



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:52 AM EDT

PDB ID : 1PBY / pdb_00001pby
Title : Structure of the Phenylhydrazine Adduct of the Quinohemoprotein Amine Dehydrogenase from *Paracoccus denitrificans* at 1.7 Å 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

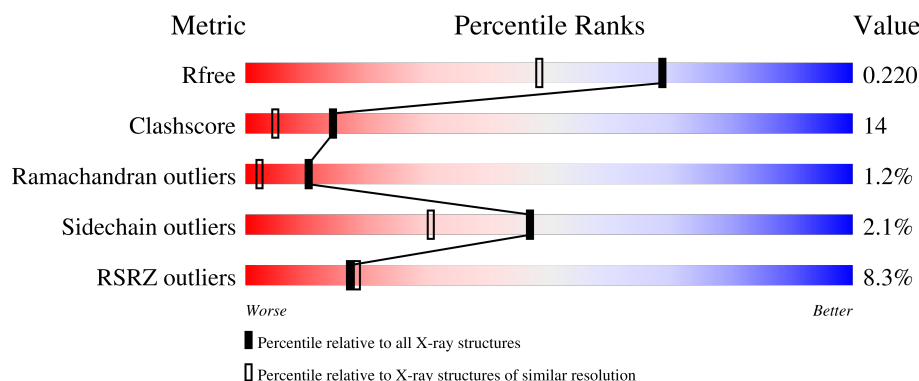
1 Overall quality at a glance

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 $\leq 5\%$. 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	13% 75% 22% .
2	B	337	2% 79% 19% .
3	C	79	9% 78% 18% .

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
4	HEC	A	991	X	-	-	-
4	HEC	A	992	X	-	-	-

2 Entry composition

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 quinoxemoprotein amine dehydrogenase 60 kDa subunit.

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

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

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

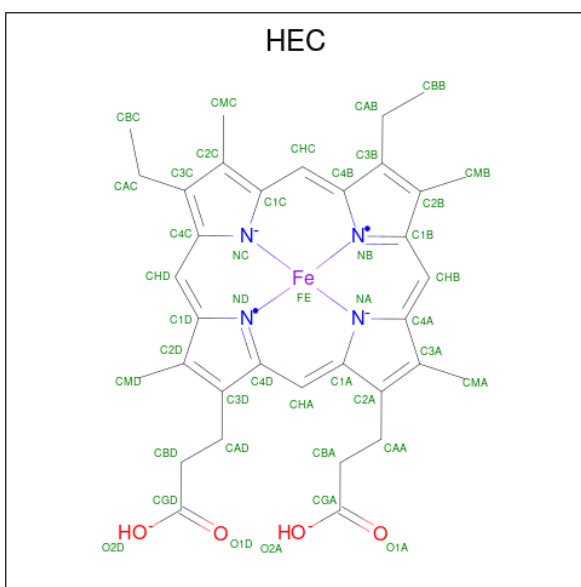
- Molecule 3 is a protein called quinoxemoprotein amine dehydrogenase 9 kDa subunit.

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

There is a discrepancy between the modelled and reference sequences:

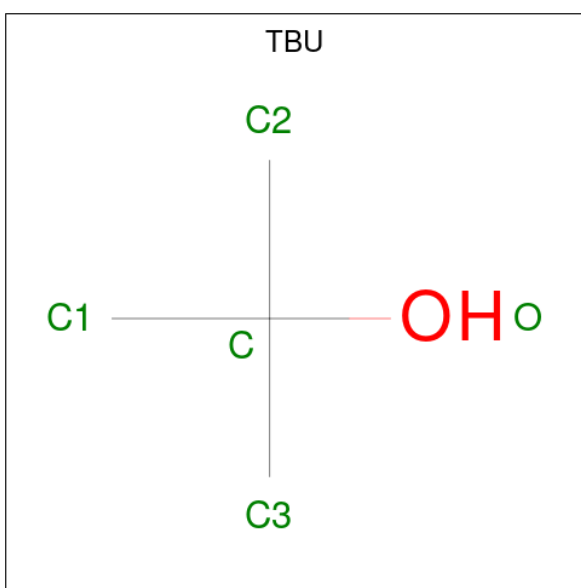
Chain	Residue	Modelled	Actual	Comment	Reference
C	43	TRW	TRP	modified residue	GB 17402570

- Molecule 4 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 5 is TERTIARY-BUTYL ALCOHOL (CCD ID: 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		

