Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 09:16 AM EDT

PDB ID	:	1PBY
Title	:	Structure of the Phenylhydrazine Adduct of the Quinohemoprotein Amine Dehydrogenase from Paracoccus denitrificans at 1.7 A Resolution
Authors	:	Datta, S.; Ikeda, T.; Kano, K.; Mathews, F.S.
Deposited on	:	2003-05-15
Resolution	:	1.70 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:

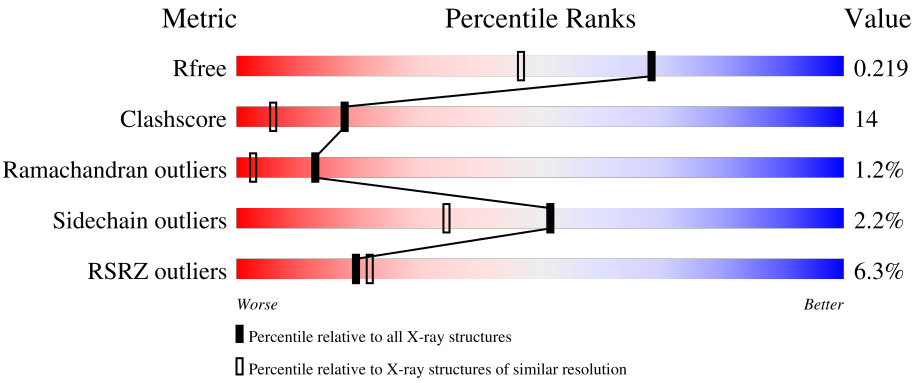
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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% 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	489	9% 77% 21%
2	B	337	% 81% 18%
3	C	79	9% 82% 14%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8443 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 quinohemoprotein amine dehydrogenase 60 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	489	3746	2329	671	734	12	0	4	0

- Molecule 2 is a protein called quinohemoprotein amine dehydrogenase 40 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	337	2668	1687	449	520	12	0	8	0

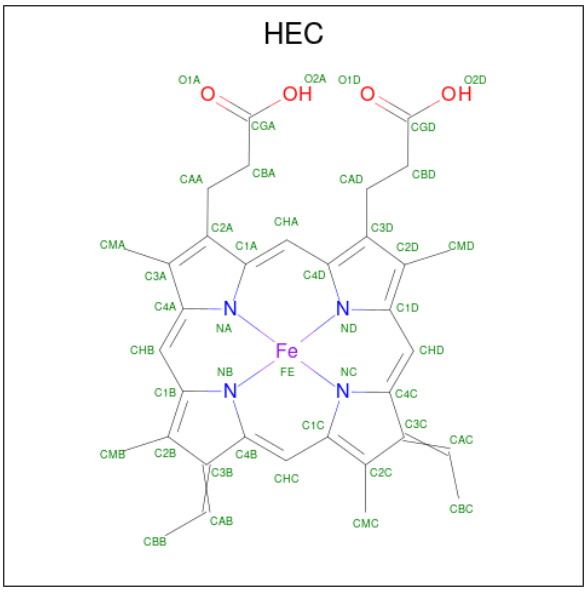
- Molecule 3 is a protein called quinohemoprotein amine dehydrogenase 9 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	79	628	398	100	123	7	0	1	0

There is a discrepancy between the modelled and reference sequences:

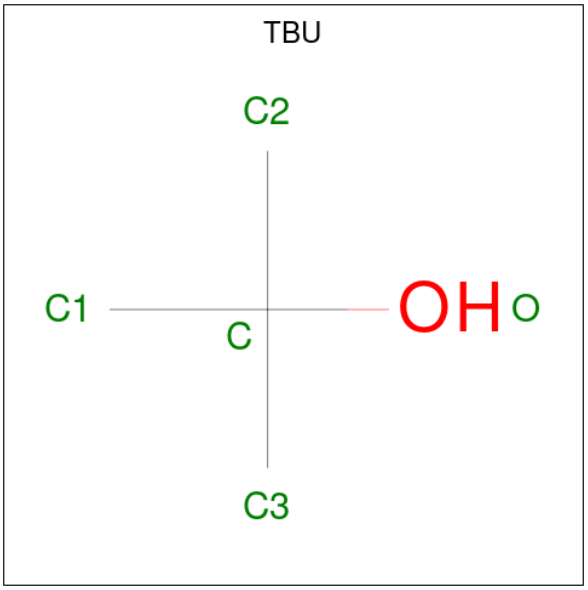
Chain	Residue	Modelled	Actual	Comment	Reference
C	43	TRW	TRP	modified residue	GB 17402570

- Molecule 4 is HEME C (three-letter code: HEC) (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 TERTIARY-BUTYL ALCOHOL (three-letter code: TBU) (formula: $C_4H_{10}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			5	4	1		
5	A	1	Total	C	O	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 5 4 1	0	0
5	B	1	Total C O 5 4 1	0	0

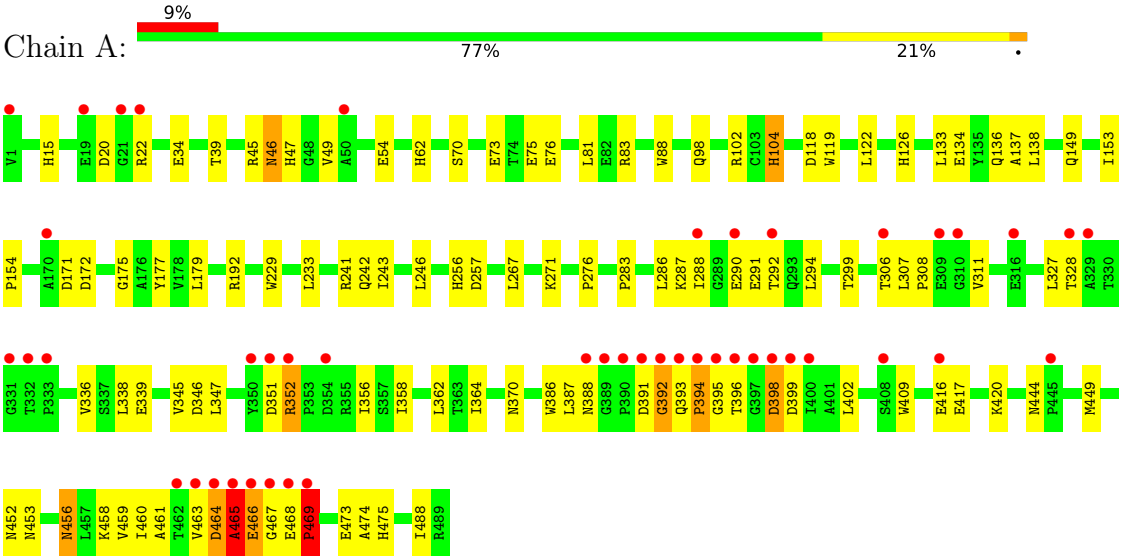
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	688	Total O 688 688	0	0
6	B	506	Total O 506 506	0	0
6	C	101	Total O 101 101	0	0

