Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 12:53 AM GMT

PDB ID	:	2C1U
Title	:	CRYSTAL STRUCTURE OF THE DI-HAEM CYTOCHROME C PEROXIDASE FROM PARACOCCUS PANTOTROPHUS - OXIDISED FORM
Authors	:	Echalier, A.; Fulop, V.
Deposited on	:	2005-09-21
Resolution	:	1.95 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 (i)) were used in the production of this report:

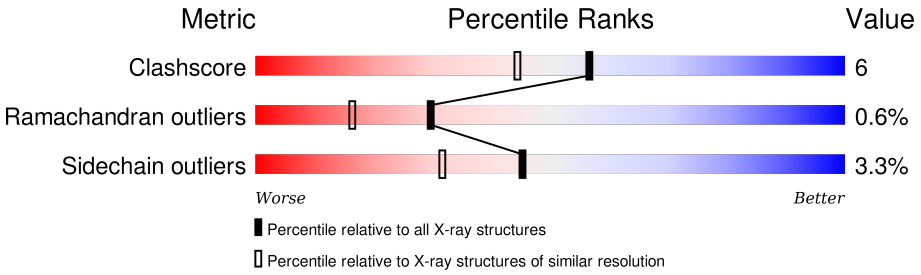
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	338	86% 10% • •
1	B	338	78% 17% • •
1	C	338	81% 14% • • •
1	D	338	80% 14% • 5%

2 Entry composition (i)

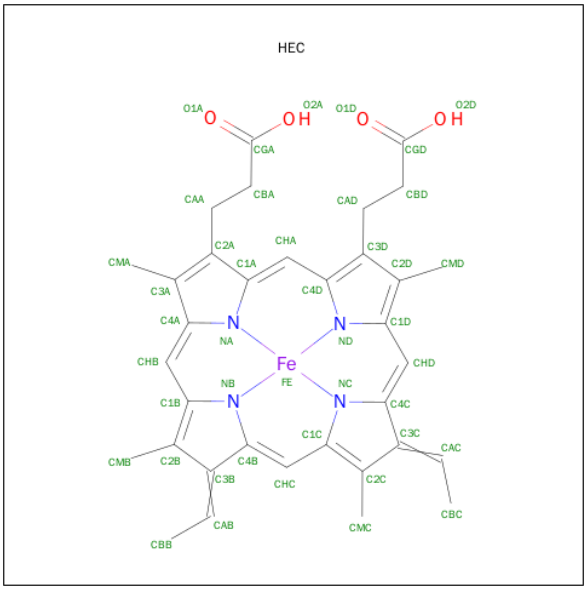
There are 4 unique types of molecules in this entry. The entry contains 11016 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DI-HAEM CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2479	1566	415	486	12			
1	B	324	Total	C	N	O	S	0	0	0
			2446	1545	410	479	12			
1	C	329	Total	C	N	O	S	0	0	0
			2479	1567	415	485	12			
1	D	322	Total	C	N	O	S	0	0	0
			2431	1537	408	474	12			

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	208	Total	O	0	0
			208	208		
4	B	199	Total	O	0	0
			199	199		
4	C	221	Total	O	0	0
			221	221		
4	D	205	Total	O	0	0
			205	205		

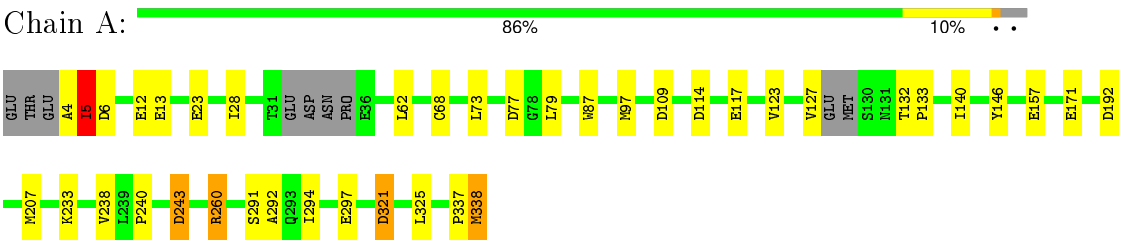
3 Residue-property plots (i)

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.