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

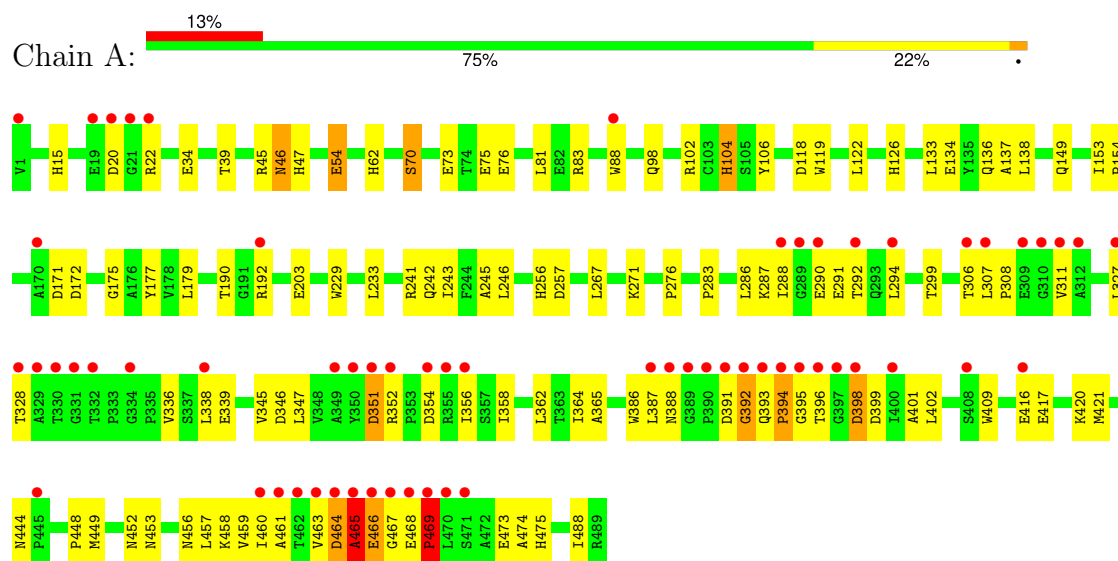
- Molecule 6 is water.

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

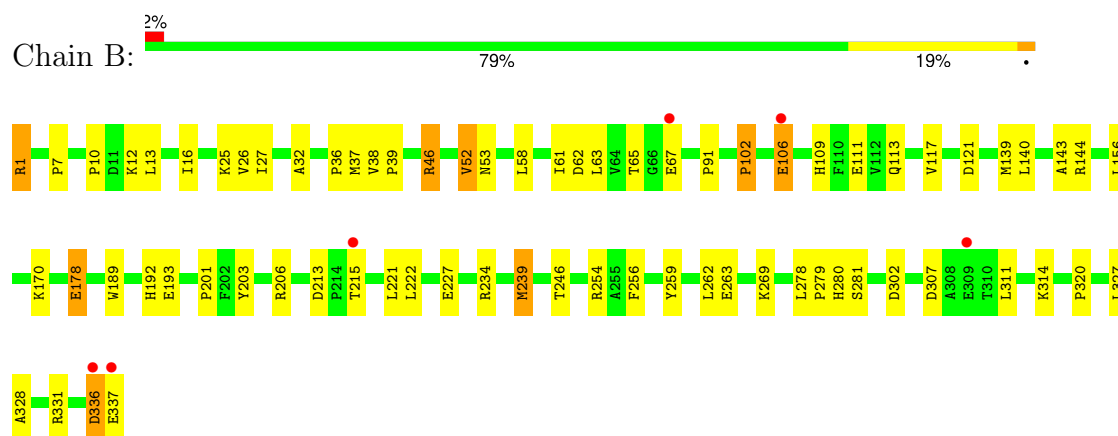
3 Residue-property plots

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.

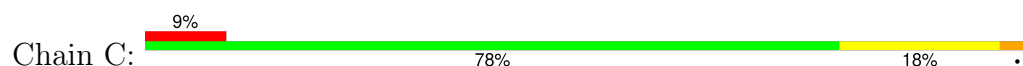
- Molecule 1: quinoxemoprotein amine dehydrogenase 60 kDa subunit

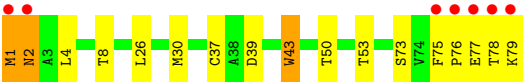


- Molecule 2: quinoxemoprotein amine dehydrogenase 40 kDa subunit



- Molecule 3: quinoxemoprotein amine dehydrogenase 9 kDa subunit





4 Data and refinement statistics

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) 90.3 (36.42-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.191 , 0.224 0.189 , 0.220	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)	0.33 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: HEC, TRW, TBU