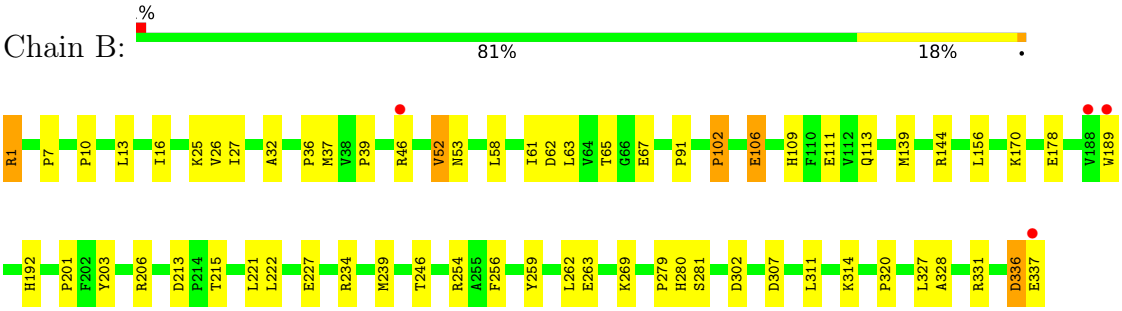
3 Residue-property plots (i)

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 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.

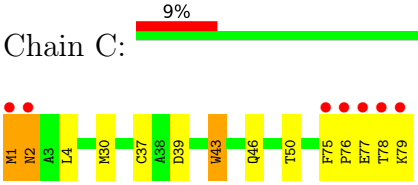
• Molecule 1: quinohemoprotein amine dehydrogenase 60 kDa subunit



• Molecule 2: quinohemoprotein amine dehydrogenase 40 kDa subunit



• Molecule 3: quinohemoprotein amine dehydrogenase 9 kDa subunit



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	99.24Å 99.24Å 213.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.42 – 1.70 36.42 – 1.70	Depositor EDS
% Data completeness (in resolution range)	90.2 (36.42-1.70) 90.4 (36.42-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.191 , 0.224 0.188 , 0.219	Depositor DCC
R_{free} test set	11032 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8443	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: TBU, HEC, TRW

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	0.38	3/3828 (0.1%)	0.68	5/5209 (0.1%)
2	B	0.37	0/2722	0.65	0/3702
3	C	0.42	0/622	0.61	0/850
All	All	0.38	3/7172 (0.0%)	0.66	5/9761 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	HIS	CE1-NE2	5.31	1.44	1.32
1	A	126	HIS	CE1-NE2	5.31	1.44	1.32
1	A	104	HIS	CE1-NE2	5.18	1.44	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	15	HIS	ND1-CG-CD2	8.09	120.12	108.80
1	A	126	HIS	ND1-CG-CD2	8.07	120.09	108.80
1	A	104	HIS	ND1-CG-CD2	8.01	120.02	108.80
1	A	465	ALA	N-CA-C	5.55	126.00	111.00
1	A	464	ASP	N-CA-C	5.54	125.97	111.00

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	3746	0	3608	117	0
2	B	2668	0	2656	63	0
3	C	628	0	562	23	0
4	A	86	0	60	4	0
5	A	10	0	20	0	0
5	B	10	0	20	0	0
6	A	688	0	0	6	0
6	B	506	0	0	13	0
6	C	101	0	0	0	0
All	All	8443	0	6926	191	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 14.

