C3C-CAC-CBC	-5.31	115.73	126.40
4	A	502	HEB	CMA-C3A-C4A	-4.96	122.07	127.13
5	A	503	HDD	CAA-CBA-CGA	-4.49	104.05	112.78
5	A	503	HDD	C2D-C1D-CHD	-4.30	117.40	123.39
5	A	503	HDD	OND-C2D-CMD	-4.10	101.85	109.37
4	A	502	HEB	CBB-CAB-C3B	-4.09	107.19	113.16
5	A	503	HDD	CAD-CBD-CGD	-3.48	98.48	104.62
4	A	502	HEB	CAA-C2A-C3A	-2.88	120.77	129.00
4	A	502	HEB	CMC-C2C-C3C	-2.81	119.59	125.09
5	A	503	HDD	C3C-CAC-CBC	-2.20	121.98	126.40
5	A	503	HDD	CAA-C2A-C3A	2.09	134.98	129.00
5	A	503	HDD	CMC-C2C-C1C	2.37	132.34	128.31
5	A	503	HDD	O1D-CGD-O2D	2.41	123.19	120.80
5	A	503	HDD	CMB-C2B-C3B	3.40	131.73	125.09
4	A	501	HEB	C4C-C3C-C2C	5.27	111.09	104.44
4	A	502	HEB	C4C-C3C-C2C	5.32	111.16	104.44
5	A	503	HDD	C3C-C4C-NC	5.37	116.15	109.21
4	A	501	HEB	C4A-C3A-C2A	6.63	111.77	105.69
4	A	502	HEB	C4A-C3A-C2A	7.01	112.12	105.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	HEB	CHC-C4B-NB	8.06	125.95	110.75
4	A	501	HEB	CHB-C1B-NB	8.34	126.49	110.75
4	A	502	HEB	CHB-C1B-NB	8.70	127.16	110.75
4	A	502	HEB	CHD-C1D-ND	8.89	127.51	110.75
4	A	502	HEB	CHC-C4B-NB	9.23	128.16	110.75
4	A	501	HEB	CHD-C1D-ND	9.56	128.78	110.75
4	A	502	HEB	CHA-C4D-ND	9.73	129.11	110.75
4	A	501	HEB	CHA-C4D-ND	10.13	129.85	110.75
4	A	501	HEB	C3C-C2C-C1C	11.37	120.05	106.51
4	A	502	HEB	C3C-C2C-C1C	11.61	120.33	106.51

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	503	HDD	C1A-C2A-CAA-CBA

There are no ring outliers.

3 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	HEB	12	0
4	A	502	HEB	2	0
5	A	503	HDD	17	0

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, 95^{th} 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	432/448 (96%)	-0.29	19 (4%) 38 25	50, 90, 158, 205	0
2	B	330/342 (96%)	-0.09	20 (6%) 25 15	78, 151, 202, 224	0
3	C	30/33 (90%)	-0.30	1 (3%) 50 34	71, 118, 179, 194	0
All	All	792/823 (96%)	-0.21	40 (5%) 32 21	50, 120, 192, 224	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	GLY	6.3
2	B	38	ALA	5.0
1	A	4	TYR	4.6
1	A	1	MET	4.3
2	B	159	ALA	4.2
2	B	39	ASN	4.1
1	A	387	ARG	4.1
1	A	277	ASP	3.9
2	B	293	ASP	3.7
2	B	148	ALA	3.5
2	B	330	LYS	3.5
2	B	1	MET	3.4
2	B	40	GLN	3.3
1	A	296	ASN	3.2
2	B	37	TRP	3.2
3	C	793	VAL	3.2
1	A	209	LYS	3.0
2	B	225	PRO	3.0
1	A	163	ASN	2.8
1	A	3	GLY	2.6
2	B	147	ALA	2.6
2	B	250	TRP	2.6
2	B	260	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	153	ASP	2.5
1	A	351	ALA	2.5
2	B	42	HIS	2.4
1	A	164	GLY	2.4
1	A	393	ALA	2.4
2	B	149	GLY	2.3
2	B	111	THR	2.3
1	A	353	ASN	2.2
1	A	52	LEU	2.2
2	B	290	THR	2.2
2	B	154	TYR	2.2
1	A	276	GLU	2.2
2	B	255	GLN	2.1
1	A	120	ASP	2.1
1	A	350	THR	2.1
1	A	127	LYS	2.1
1	A	92	GLN	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	HDD	A	503	44/44	0.85	0.34	0.94	113,113,113,113	0
4	HEB	A	502	43/43	0.95	0.23	0.45	92,92,92,92	0
4	HEB	A	501	43/43	0.95	0.21	0.37	75,75,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.