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	0.66	6/3828 (0.2%)	1.01	22/5209 (0.4%)
2	B	0.54	0/2722	0.92	8/3702 (0.2%)
3	C	0.61	0/622	0.98	3/850 (0.4%)
All	All	0.61	6/7172 (0.1%)	0.98	33/9761 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	HIS	CE1-NE2	12.32	1.44	1.32
1	A	126	HIS	CE1-NE2	12.32	1.44	1.32
1	A	104	HIS	CE1-NE2	12.01	1.44	1.32
1	A	104	HIS	ND1-CE1	5.98	1.38	1.32
1	A	15	HIS	ND1-CE1	5.82	1.38	1.32
1	A	126	HIS	ND1-CE1	5.68	1.38	1.32

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	HIS	ND1-CG-CD2	14.02	120.12	106.10
1	A	126	HIS	ND1-CG-CD2	13.99	120.09	106.10
1	A	104	HIS	ND1-CG-CD2	13.92	120.02	106.10
1	A	464	ASP	N-CA-C	10.96	125.97	109.63
1	A	104	HIS	CB-CG-CD2	-9.94	118.27	131.20
1	A	126	HIS	CB-CG-CD2	-9.53	118.81	131.20
1	A	15	HIS	CB-CG-CD2	-9.52	118.83	131.20
1	A	203	GLU	N-CA-C	-7.27	98.71	110.20
1	A	465	ALA	N-CA-C	7.13	126.00	110.80
3	C	53	THR	N-CA-C	6.80	118.69	111.28
1	A	365	ALA	N-CA-C	-6.67	99.17	109.24
1	A	70	SER	N-CA-C	-6.57	102.05	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	143	ALA	N-CA-C	-6.41	101.46	110.50
1	A	106	TYR	N-CA-C	-6.38	104.98	112.89
2	B	193	GLU	N-CA-C	6.30	118.96	111.33
2	B	38	VAL	N-CA-C	6.14	114.23	108.15
1	A	15	HIS	CG-CD2-NE2	-5.96	101.24	107.20
1	A	126	HIS	CG-CD2-NE2	-5.94	101.26	107.20
2	B	140	LEU	N-CA-C	-5.81	99.93	109.40
1	A	190	THR	N-CA-C	-5.72	101.45	109.69
2	B	239	MET	N-CA-C	5.72	117.38	109.15
3	C	26	LEU	N-CA-C	-5.68	103.20	110.53
1	A	104	HIS	CG-CD2-NE2	-5.58	101.62	107.20
2	B	12	LYS	N-CA-C	5.50	118.04	109.52
3	C	73	SER	N-CA-C	-5.45	101.58	110.20
1	A	245	ALA	N-CA-C	-5.40	100.89	109.59
1	A	351	ASP	N-CA-C	-5.38	106.40	113.12
1	A	457	LEU	N-CA-C	5.37	118.03	110.14
1	A	126	HIS	CG-ND1-CE1	-5.18	100.48	109.30
2	B	121	ASP	N-CA-C	-5.18	102.18	109.96
2	B	117	VAL	N-CA-C	-5.16	100.88	108.11
1	A	104	HIS	CG-ND1-CE1	-5.16	100.53	109.30
1	A	15	HIS	CG-ND1-CE1	-5.12	100.59	109.30