Note EDS was not executed.

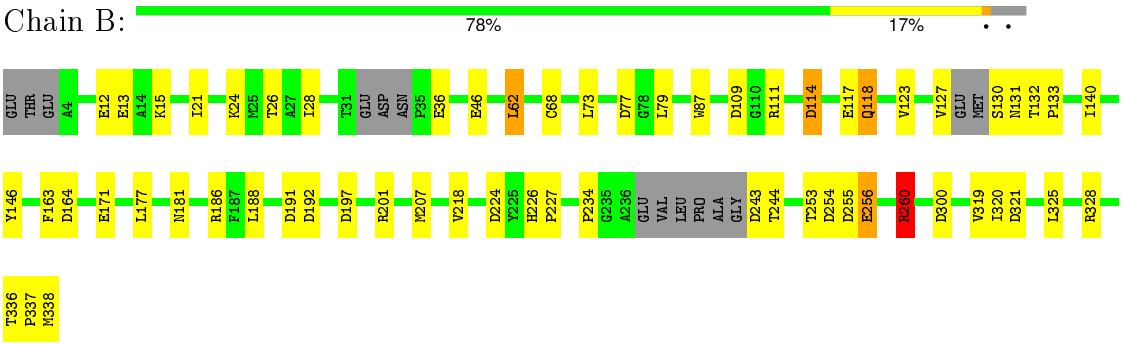
• Molecule 1: DI-HAEM CYTOCHROME C PEROXIDASE

Chain A:



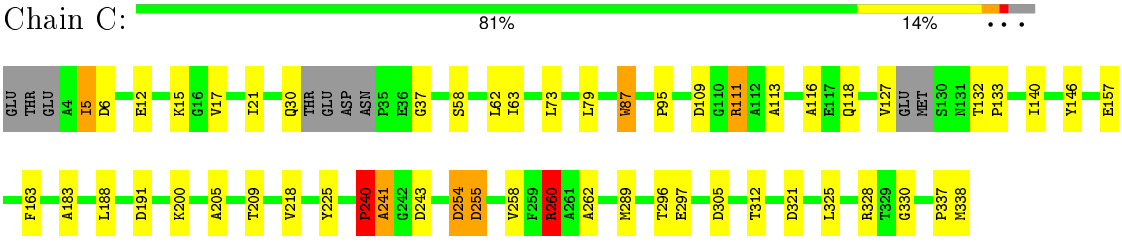
• Molecule 1: DI-HAEM CYTOCHROME C PEROXIDASE

Chain B:



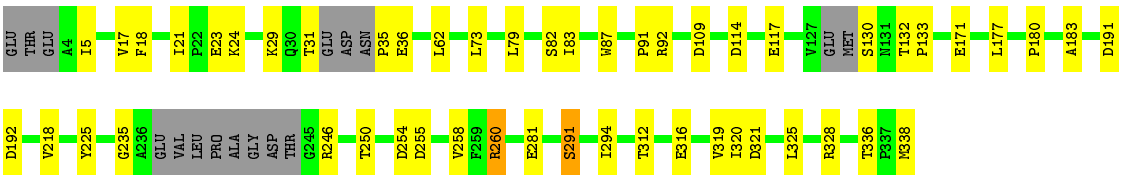
• Molecule 1: DI-HAEM CYTOCHROME C PEROXIDASE

Chain C:



• Molecule 1: DI-HAEM CYTOCHROME C PEROXIDASE

Chain D:


GLU THR GLU A4 I5 V17 F18 I21 P22 E23 K24 K29 Q30 T31 GLU ASP ASN P35 E36 L62 L73 L79 S82 I83 W87 P91 R92 D109 D114 E117 V127 GLU MET S130 N131 T132 P133 E171 L177 P180 A183 D191
D192 V218 Y225 G235 A236 GLU VAL LEU PRO ALA GLY ASP THR G245 R246 T250 D254 D255 V258 P259 R260 E281 S291 I294 T312 E316 V319 I320 D321 L325 R328 T336 P337 M338