All (191) 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)
2:B:144:ARG:HG3	2:B:227[A]:GLU:HG2	1.38	1.04
2:B:32:ALA:HB1	2:B:52[B]:VAL:HG21	1.41	1.03
1:A:387:LEU:HG	1:A:402:LEU:HD11	1.45	0.97
1:A:444:ASN:HD22	1:A:453:ASN:HD21	1.08	0.96
1:A:452:ASN:HD21	3:C:30:MET:H	0.96	0.96
3:C:78:THR:HG22	3:C:79:LYS:H	1.30	0.93
1:A:456:ASN:HD21	1:A:475:HIS:HE1	1.17	0.87
1:A:102:ARG:HH12	1:A:136:GLN:HE21	1.21	0.86
1:A:175:GLY:HA3	1:A:271:LYS:HZ1	1.41	0.83
2:B:254:ARG:HH11	2:B:254:ARG:HG3	1.43	0.82
1:A:456:ASN:ND2	1:A:475:HIS:HE1	1.78	0.81
1:A:388:ASN:HB3	1:A:392:GLY:O	1.83	0.78
2:B:307:ASP:HA	2:B:314:LYS:HE3	1.66	0.78
1:A:306:THR:CG2	1:A:339:GLU:HB2	2.14	0.78
2:B:32:ALA:O	2:B:52[B]:VAL:HG22	1.83	0.78
1:A:456:ASN:HD21	1:A:475:HIS:CE1	2.01	0.77
1:A:467:GLY:C	1:A:469:PRO:HD3	2.05	0.77
2:B:213:ASP:OD1	2:B:215[B]:THR:HG22	1.85	0.77
1:A:175:GLY:HA3	1:A:271:LYS:NZ	1.99	0.76
1:A:392:GLY:O	1:A:393:GLN:HG2	1.84	0.76
1:A:452:ASN:ND2	3:C:30:MET:H	1.80	0.73
2:B:32:ALA:HB1	2:B:52[B]:VAL:CG2	2.18	0.73
1:A:393:GLN:HE22	1:A:398:ASP:HB3	1.54	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ARG:HG3	1:A:241:ARG:HH11	1.53	0.72
3:C:78:THR:HG22	3:C:79:LYS:N	2.05	0.71
1:A:393:GLN:O	1:A:395:GLY:N	2.25	0.70
2:B:36:PRO:HA	2:B:52[B]:VAL:HG23	1.74	0.69
1:A:358:ILE:HD11	1:A:461:ALA:HB3	1.75	0.69
1:A:364:ILE:HG23	3:C:4:LEU:HD22	1.74	0.69
1:A:393:GLN:HE22	1:A:398:ASP:CA	2.06	0.69
1:A:393:GLN:NE2	1:A:398:ASP:HB3	2.09	0.68
1:A:466:GLU:C	1:A:468:GLU:H	1.96	0.68
3:C:1:MET:HG2	3:C:4:LEU:HD12	1.76	0.68
1:A:137:ALA:O	1:A:138:LEU:HB2	1.94	0.68
2:B:102:PRO:HG2	2:B:113:GLN:HB2	1.78	0.65
1:A:102:ARG:HH12	1:A:136:GLN:NE2	1.94	0.65
2:B:280:HIS:HD2	2:B:281:SER:O	1.78	0.65
1:A:393:GLN:HE22	1:A:398:ASP:CB	2.10	0.65
2:B:1:ARG:HG3	2:B:1:ARG:HH11	1.62	0.64
3:C:1:MET:HB3	3:C:4:LEU:HG	1.78	0.64
2:B:156:LEU:HB3	2:B:170:LYS:HB2	1.79	0.64
2:B:178[A]:GLU:H	2:B:178[A]:GLU:CD	2.01	0.64
2:B:13:LEU:HD12	2:B:61:ILE:HD13	1.81	0.63
1:A:460:ILE:N	1:A:460:ILE:HD12	2.15	0.62
1:A:444:ASN:HD22	1:A:453:ASN:ND2	1.91	0.61
2:B:109:HIS:HE1	2:B:111:GLU:OE1	1.84	0.61
2:B:215[A]:THR:HG22	6:B:2178:HOH:O	1.99	0.61
3:C:75:PHE:O	3:C:77:GLU:N	2.34	0.61
2:B:262[B]:LEU:HD22	2:B:311:LEU:HD13	1.82	0.61
2:B:170:LYS:HE3	6:B:2135:HOH:O	2.02	0.60
2:B:52[B]:VAL:HG13	2:B:53:ASN:N	2.17	0.60
1:A:81:LEU:O	1:A:243:ILE:HD13	2.01	0.60
1:A:229:TRP:HE1	1:A:242:GLN:HE21	1.50	0.60
2:B:13:LEU:HD12	2:B:61:ILE:CD1	2.32	0.60
3:C:78:THR:CG2	3:C:79:LYS:H	2.12	0.59
2:B:213:ASP:CG	2:B:215[B]:THR:HG22	2.22	0.59
1:A:416:GLU:O	1:A:420:LYS:HG3	2.03	0.59
2:B:192:HIS:HE1	6:B:2006:HOH:O	1.86	0.58
1:A:229:TRP:HE1	1:A:242:GLN:NE2	2.00	0.58
3:C:37:CYS:SG	3:C:43:TRW:HB3	2.42	0.58
1:A:393:GLN:O	1:A:393:GLN:HG3	2.04	0.58
1:A:287:LYS:HD3	1:A:290:GLU:OE1	2.02	0.58
1:A:292:THR:HG21	6:A:2172:HOH:O	2.03	0.57
1:A:352:ARG:HD3	6:A:2322:HOH:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:ARG:HG3	2:B:254:ARG:NH1	2.13	0.57
1:A:391:ASP:OD2	1:A:393:GLN:HB3	2.03	0.57
1:A:46:ASN:HD22	1:A:46:ASN:N	2.01	0.56
1:A:356:ILE:HG21	1:A:463:VAL:HG21	1.88	0.56
1:A:39:THR:HG21	4:A:991:HEC:HMA2	1.88	0.56
1:A:47:HIS:HE1	4:A:991:HEC:O1D	1.88	0.56
1:A:62:HIS:HD2	6:A:2091:HOH:O	1.88	0.56
2:B:46:ARG:HH21	2:B:46:ARG:HG3	1.70	0.56
1:A:409:TRP:CZ3	1:A:461:ALA:HB2	2.41	0.55
2:B:280:HIS:HE1	2:B:302:ASP:OD2	1.89	0.55
1:A:468:GLU:N	1:A:469:PRO:HD3	2.22	0.55
1:A:345:VAL:HG12	1:A:347:LEU:HD21	1.90	0.54
1:A:346:ASP:C	1:A:347:LEU:HD22	2.28	0.54
1:A:283:PRO:HG2	1:A:294:LEU:CD2	2.38	0.54
3:C:75:PHE:C	3:C:77:GLU:H	2.11	0.54
1:A:306:THR:HG23	1:A:339:GLU:HB2	1.88	0.54
1:A:241:ARG:HG3	1:A:241:ARG:NH1	2.19	0.54
1:A:45:ARG:HH11	1:A:46:ASN:HD21	1.56	0.53
1:A:386:TRP:HA	1:A:402:LEU:HD13	1.89	0.53
2:B:10:PRO:HB3	6:B:2053:HOH:O	2.09	0.53
3:C:1:MET:HB2	3:C:4:LEU:HB2	1.90	0.53
1:A:393:GLN:HB2	1:A:396:THR:OG1	2.10	0.52
2:B:25:LYS:HD3	2:B:26:VAL:N	2.25	0.52
1:A:177:TYR:O	1:A:192:ARG:HD2	2.09	0.52
1:A:393:GLN:NE2	1:A:396:THR:OG1	2.42	0.52
2:B:32:ALA:CB	2:B:52[B]:VAL:HG21	2.28	0.52
2:B:262[B]:LEU:C	2:B:262[B]:LEU:HD23	2.30	0.52
1:A:459:VAL:HB	1:A:474:ALA:HB3	1.92	0.52
2:B:25:LYS:HD3	2:B:26:VAL:H	1.74	0.52
1:A:388:ASN:O	1:A:393:GLN:HG2	2.10	0.52
2:B:327:LEU:H	2:B:327:LEU:HD23	1.75	0.51
1:A:391:ASP:O	1:A:393:GLN:N	2.42	0.51
1:A:267:LEU:C	1:A:267:LEU:HD12	2.31	0.51
2:B:46:ARG:NH2	2:B:62:ASP:OD2	2.44	0.51