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	124	0
2	B	2668	0	2656	63	0
3	C	628	0	562	25	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	101	0	0	1	0
All	All	8443	0	6926	199	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 (199) 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:175:GLY:HA3	1:A:271:LYS:HZ1	1.35	0.91
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
2:B:254:ARG:HH11	2:B:254:ARG:HG3	1.43	0.82
1:A:467:GLY:C	1:A:469:PRO:HD3	2.05	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
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
1:A:466:GLU:C	1:A:468:GLU:H	1.96	0.72
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
2:B:178[A]:GLU:H	2:B:178[A]:GLU:CD	2.01	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLN:NE2	1:A:398:ASP:HB3	2.09	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
3:C:1:MET:HE1	3:C:8:THR:O	1.97	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
1:A:122:LEU:HD21	4:A:992:HEC:HMA3	1.77	0.64
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:213:ASP:CG	2:B:215[B]:THR:HG22	2.22	0.64
2:B:156:LEU:HB3	2:B:170:LYS:HB2	1.79	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
1:A:346:ASP:C	1:A:347:LEU:HD22	2.28	0.59
3:C:75:PHE:C	3:C:77:GLU:H	2.11	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
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
2:B:262[B]:LEU:C	2:B:262[B]:LEU:HD23	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:C	1:A:267:LEU:HD12	2.31	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:54:GLU:H	1:A:54:GLU:CD	2.13	0.55
1:A:393:GLN:HE22	1:A:398:ASP:C	2.15	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:133[B]:LEU:C	1:A:133[B]:LEU:HD12	2.32	0.54
1:A:283:PRO:HG2	1:A:294:LEU:CD2	2.38	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
3:C:1:MET:SD	3:C:1:MET:N	2.81	0.53
1:A:45:ARG:HH11	1:A:46:ASN:HD21	1.56	0.53
2:B:222:LEU:C	2:B:222:LEU:HD23	2.34	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
1:A:466:GLU:C	1:A:468:GLU:N	2.66	0.53
3:C:1:MET:HB2	3:C:4:LEU:HB2	1.90	0.53
1:A:179:LEU:HD12	1:A:179:LEU:C	2.34	0.52
1:A:352:ARG:HD2	1:A:352:ARG:C	2.34	0.52
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
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
2:B:58:LEU:C	2:B:58:LEU:HD23	2.35	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
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:133[A]:LEU:C	1:A:133[A]:LEU:HD23	2.36	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:458:LYS:HD2	1:A:473:GLU:CD	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:C:1:MET:HE2	6:C:178: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:393:GLN:O	1:A:394:PRO:C	2.56	0.48
1:A:417:GLU:HG2	6:A:2146:HOH:O	2.13	0.48
1:A:393:GLN:NE2	1:A:399:ASP:OD1	2.47	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
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
2:B:201:PRO:HD3	2:B:246:THR:HG23	1.96	0.47
1:A:286:LEU:HD21	1:A:294:LEU:HD11	1.95	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:75:GLU:O	1:A:76:GLU:HB2	2.14	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:338:LEU:C	1:A:338:LEU:HD12	2.40	0.46
1:A:393:GLN:CD	1:A:398:ASP:HB3	2.40	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
1:A:70:SER:OG	1:A:73:GLU:HG3	2.16	0.45
1:A:171:ASP:CG	1:A:172:ASP:H	2.24	0.45
2:B:91:PRO:HB3	2:B:144:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:133[B]:LEU:HD12	1:A:134:GLU:N	2.33	0.44
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
1:A:421:MET:HE1	1:A:448:PRO:HG2	2.00	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:449:MET:HE3	2:B:278:LEU:O	2.19	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
1:A:387:LEU:O	1:A:388:ASN:C	2.62	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:392:GLY:C	1:A:394:PRO:HD3	2.45	0.42
1:A:104:HIS:CD2	4:A:992:HEC:ND	2.87	0.41
1:A:459:VAL:C	1:A:460:ILE:HD12	2.44	0.41
1:A:39:THR:HG21	4:A:991:HEC:CMA	2.50	0.41
2:B:109:HIS:HD2	6:B:2031:HOH:O	2.03	0.41
3:C:1:MET:HB3	3:C:4:LEU:CG	2.48	0.41
1:A:401:ALA:C	1:A:402:LEU:HD12	2.46	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:449:MET:HA	2:B:279:PRO:O	2.20	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:354:ASP:CG	1:A:388:ASN:ND2	2.79	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%)	10	2
2	B	343/337 (102%)	326 (95%)	12 (4%)	5 (2%)	8	1
3	C	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	9	2
All	All	911/905 (101%)	857 (94%)	42 (5%)	12 (1%)	10	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 ⓘ

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%)	373 (98%)	6 (2%)	55	41
2	B	287/279 (103%)	278 (97%)	9 (3%)	35	18
3	C	65/64 (102%)	63 (97%)	2 (3%)	35	18
All	All	731/718 (102%)	714 (98%)	17 (2%)	47	27

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

Mol	Chain	Res	Type
1	A	46	ASN
1	A	54	GLU
1	A	118	ASP
1	A	246	LEU
1	A	464	ASP
1	A	469	PRO
2	B	1	ARG
2	B	46	ARG
2	B	63	LEU
2	B	106	GLU
2	B	178[A]	GLU
2	B	178[B]	GLU
2	B	221[A]	LEU
2	B	221[B]	LEU
2	B	234	ARG
3	C	1	MET
3	C	2	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) 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

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Mol	Chain	Res	Type
1	A	47	HIS
1	A	62	HIS
1	A	136	GLN
1	A	149	GLN
1	A	183	GLN
1	A	242	GLN
1	A	256	HIS
1	A	277	GLN
1	A	293	GLN
1	A	320	ASN
1	A	370	ASN
1	A	380	GLN
1	A	393	GLN
1	A	422	GLN
1	A	450	GLN
1	A	452	ASN
1	A	453	ASN
1	A	456	ASN
1	A	475	HIS
2	B	53	ASN
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	$\# Z > 2$
3	TRW	C	43	3	24,25,25	3.24	10 (41%)	24,34,34	1.57	4 (16%)