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.80Å 51.10Å 167.90Å 90.00° 98.20° 90.00°	Depositor
Resolution (Å)	29.88 – 1.95	Depositor
% Data completeness (in resolution range)	88.6 (29.88-1.95)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.169 , 0.220	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11016	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, HEC

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	0.74	0/2535	0.89	8/3449 (0.2%)
1	B	0.72	0/2501	0.89	10/3400 (0.3%)
1	C	0.80	2/2536 (0.1%)	0.89	10/3450 (0.3%)
1	D	0.71	0/2486	0.87	10/3379 (0.3%)
All	All	0.74	2/10058 (0.0%)	0.88	38/13678 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	12	GLU	CD-OE2	11.62	1.38	1.25
1	C	12	GLU	CD-OE1	5.39	1.31	1.25

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	260	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	B	328	ARG	NE-CZ-NH1	9.75	125.18	120.30
1	B	328	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	C	328	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	321	ASP	CB-CG-OD2	7.02	124.61	118.30
1	B	260	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	D	260	ARG	NE-CZ-NH2	-6.81	116.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	328	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	C	260	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	D	191	ASP	CB-CG-OD2	6.15	123.84	118.30
1	D	260	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	C	321	ASP	CB-CG-OD2	6.03	123.72	118.30
1	C	328	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	109	ASP	CB-CG-OD2	5.84	123.56	118.30
1	D	109	ASP	CB-CG-OD2	5.73	123.46	118.30
1	B	164	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	300	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	243	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	191	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	192	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	260	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	197	ASP	CB-CG-OD2	5.54	123.28	118.30
1	C	260	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	109	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	6	ASP	CB-CG-OD2	5.47	123.22	118.30
1	C	254	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	192	ASP	CB-CG-OD2	5.37	123.14	118.30
1	B	109	ASP	CB-CG-OD2	5.32	123.09	118.30
1	D	254	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	305	ASP	CB-CG-OD2	5.26	123.03	118.30
1	D	92	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	D	255	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	243	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	191	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	192	ASP	CB-CG-OD2	5.12	122.91	118.30
1	C	255	ASP	CB-CG-OD2	5.11	122.89	118.30
1	A	114	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	321	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	234	PRO	Peptide