1:A:356:ILE:HD13	1:A:463:VAL:HG22	1.92	0.51
2:B:16:ILE:N	2:B:16:ILE:HD12	2.25	0.51
1:A:47:HIS:HD2	6:A:2119:HOH:O	1.92	0.51
2:B:1:ARG:HG3	2:B:1:ARG:NH1	2.26	0.51
1:A:54:GLU:H	1:A:54:GLU:CD	2.13	0.50
1:A:393:GLN:NE2	1:A:399:ASP:N	2.57	0.50
2:B:307:ASP:CA	2:B:314:LYS:HE3	2.38	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLN:HE22	1:A:398:ASP:C	2.15	0.50
1:A:444:ASN:ND2	1:A:453:ASN:HD21	1.92	0.50
1:A:241:ARG:NH1	3:C:79:LYS:N	2.59	0.50
2:B:7:PRO:HG3	2:B:328:ALA:HB1	1.94	0.50
1:A:133[B]:LEU:C	1:A:133[B]:LEU:HD12	2.32	0.49
2:B:144:ARG:HD2	6:B:2342:HOH:O	2.12	0.49
2:B:192:HIS:HD2	6:B:2047:HOH:O	1.95	0.49
1:A:393:GLN:HE22	1:A:398:ASP:N	2.10	0.49
2:B:269:LYS:HE3	6:B:2397:HOH:O	2.12	0.49
1:A:393:GLN:O	1:A:396:THR:HG23	2.12	0.49
2:B:46:ARG:HH21	2:B:46:ARG:CG	2.24	0.49
1:A:241:ARG:CZ	3:C:78:THR:HG23	2.43	0.49
1:A:358:ILE:CD1	1:A:461:ALA:HB3	2.43	0.49
1:A:276:PRO:HA	1:A:299:THR:O	2.12	0.48
1:A:417:GLU:HG2	6:A:2146:HOH:O	2.13	0.48
1:A:466:GLU:C	1:A:468:GLU:N	2.66	0.48
1:A:393:GLN:NE2	1:A:399:ASP:OD1	2.47	0.48
1:A:179:LEU:HD12	1:A:179:LEU:C	2.34	0.48
1:A:256:HIS:HD2	1:A:257:ASP:O	1.96	0.48
1:A:83:ARG:NE	3:C:79:LYS:O	2.47	0.48
2:B:222:LEU:C	2:B:222:LEU:HD23	2.34	0.48
1:A:241:ARG:NH2	3:C:78:THR:HG23	2.29	0.48
2:B:7:PRO:HG3	2:B:328:ALA:CB	2.44	0.48
2:B:203:TYR:HB3	2:B:239:MET:CE	2.43	0.48
1:A:308:PRO:HG2	1:A:311:VAL:HG12	1.95	0.48
1:A:352:ARG:HD2	1:A:352:ARG:C	2.34	0.47
2:B:201:PRO:HD3	2:B:246:THR:HG23	1.96	0.47
1:A:75:GLU:O	1:A:76:GLU:HB2	2.14	0.47
1:A:286:LEU:HD21	1:A:294:LEU:HD11	1.95	0.47
2:B:58:LEU:C	2:B:58:LEU:HD23	2.35	0.47
2:B:106:GLU:HG3	6:B:2464:HOH:O	2.13	0.47
1:A:153:ILE:HB	1:A:154:PRO:HD3	1.95	0.47
1:A:458:LYS:HD2	1:A:473:GLU:CD	2.35	0.47
2:B:39:PRO:HG2	2:B:331:ARG:HG2	1.96	0.47
1:A:307:LEU:HB3	1:A:311:VAL:HG13	1.97	0.46
1:A:393:GLN:N	1:A:394:PRO:HD3	2.30	0.46
1:A:88[B]:TRP:CE2	3:C:2:ASN:HB2	2.50	0.46
1:A:133[A]:LEU:C	1:A:133[A]:LEU:HD23	2.36	0.46
1:A:233:LEU:HD12	1:A:233:LEU:N	2.31	0.45
2:B:37:MET:HG2	6:B:2218:HOH:O	2.17	0.45
1:A:336:VAL:HG23	1:A:347:LEU:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:SER:OG	1:A:73:GLU:HG3	2.16	0.45
2:B:203:TYR:HB3	2:B:239:MET:HE1	1.98	0.45
2:B:91:PRO:HB3	2:B:144:ARG:NH2	2.32	0.45
2:B:91:PRO:HG2	6:B:2040:HOH:O	2.16	0.45
1:A:358:ILE:HG21	1:A:474:ALA:HB2	1.98	0.45
1:A:241:ARG:HH12	3:C:79:LYS:N	2.13	0.44
1:A:288:ILE:HD12	1:A:351:ASP:OD1	2.17	0.44
1:A:34:GLU:HB3	1:A:488:ILE:HG13	1.99	0.44
2:B:36:PRO:CA	2:B:52[B]:VAL:HG23	2.44	0.44
1:A:119:TRP:CZ3	1:A:122:LEU:HD23	2.53	0.44
1:A:291:GLU:HA	1:A:327:LEU:O	2.17	0.44
1:A:393:GLN:O	1:A:394:PRO:C	2.56	0.44
1:A:133[B]:LEU:HD12	1:A:134:GLU:N	2.33	0.44
1:A:49:VAL:HG22	4:A:991:HEC:HMC2	2.00	0.43
2:B:213:ASP:OD1	2:B:215[A]:THR:HG23	2.18	0.43
3:C:39:ASP:HA	3:C:50:THR:OG1	2.19	0.43
1:A:20:ASP:OD1	1:A:22:ARG:HB2	2.18	0.43
1:A:328:THR:HG23	1:A:328:THR:O	2.17	0.43
1:A:347:LEU:HD22	1:A:347:LEU:N	2.34	0.43
2:B:27:ILE:HD12	2:B:27:ILE:N	2.34	0.43
1:A:345:VAL:HG12	1:A:347:LEU:CD2	2.48	0.43
1:A:362:LEU:CD2	3:C:4:LEU:HD21	2.49	0.42
1:A:149:GLN:NE2	6:A:2192:HOH:O	2.45	0.42
2:B:206:ARG:HD2	6:B:2238:HOH:O	2.19	0.42
2:B:320:PRO:HG2	6:B:2324:HOH:O	2.18	0.42
2:B:262[B]:LEU:HD23	2:B:263:GLU:N	2.34	0.42
1:A:294:LEU:HD12	1:A:327:LEU:HD12	2.00	0.42
2:B:336:ASP:O	2:B:337:GLU:OXT	2.37	0.42
1:A:241:ARG:NH1	3:C:79:LYS:H	2.16	0.42
1:A:104:HIS:CD2	4:A:992:HEC:ND	2.87	0.41
2:B:109:HIS:HD2	6:B:2031:HOH:O	2.03	0.41
1:A:338:LEU:C	1:A:338:LEU:HD12	2.40	0.41
1:A:393:GLN:CD	1:A:398:ASP:HB3	2.40	0.41
3:C:1:MET:HB3	3:C:4:LEU:CG	2.48	0.41
3:C:1:MET:SD	3:C:1:MET:N	2.81	0.41
1:A:458:LYS:HD2	1:A:473:GLU:OE2	2.21	0.41
1:A:465:ALA:HA	1:A:468:GLU:CG	2.51	0.41
2:B:65:THR:OG1	2:B:67:GLU:HG2	2.21	0.41
2:B:139[B]:MET:SD	2:B:189:TRP:O	2.79	0.41
1:A:171:ASP:CG	1:A:172:ASP:H	2.24	0.40
1:A:449:MET:HA	2:B:279:PRO:O	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ASN:ND2	1:A:475:HIS:CE1	2.70	0.40
2:B:246:THR:HA	2:B:256:PHE:O	2.21	0.40
1:A:460:ILE:N	1:A:460:ILE:CD1	2.84	0.40
1:A:98:GLN:O	1:A:102:ARG:HD3	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	491/489 (100%)	461 (94%)	24 (5%)	6 (1%)	13	3
2	B	343/337 (102%)	326 (95%)	12 (4%)	5 (2%)	10	2
3	C	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	12	2
All	All	911/905 (101%)	857 (94%)	42 (5%)	12 (1%)	13	2