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	-	0/10/11/11	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	5.86	1.48	1.38
3	C	43	TRW	C5-C6	5.72	1.48	1.38
3	C	43	TRW	O7-CZ2	-5.14	1.25	1.36
3	C	43	TRW	C5-C4	4.25	1.47	1.38
3	C	43	TRW	C4-C3	3.32	1.45	1.38
3	C	43	TRW	CZ3-CE3	2.82	1.43	1.38
3	C	43	TRW	CH2-N6	-2.74	1.31	1.39
3	C	43	TRW	CZ3-CH2	2.57	1.43	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	43	TRW	C6-C1-C2	-3.93	113.83	119.04
3	C	43	TRW	O7-CZ2-CH2	3.51	127.63	118.32
3	C	43	TRW	C3-C2-C1	3.36	123.61	119.73
3	C	43	TRW	C5-C6-C1	2.47	122.58	119.73

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 oligosaccharides 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	$\# Z > 2$
4	HEC	A	991	1	50,50,50	1.21	5 (10%)	68,82,82	0.77	1 (1%)
5	TBU	A	1994	-	4,4,4	0.48	0	6,6,6	0.51	0
5	TBU	A	1993	-	4,4,4	0.47	0	6,6,6	0.53	0
5	TBU	B	1995	-	4,4,4	0.47	0	6,6,6	0.52	0
5	TBU	B	1996	-	4,4,4	0.48	0	6,6,6	0.54	0
4	HEC	A	992	1	50,50,50	1.23	5 (10%)	68,82,82	0.80	1 (1%)

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	991	1	1/1/3/7	6/14/54/54	-
4	HEC	A	992	1	1/1/3/7	4/14/54/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	992	HEC	FE-NA	2.76	2.04	1.95
4	A	991	HEC	CMC-C2C	2.63	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	992	HEC	CMC-C2C	2.53	1.56	1.50
4	A	991	HEC	FE-NB	2.42	2.02	1.94
4	A	991	HEC	FE-NA	2.32	2.02	1.95
4	A	992	HEC	FE-NB	2.31	2.02	1.94
4	A	991	HEC	O2A-CGA	-2.12	1.23	1.30
4	A	992	HEC	O2A-CGA	-2.12	1.23	1.30
4	A	992	HEC	O1A-CGA	2.08	1.28	1.22
4	A	991	HEC	CBD-CAD	2.02	1.58	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	991	HEC	O1A-CGA-CBA	-2.73	114.44	123.09
4	A	992	HEC	O1A-CGA-CBA	-2.49	115.18	123.09

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	991	HEC	NA
4	A	992	HEC	NA

All (10) torsion outliers are listed below:

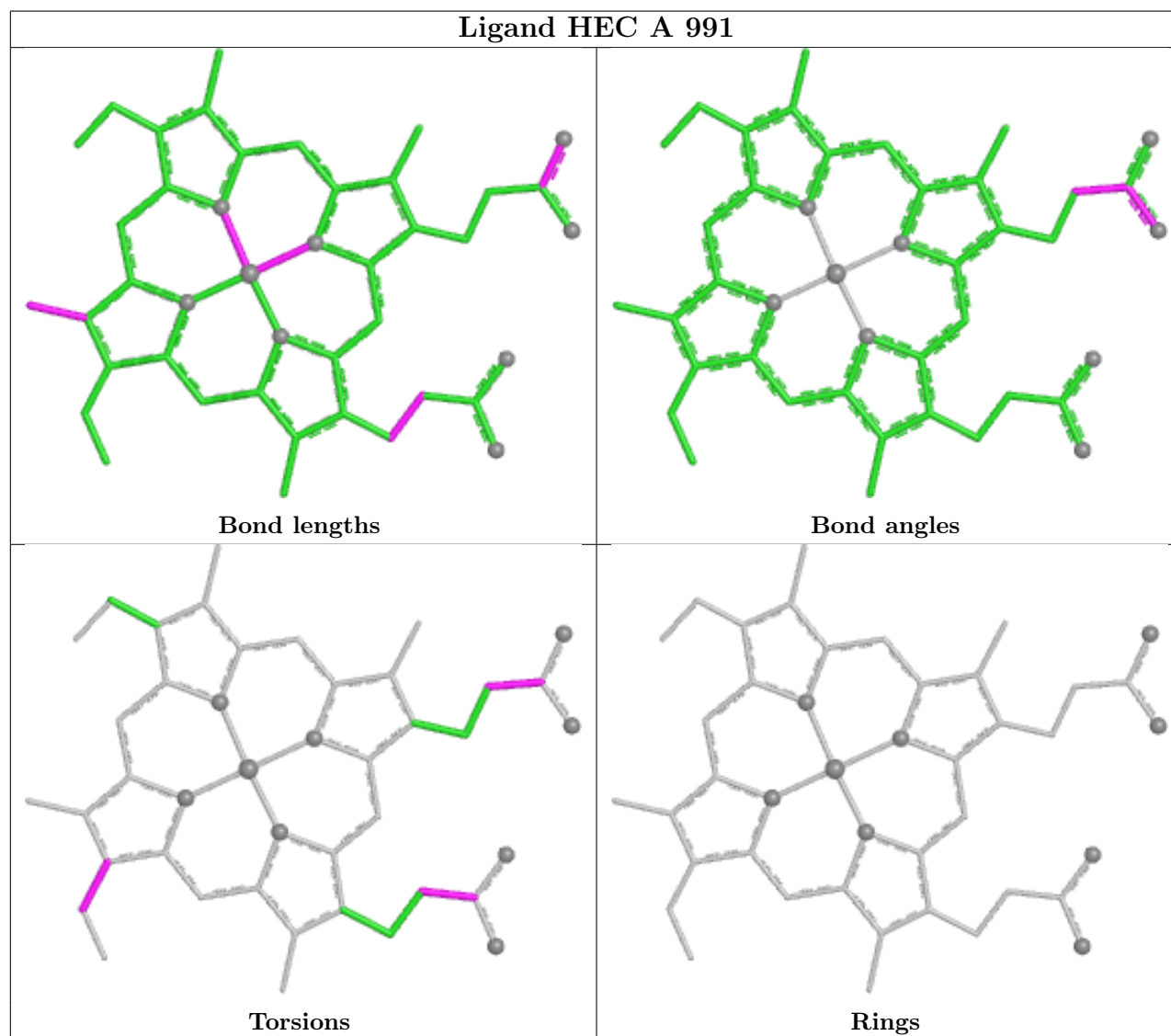
Mol	Chain	Res	Type	Atoms
4	A	992	HEC	CAD-CBD-CGD-O2D
4	A	991	HEC	CAA-CBA-CGA-O1A
4	A	992	HEC	CAD-CBD-CGD-O1D
4	A	991	HEC	CAA-CBA-CGA-O2A
4	A	991	HEC	CAD-CBD-CGD-O1D
4	A	991	HEC	C4C-C3C-CAC-CBC
4	A	991	HEC	CAD-CBD-CGD-O2D
4	A	992	HEC	CAA-CBA-CGA-O2A
4	A	991	HEC	C2C-C3C-CAC-CBC
4	A	992	HEC	CAA-CBA-CGA-O1A

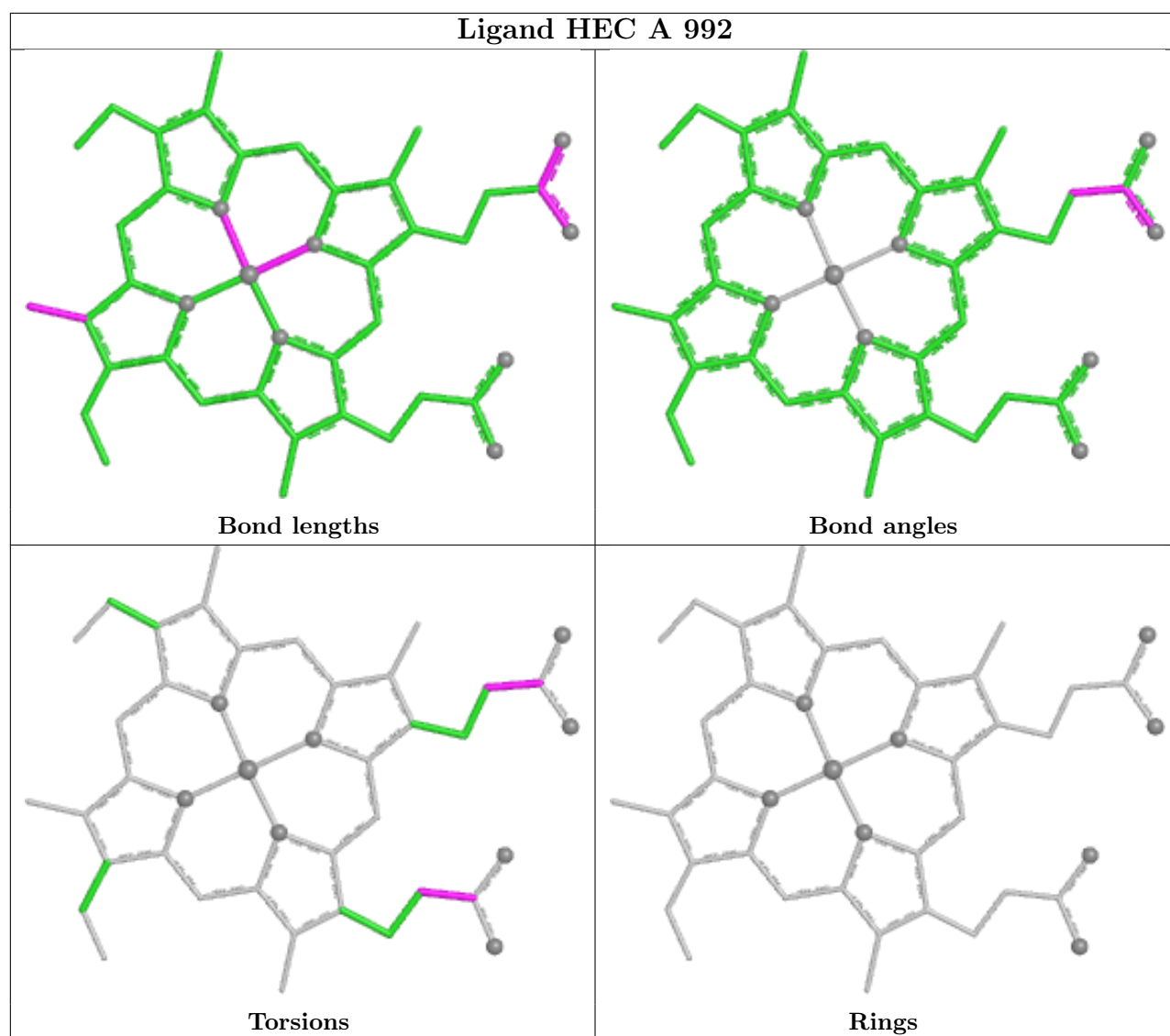
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	991	HEC	2	0
4	A	992	HEC	2	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 than 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.