5.2 Too-close contacts (i)

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	2479	0	2392	24	0
1	B	2446	0	2358	33	0
1	C	2479	0	2393	38	0
1	D	2431	0	2347	31	0
2	A	86	0	60	5	0
2	B	86	0	60	6	0
2	C	86	0	60	7	0
2	D	86	0	60	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	208	0	0	2	0
4	B	199	0	0	4	0
4	C	221	0	0	3	0
4	D	205	0	0	3	0
All	All	11016	0	9730	122	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 (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:THR:O	1:C:297:GLU:HG2	1.48	1.12
1:D:83:ILE:CD1	1:D:91:PRO:HA	1.96	0.96
1:D:83:ILE:HD13	1:D:91:PRO:HA	1.59	0.83
1:D:83:ILE:HD11	1:D:91:PRO:CA	2.13	0.79
1:C:79:LEU:HD11	1:D:62:LEU:HG	1.69	0.74
1:D:180:PRO:O	1:D:316:GLU:HG3	1.88	0.73
1:B:127:VAL:HG11	1:B:163:PHE:CE2	2.28	0.69
1:C:297:GLU:HG3	4:C:2188:HOH:O	1.91	0.68
1:B:260:ARG:HD2	4:B:2143:HOH:O	1.92	0.68
1:D:117:GLU:HG2	1:D:117:GLU:O	1.95	0.66
1:D:83:ILE:HD11	1:D:91:PRO:HA	1.70	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ARG:HH11	1:C:111:ARG:HG2	1.61	0.66
1:D:260:ARG:HD2	4:D:2141:HOH:O	1.95	0.65
1:A:132:THR:OG1	1:A:133:PRO:HD3	1.95	0.65
1:B:227:PRO:HB3	1:B:255:ASP:HA	1.77	0.65
1:B:140:ILE:HG23	1:B:146:TYR:HB3	1.79	0.65
1:A:337:PRO:O	1:A:338:MET:HB2	1.97	0.64
1:C:240:PRO:O	1:C:241:ALA:HB2	1.98	0.63
1:C:330:GLY:HA2	1:D:281:GLU:OE2	1.98	0.63
1:B:13:GLU:HG2	1:B:207:MET:SD	2.38	0.63
2:A:402:HEC:HBB3	2:A:402:HEC:HMB1	1.80	0.63
1:A:62:LEU:HG	1:B:79:LEU:HD11	1.80	0.62
1:A:292:ALA:HA	1:A:297:GLU:OE2	1.99	0.62
1:C:87:TRP:HE1	1:C:118:GLN:HE21	1.48	0.60
1:C:62:LEU:HG	1:D:79:LEU:HD11	1.85	0.59
2:D:401:HEC:HMB1	2:D:401:HEC:HBB3	1.84	0.58
1:C:337:PRO:O	1:C:338:MET:HB3	2.03	0.58
1:C:205:ALA:O	1:C:209:THR:HG23	2.04	0.58
1:A:321:ASP:OD1	1:B:321:ASP:OD1	2.21	0.58
1:C:5:ILE:HG21	1:C:200:LYS:HD3	1.86	0.57
1:D:246:ARG:HH11	1:D:246:ARG:HB2	1.69	0.57
1:C:21:ILE:HD13	1:C:218:VAL:HG22	1.85	0.57
2:B:401:HEC:HMC1	2:B:401:HEC:HBC3	1.87	0.56
1:C:15:LYS:HG2	1:C:188:LEU:HD22	1.88	0.56
1:C:111:ARG:NH1	1:C:111:ARG:HG2	2.19	0.56
1:C:260:ARG:HD2	4:C:2165:HOH:O	2.04	0.56
1:A:5:ILE:HG23	1:A:5:ILE:O	2.05	0.56
1:B:68:CYS:HA	1:B:77:ASP:HB3	1.88	0.55
2:B:402:HEC:HBB3	2:B:402:HEC:HMB1	1.88	0.55
1:A:127:VAL:HG12	1:A:133:PRO:HG3	1.89	0.54
1:B:123:VAL:CG2	2:B:401:HEC:HMB2	2.38	0.54
1:A:123:VAL:HG21	2:A:401:HEC:HMB2	1.90	0.54
1:D:83:ILE:CD1	1:D:91:PRO:CA	2.70	0.54
1:B:132:THR:HB	1:B:133:PRO:HD3	1.89	0.54
2:C:402:HEC:HMB1	2:C:402:HEC:HBB3	1.89	0.53
1:D:235:GLY:HA3	4:D:2133:HOH:O	2.07	0.53
1:D:132:THR:HB	1:D:133:PRO:HD3	1.90	0.52
1:B:201:ARG:HD3	4:B:2130:HOH:O	2.10	0.52
1:D:83:ILE:HD11	1:D:91:PRO:N	2.24	0.52
1:A:73:LEU:HG	1:B:325:LEU:HD12	1.92	0.52
1:B:114:ASP:N	1:B:114:ASP:OD1	2.43	0.52
1:B:260:ARG:HH22	2:B:401:HEC:CGA	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:HEC:HBC3	2:A:401:HEC:HMC1	1.91	0.51
1:B:15:LYS:HG3	1:B:188:LEU:HD22	1.92	0.51
1:C:260:ARG:CD	4:C:2165:HOH:O	2.57	0.51
1:B:177:LEU:HD21	1:B:320:ILE:HD11	1.91	0.51
1:D:21:ILE:HD13	1:D:218:VAL:HG22	1.93	0.51
2:B:401:HEC:HMB1	2:B:401:HEC:HBB3	1.94	0.50
1:C:127:VAL:HG12	1:C:133:PRO:HG3	1.92	0.50
1:B:130:SER:HB2	4:B:2083:HOH:O	2.11	0.49
1:A:123:VAL:CG2	2:A:401:HEC:HMB2	2.43	0.49
1:B:21:ILE:HD13	1:B:218:VAL:HG22	1.94	0.49
1:C:325:LEU:HD12	1:D:73:LEU:HG	1.94	0.49