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	PRO
1	A	465	ALA
1	A	466	GLU
1	A	469	PRO
3	C	76	PRO
2	B	259	TYR
1	A	398	ASP
2	B	336	ASP
1	A	392	GLY
2	B	52[A]	VAL
2	B	52[B]	VAL
2	B	102	PRO

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	379/375 (101%)	371 (98%)	8 (2%)	53	36
2	B	287/279 (103%)	281 (98%)	6 (2%)	53	36
3	C	65/64 (102%)	62 (95%)	3 (5%)	27	10
All	All	731/718 (102%)	714 (98%)	17 (2%)	52	33

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	118	ASP
1	A	246	LEU
1	A	352	ARG
1	A	370	ASN
1	A	456	ASN
1	A	464	ASP
1	A	469	PRO
2	B	1	ARG
2	B	63	LEU
2	B	106	GLU
2	B	221[A]	LEU
2	B	221[B]	LEU
2	B	234	ARG
3	C	1	MET
3	C	2	ASN
3	C	46	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	9	ASN
1	A	17	GLN
1	A	46	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	47	HIS
1	A	62	HIS
1	A	136	GLN
1	A	242	GLN
1	A	256	HIS
1	A	277	GLN
1	A	293	GLN
1	A	320	ASN
1	A	343	GLN
1	A	370	ASN
1	A	393	GLN
1	A	422	GLN
1	A	452	ASN
1	A	453	ASN
1	A	456	ASN
1	A	475	HIS
2	B	109	HIS
2	B	192	HIS
2	B	280	HIS
3	C	25	ASN
3	C	28	GLN
3	C	46	GLN
3	C	72	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	TRW	C	43	3	22,25,25	3.01	10 (45%)	21,34,34	1.84	6 (28%)

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
3	TRW	C	43	3	-	0/9/11/11	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	43	TRW	C2-C1	6.99	1.51	1.39
3	C	43	TRW	C6-C1	6.93	1.50	1.39
3	C	43	TRW	C3-C2	4.75	1.48	1.38
3	C	43	TRW	C5-C6	4.64	1.48	1.38
3	C	43	TRW	C5-C4	3.61	1.47	1.38
3	C	43	TRW	CE3-CZ3	3.21	1.43	1.36
3	C	43	TRW	O7-CZ2	-3.14	1.25	1.35
3	C	43	TRW	C4-C3	2.84	1.45	1.38
3	C	43	TRW	CH2-N6	-2.49	1.31	1.38
3	C	43	TRW	CZ3-CH2	2.48	1.43	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	43	TRW	C6-C1-C2	-3.80	113.83	119.03
3	C	43	TRW	O7-CZ2-CH2	3.64	127.63	118.27
3	C	43	TRW	C3-C2-C1	3.25	123.61	119.72
3	C	43	TRW	CH2-N6-N1	2.91	124.60	118.50
3	C	43	TRW	O7-CZ2-CE2	-2.61	114.83	119.62
3	C	43	TRW	C5-C6-C1	2.39	122.58	119.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	43	TRW	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
5	TBU	A	1994	-	4,4,4	0.48	0	6,6,6	0.55	0
5	TBU	B	1995	-	4,4,4	0.47	0	6,6,6	0.56	0
5	TBU	A	1993	-	4,4,4	0.46	0	6,6,6	0.57	0
4	HEC	A	991	1	32,50,50	1.91	4 (12%)	24,82,82	1.51	6 (25%)
5	TBU	B	1996	-	4,4,4	0.47	0	6,6,6	0.58	0
4	HEC	A	992	1	32,50,50	1.96	5 (15%)	24,82,82	1.59	6 (25%)