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, 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	489/489 (100%)	0.59	62 (12%) 8 7	5, 19, 43, 60	4 (0%)
2	B	337/337 (100%)	-0.02	6 (1%) 67 72	7, 17, 27, 44	8 (2%)
3	C	78/79 (98%)	0.37	7 (8%) 15 16	8, 16, 41, 53	1 (1%)
All	All	904/905 (99%)	0.34	75 (8%) 17 18	5, 18, 39, 60	13 (1%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	469	PRO	10.0
1	A	465	ALA	9.3
3	C	1	MET	7.9
1	A	467	GLY	7.7
3	C	78	THR	7.5
1	A	392	GLY	7.4
1	A	463	VAL	6.3
3	C	79	LYS	5.7
1	A	390	PRO	5.5
3	C	76	PRO	5.4
3	C	2	ASN	5.3
1	A	389	GLY	5.1
1	A	466	GLU	5.0
1	A	464	ASP	5.0
1	A	468	GLU	4.6
3	C	77	GLU	4.4
1	A	397	GLY	4.2
1	A	462	THR	4.0
1	A	398	ASP	3.8
1	A	290	GLU	3.8
1	A	354	ASP	3.7
1	A	470	LEU	3.7
1	A	351	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	337	GLU	3.5
1	A	21	GLY	3.5
1	A	19	GLU	3.3
1	A	461	ALA	3.2
1	A	311	VAL	3.2
1	A	352	ARG	3.2
1	A	391	ASP	3.2
1	A	288	ILE	3.1
1	A	388	ASN	3.1
1	A	292	THR	3.1
1	A	393	GLN	3.0
1	A	289	GLY	3.0
1	A	394	PRO	2.9
3	C	75	PHE	2.8
1	A	350	TYR	2.8
2	B	215[A]	THR	2.8
1	A	88[A]	TRP	2.8
1	A	387	LEU	2.8
1	A	22	ARG	2.7
1	A	307	LEU	2.7
1	A	356	ILE	2.7
1	A	408	SER	2.6
1	A	396	THR	2.6
1	A	294	LEU	2.6
1	A	328	THR	2.5
1	A	471	SER	2.5
1	A	460	ILE	2.5
2	B	67	GLU	2.5
1	A	170	ALA	2.5
1	A	331	GLY	2.5
1	A	327	LEU	2.5
2	B	106	GLU	2.4
1	A	310	GLY	2.4
2	B	336	ASP	2.4
1	A	349	ALA	2.4
2	B	309	GLU	2.4
1	A	1	VAL	2.4
1	A	416	GLU	2.3
1	A	306	THR	2.3
1	A	445	PRO	2.3
1	A	309	GLU	2.3
1	A	332	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	338	LEU	2.2
1	A	192	ARG	2.2
1	A	395	GLY	2.2
1	A	312	ALA	2.1
1	A	330	THR	2.1
1	A	400	ILE	2.1
1	A	329	ALA	2.1
1	A	334	GLY	2.1
1	A	355	ARG	2.1
1	A	20	ASP	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, 95th 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	0.07	10,13,17,18	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