1:B:123:VAL:HG21	2:B:401:HEC:HMB2	1.94	0.48
1:C:240:PRO:HG2	1:C:243:ASP:OD2	2.13	0.48
1:C:262:ALA:HB3	2:C:402:HEC:HBA1	1.96	0.48
1:C:254:ASP:O	1:C:255:ASP:HB2	2.14	0.48
1:A:97:MET:HE1	2:A:401:HEC:CHB	2.44	0.47
1:D:82:SER:O	1:D:83:ILE:HD13	2.14	0.47
1:A:140:ILE:HG23	1:A:146:TYR:HB3	1.95	0.47
1:C:240:PRO:O	1:C:241:ALA:CB	2.63	0.47
1:A:325:LEU:HD12	1:B:73:LEU:HG	1.96	0.47
1:A:12:GLU:OE1	1:D:24:LYS:NZ	2.43	0.47
1:A:23:GLU:HG3	4:A:2016:HOH:O	2.13	0.47
1:A:238:VAL:O	1:A:238:VAL:CG1	2.61	0.47
1:A:291:SER:HB3	1:A:294:ILE:HG12	1.97	0.47
1:B:111:ARG:HB2	1:B:114:ASP:OD1	2.15	0.47
1:D:291:SER:HB3	1:D:294:ILE:HG12	1.96	0.46
1:B:117:GLU:O	1:B:118:GLN:HB2	2.15	0.46
1:C:127:VAL:HG11	1:C:163:PHE:CE2	2.51	0.46
1:C:73:LEU:HG	1:D:325:LEU:HD12	1.98	0.46
1:D:177:LEU:HD21	1:D:320:ILE:HD11	1.98	0.46
1:C:337:PRO:O	1:C:338:MET:CB	2.64	0.45
1:C:183:ALA:HB3	1:C:312:THR:HB	1.98	0.45
1:C:225:TYR:HB3	1:C:258:VAL:HB	1.98	0.45
1:B:13:GLU:HG2	1:B:207:MET:CE	2.47	0.45
1:C:113:ALA:O	1:C:116:ALA:HB3	2.17	0.44
1:D:17:VAL:HG13	1:D:18:PHE:CD2	2.53	0.44
1:A:68:CYS:HA	1:A:77:ASP:HB3	1.99	0.44
1:A:79:LEU:HD11	1:B:62:LEU:HG	2.00	0.44
1:A:238:VAL:HG12	1:A:238:VAL:O	2.18	0.43
1:B:336:THR:HG22	1:B:338:MET:H	1.83	0.43
1:B:181:ASN:O	1:B:186:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:401:HEC:HMB1	2:C:401:HEC:HBB3	2.01	0.43
1:D:29:LYS:HE3	1:D:171:GLU:OE2	2.19	0.43
1:A:233:LYS:HD3	4:A:2146:HOH:O	2.19	0.42
1:B:28:ILE:HD12	1:B:171:GLU:HG2	2.01	0.42
1:D:336:THR:HG22	1:D:338:MET:H	1.84	0.42
1:C:30:GLN:HG3	1:C:37:GLY:HA3	2.02	0.42
1:C:58:SER:HB3	1:C:63:ILE:O	2.19	0.42
1:B:224:ASP:HB2	4:B:2136:HOH:O	2.20	0.42
1:D:183:ALA:HB3	1:D:312:THR:HB	2.02	0.42
1:B:226:HIS:HA	1:B:227:PRO:HD3	1.85	0.42
1:C:260:ARG:HH22	2:C:401:HEC:CGA	2.32	0.42
1:B:337:PRO:O	1:B:338:MET:CB	2.67	0.42
1:D:83:ILE:O	2:D:401:HEC:HBC2	2.20	0.41
1:C:262:ALA:CB	2:C:402:HEC:HBA1	2.49	0.41
1:C:95:PRO:HG2	2:C:401:HEC:HBA1	2.02	0.41
1:B:254:ASP:O	1:B:255:ASP:HB2	2.20	0.41
1:D:225:TYR:HB3	1:D:258:VAL:HB	2.03	0.41
1:C:140:ILE:HG23	1:C:146:TYR:HB3	2.02	0.41
1:D:87:TRP:HB2	4:D:2078:HOH:O	2.19	0.41
1:C:62:LEU:CG	1:D:79:LEU:HD11	2.50	0.41
1:C:289:MET:HG3	2:C:402:HEC:C4A	2.50	0.41
1:D:31:THR:HG1	1:D:35:PRO:N	2.17	0.41
1:B:256:GLU:CD	1:B:256:GLU:H	2.24	0.41
1:C:132:THR:O	1:C:133:PRO:C	2.59	0.41
1:C:296:THR:C	1:C:297:GLU:HG2	2.30	0.41
1:A:4:ALA:O	1:A:5:ILE:HG22	2.20	0.40
1:A:28:ILE:HD12	1:A:171:GLU:HG2	2.04	0.40
1:A:13:GLU:HG2	1:A:207:MET:SD	2.62	0.40
1:B:13:GLU:HG2	1:B:207:MET:HE3	2.03	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	323/338 (96%)	309 (96%)	12 (4%)	2 (1%)	30 16
1	B	316/338 (94%)	299 (95%)	15 (5%)	2 (1%)	30 16
1	C	323/338 (96%)	312 (97%)	8 (2%)	3 (1%)	21 9
1	D	314/338 (93%)	300 (96%)	13 (4%)	1 (0%)	46 35
All	All	1276/1352 (94%)	1220 (96%)	48 (4%)	8 (1%)	30 16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	C	5	ILE
1	C	240	PRO
1	C	241	ALA
1	B	244	THR
1	B	118	GLN
1	D	5	ILE
1	A	240	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	258/267 (97%)	251 (97%)	7 (3%)	52 41
1	B	255/267 (96%)	242 (95%)	13 (5%)	29 13
1	C	258/267 (97%)	251 (97%)	7 (3%)	52 41
1	D	253/267 (95%)	246 (97%)	7 (3%)	51 39
All	All	1024/1068 (96%)	990 (97%)	34 (3%)	45 32