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	HEC	A	992	1	-	4/10/54/54	-
4	HEC	A	991	1	-	4/10/54/54	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	992	HEC	C3C-C2C	-6.55	1.33	1.40
4	A	991	HEC	C3C-C2C	-6.26	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	991	HEC	C2B-C3B	-4.61	1.35	1.40
4	A	992	HEC	C2B-C3B	-4.36	1.36	1.40
4	A	992	HEC	C1D-ND	2.22	1.40	1.36
4	A	991	HEC	O2A-CGA	-2.06	1.23	1.30
4	A	992	HEC	O2A-CGA	-2.06	1.23	1.30
4	A	992	HEC	O1A-CGA	2.03	1.28	1.22
4	A	991	HEC	C3C-C4C	2.03	1.46	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	992	HEC	CMC-C2C-C3C	3.06	129.42	125.82
4	A	991	HEC	CMC-C2C-C3C	3.02	129.37	125.82
4	A	992	HEC	CMC-C2C-C1C	-2.93	123.96	128.46
4	A	991	HEC	CMC-C2C-C1C	-2.93	123.97	128.46
4	A	991	HEC	O1A-CGA-CBA	-2.69	114.44	123.08
4	A	992	HEC	CMD-C2D-C1D	-2.57	124.51	128.46
4	A	992	HEC	O1A-CGA-CBA	-2.46	115.18	123.08
4	A	991	HEC	CMD-C2D-C1D	-2.32	124.89	128.46
4	A	992	HEC	CMB-C2B-C3B	2.26	128.48	125.82
4	A	991	HEC	CMB-C2B-C3B	2.14	128.34	125.82
4	A	991	HEC	CMB-C2B-C1B	-2.13	125.20	128.46
4	A	992	HEC	CMB-C2B-C1B	-2.12	125.21	128.46

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	991	HEC	CAA-CBA-CGA-O1A
4	A	991	HEC	CAD-CBD-CGD-O1D
4	A	991	HEC	CAA-CBA-CGA-O2A
4	A	992	HEC	CAD-CBD-CGD-O2D
4	A	992	HEC	CAD-CBD-CGD-O1D
4	A	991	HEC	CAD-CBD-CGD-O2D
4	A	992	HEC	CAA-CBA-CGA-O2A
4	A	992	HEC	CAA-CBA-CGA-O1A

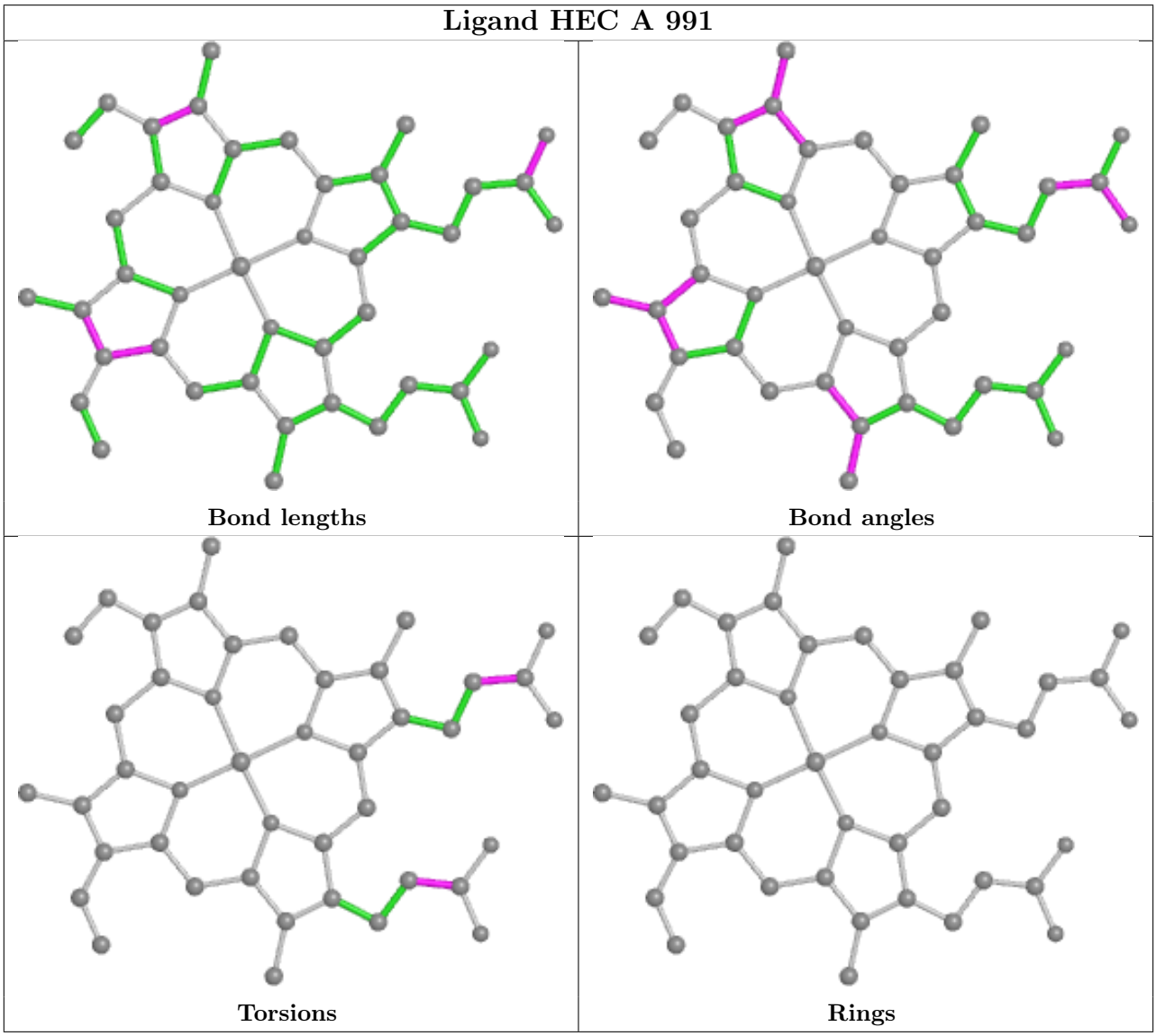
There are no ring outliers.