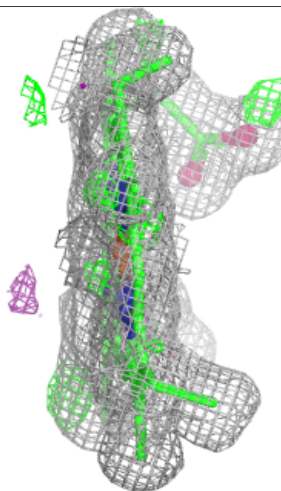
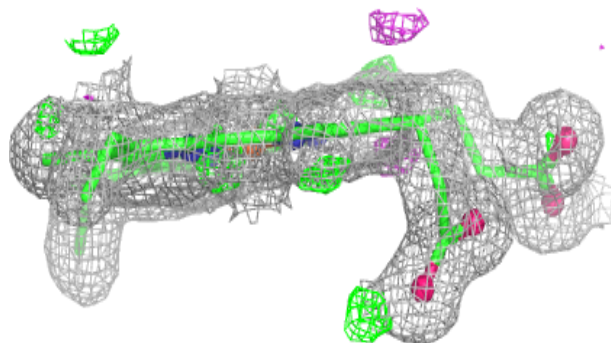
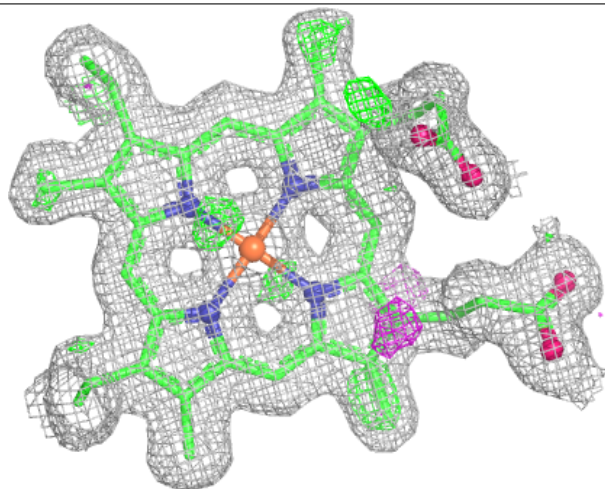
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	0.76	0.20	45,45,46,46	0
5	TBU	B	1995	5/5	0.77	0.25	46,46,46,46	0
5	TBU	A	1993	5/5	0.82	0.17	41,41,41,41	0
5	TBU	A	1994	5/5	0.85	0.18	36,36,36,36	0
4	HEC	A	991	43/43	0.97	0.08	12,14,17,18	0
4	HEC	A	992	43/43	0.98	0.06	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.

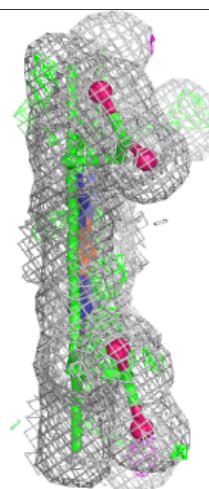
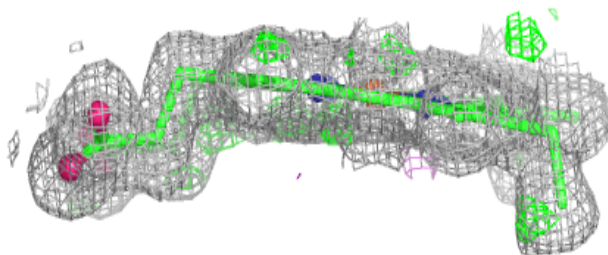
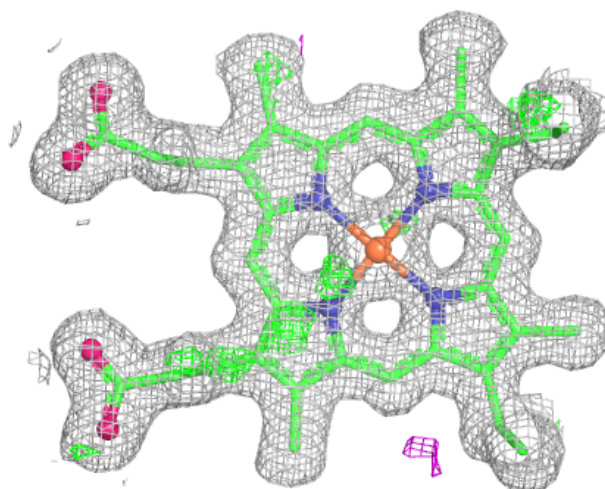
Electron density around HEC A 991:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.