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	87	TRP
1	A	117	GLU

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Mol	Chain	Res	Type
1	A	157	GLU
1	A	243	ASP
1	A	260	ARG
1	A	338	MET
1	B	12	GLU
1	B	24	LYS
1	B	26	THR
1	B	36	GLU
1	B	46	GLU
1	B	62	LEU
1	B	87	TRP
1	B	114	ASP
1	B	131	ASN
1	B	253	THR
1	B	256	GLU
1	B	260	ARG
1	B	319	VAL
1	C	6	ASP
1	C	17	VAL
1	C	87	TRP
1	C	111	ARG
1	C	157	GLU
1	C	240	PRO
1	C	260	ARG
1	D	23	GLU
1	D	36	GLU
1	D	114	ASP
1	D	130	SER
1	D	250	THR
1	D	291	SER
1	D	319	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	30	GLN
1	B	106	GLN
1	B	131	ASN
1	C	118	GLN
1	D	181	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	$\#\|Z\| > 2$
2	HEC	A	401	1	24,50,50	2.34	5 (20%)	19,82,82	2.82	6 (31%)
2	HEC	A	402	1	24,50,50	2.52	4 (16%)	19,82,82	2.70	4 (21%)
2	HEC	B	401	1	24,50,50	2.25	5 (20%)	19,82,82	3.45	9 (47%)
2	HEC	B	402	1	24,50,50	2.21	6 (25%)	19,82,82	2.57	5 (26%)
2	HEC	C	401	1	24,50,50	2.69	8 (33%)	19,82,82	2.74	6 (31%)
2	HEC	C	402	1	24,50,50	2.33	8 (33%)	19,82,82	2.97	9 (47%)
2	HEC	D	401	1	24,50,50	2.42	5 (20%)	19,82,82	3.29	8 (42%)
2	HEC	D	402	1	24,50,50	2.12	3 (12%)	19,82,82	2.53	5 (26%)