2 monomers are involved in 4 short contacts:

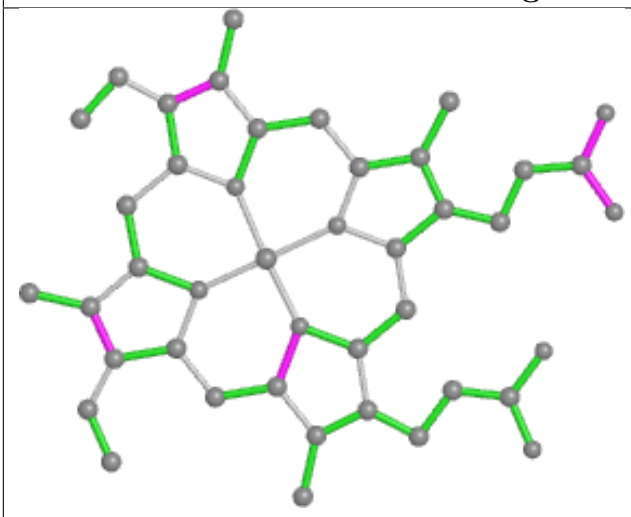
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	991	HEC	3	0
4	A	992	HEC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

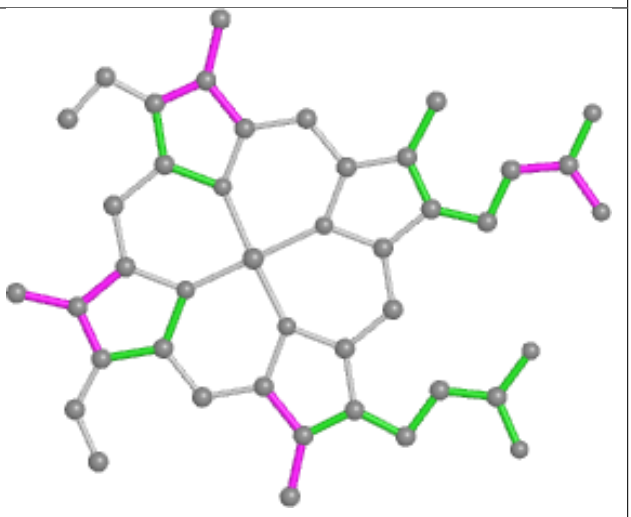
Ligand HEC A 991



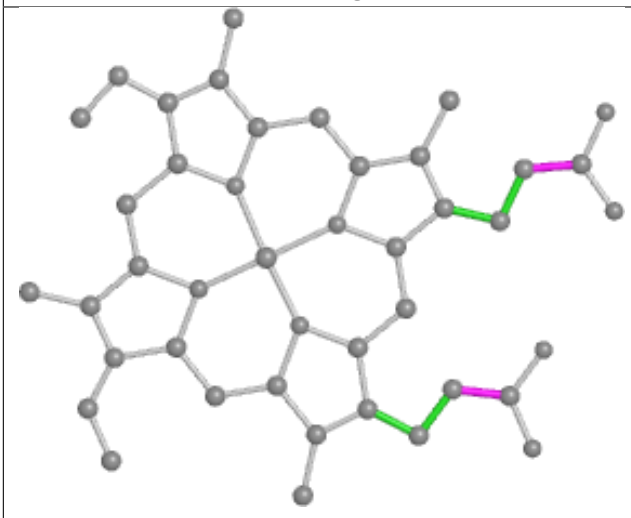
Ligand HEC A 992



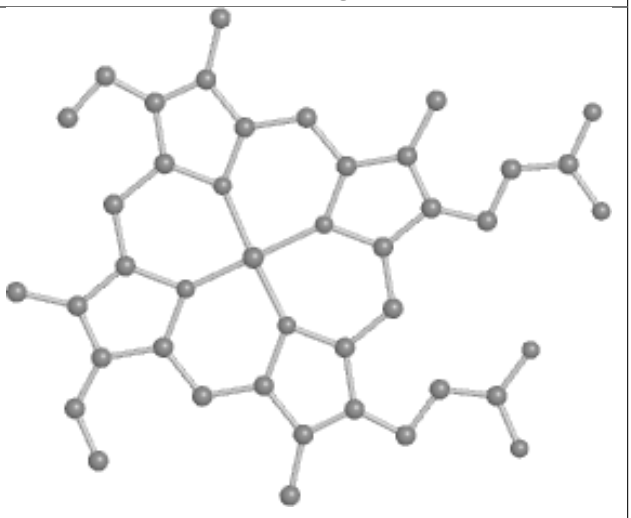
Bond lengths



Bond angles



Torsions



Rings

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	489/489 (100%)	0.37	46 (9%) 8 9	10, 19, 43, 60	0
2	B	337/337 (100%)	0.04	4 (1%) 79 82	12, 17, 27, 44	0
3	C	78/79 (98%)	0.55	7 (8%) 9 10	10, 16, 41, 53	0
All	All	904/905 (99%)	0.26	57 (6%) 20 22	10, 18, 39, 60	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	78	THR	12.1
3	C	1	MET	11.9
1	A	469	PRO	11.0
1	A	465	ALA	10.1
3	C	79	LYS	8.8
1	A	397	GLY	8.7
1	A	466	GLU	6.7
1	A	392	GLY	6.5
1	A	390	PRO	6.5
3	C	2	ASN	6.0
1	A	467	GLY	5.9
3	C	77	GLU	5.9
1	A	398	ASP	5.8
1	A	396	THR	5.4
1	A	332	THR	5.2
1	A	389	GLY	5.1
3	C	76	PRO	5.1
2	B	337	GLU	4.9
1	A	394	PRO	4.9
1	A	391	ASP	4.9
1	A	468	GLU	4.8
1	A	393	GLN	4.1
1	A	290	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	463	VAL	3.9
1	A	464	ASP	3.8
1	A	22	ARG	3.8
1	A	21	GLY	3.6
1	A	331	GLY	3.6
1	A	19	GLU	3.5
1	A	354	ASP	3.4
1	A	309	GLU	3.1
1	A	352	ARG	3.0
1	A	333	PRO	3.0
2	B	188	VAL	3.0
1	A	395	GLY	3.0
1	A	388	ASN	2.9
1	A	170	ALA	2.9
1	A	292	THR	2.9
1	A	462	THR	2.6
1	A	351	ASP	2.5
1	A	399	ASP	2.4
1	A	416	GLU	2.4
1	A	445	PRO	2.4
2	B	189	TRP	2.3
1	A	306	THR	2.3
1	A	328	THR	2.2
1	A	1	VAL	2.2
1	A	288	ILE	2.2
1	A	350	TYR	2.2
2	B	46	ARG	2.2
1	A	329	ALA	2.2
1	A	310	GLY	2.1
1	A	408	SER	2.1
3	C	75	PHE	2.1
1	A	316	GLU	2.1
1	A	400	ILE	2.0
1	A	50	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. 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	B-factors(Å^2)	Q<0.9
3	TRW	C	43	23/23	0.94	0.12	10,13,17,18	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

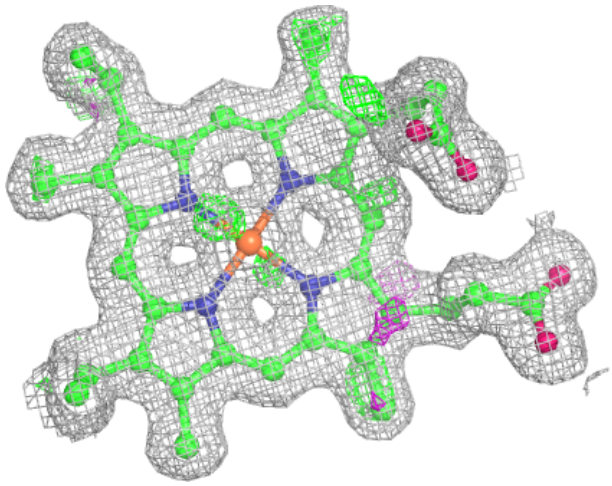
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

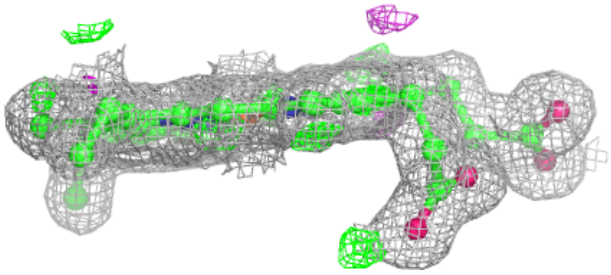
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	TBU	B	1996	5/5	0.59	0.23	45,45,46,46	0
5	TBU	B	1995	5/5	0.72	0.20	46,46,46,46	0
5	TBU	A	1994	5/5	0.82	0.19	36,36,36,36	0
5	TBU	A	1993	5/5	0.84	0.17	41,41,41,41	0
4	HEC	A	991	43/43	0.97	0.10	12,14,17,18	0
4	HEC	A	992	43/43	0.98	0.10	9,11,13,13	0

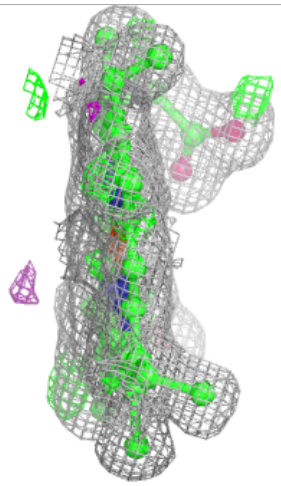
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEC A 991:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

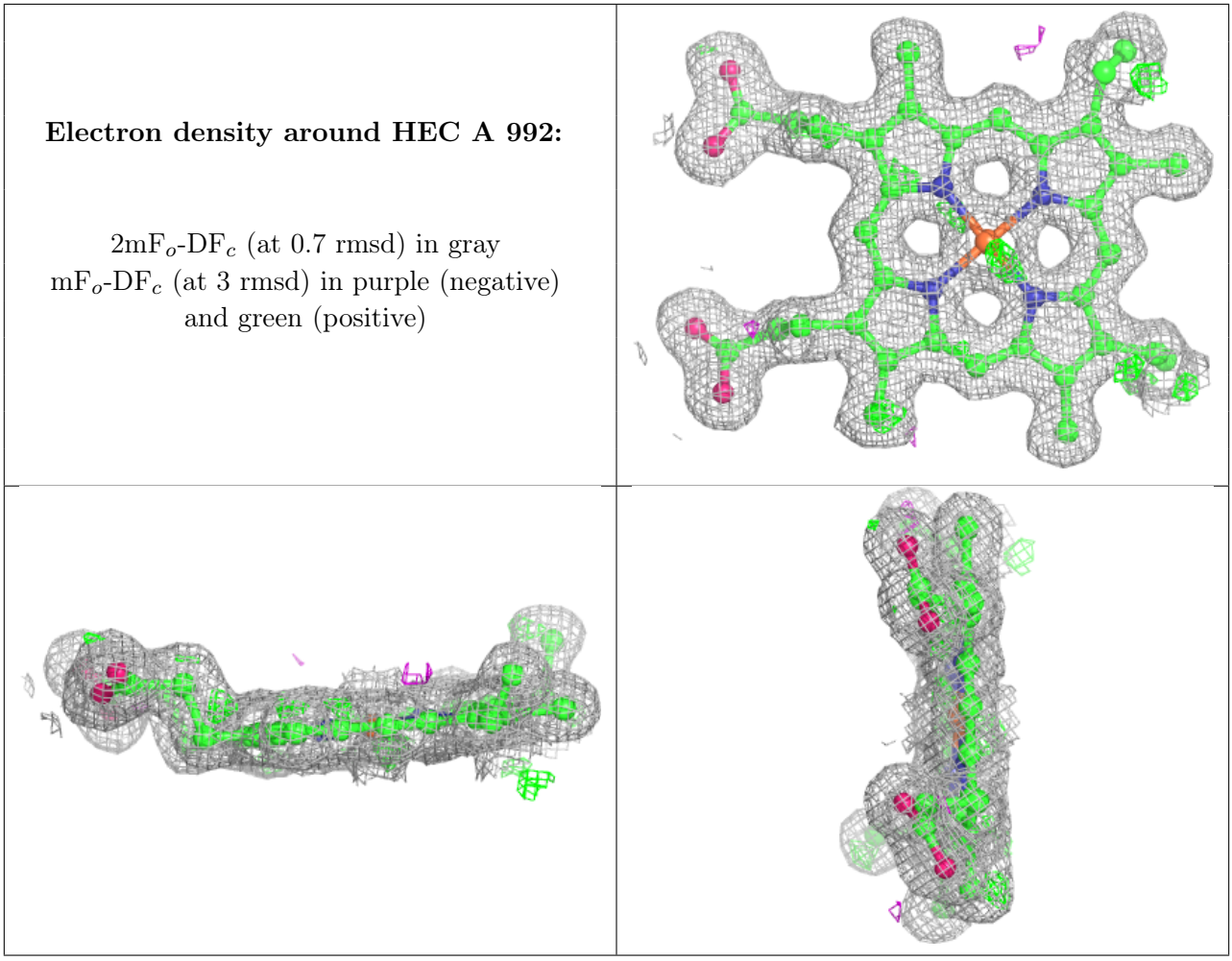






Electron density around HEC A 992:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.