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
2	HEC	A	401	1	-	0/6/54/54	0/0/8/8
2	HEC	A	402	1	-	0/6/54/54	0/0/8/8
2	HEC	B	401	1	-	0/6/54/54	0/0/8/8
2	HEC	B	402	1	-	0/6/54/54	0/0/8/8
2	HEC	C	401	1	-	0/6/54/54	0/0/8/8
2	HEC	C	402	1	-	0/6/54/54	0/0/8/8
2	HEC	D	401	1	-	0/6/54/54	0/0/8/8
2	HEC	D	402	1	-	0/6/54/54	0/0/8/8

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	HEC	C3B-C2B	-7.94	1.32	1.40
2	A	402	HEC	C3B-C2B	-7.22	1.33	1.40
2	A	401	HEC	C3B-C2B	-7.15	1.33	1.40
2	C	401	HEC	C3C-C2C	-6.51	1.34	1.40
2	C	402	HEC	C3B-C2B	-6.43	1.34	1.40
2	B	401	HEC	C3B-C2B	-6.40	1.34	1.40
2	D	402	HEC	C3B-C2B	-5.79	1.34	1.40
2	C	401	HEC	C3B-C2B	-5.62	1.34	1.40
2	B	402	HEC	C3B-C2B	-5.49	1.35	1.40
2	A	402	HEC	C3C-C2C	-5.45	1.35	1.40
2	B	402	HEC	C3C-C2C	-5.06	1.35	1.40
2	D	402	HEC	C3C-C2C	-4.94	1.35	1.40
2	B	401	HEC	C3C-C2C	-4.87	1.35	1.40
2	D	401	HEC	C3C-C2C	-4.12	1.36	1.40
2	C	402	HEC	C3C-C2C	-3.96	1.36	1.40
2	A	401	HEC	C3C-C2C	-3.72	1.36	1.40
2	C	402	HEC	C1A-NA	2.05	1.39	1.36
2	B	402	HEC	C3C-C4C	2.05	1.47	1.42
2	B	402	HEC	C4C-NC	2.16	1.39	1.36
2	C	402	HEC	C3C-C4C	2.20	1.47	1.42
2	B	401	HEC	C4B-NB	2.23	1.39	1.36
2	C	401	HEC	CMA-C3A	2.27	1.56	1.51
2	C	402	HEC	CMA-C3A	2.29	1.56	1.51
2	D	401	HEC	CAD-C3D	2.31	1.56	1.52
2	D	401	HEC	CAA-C2A	2.32	1.56	1.52
2	A	401	HEC	CAA-C2A	2.34	1.56	1.52
2	C	401	HEC	CAA-C2A	2.46	1.57	1.52
2	B	401	HEC	CMA-C3A	2.47	1.57	1.51
2	C	402	HEC	CMC-C2C	2.51	1.57	1.51
2	A	401	HEC	CMA-C3A	2.51	1.57	1.51
2	C	402	HEC	C4C-NC	2.58	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	HEC	CMD-C2D	2.75	1.57	1.51
2	A	402	HEC	CAD-C3D	3.05	1.57	1.52
2	C	401	HEC	C3C-C4C	3.09	1.49	1.42
2	C	401	HEC	C4B-NB	3.10	1.40	1.36
2	B	402	HEC	C3D-C2D	4.60	1.51	1.37
2	D	402	HEC	C3D-C2D	4.60	1.51	1.37
2	B	401	HEC	C3D-C2D	4.78	1.51	1.37
2	D	401	HEC	C3D-C2D	5.09	1.52	1.37
2	C	401	HEC	CMC-C2C	5.25	1.63	1.51
2	A	401	HEC	C3D-C2D	5.25	1.53	1.37
2	C	401	HEC	C3D-C2D	5.25	1.53	1.37
2	A	402	HEC	C3D-C2D	5.37	1.53	1.37
2	C	402	HEC	C3D-C2D	5.53	1.54	1.37

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	HEC	CBB-CAB-C3B	-9.64	105.93	127.35
2	D	401	HEC	CBB-CAB-C3B	-9.02	107.30	127.35
2	A	402	HEC	CBB-CAB-C3B	-8.20	109.14	127.35
2	A	401	HEC	CBB-CAB-C3B	-7.82	109.96	127.35
2	D	402	HEC	CBB-CAB-C3B	-7.27	111.19	127.35
2	C	402	HEC	CBB-CAB-C3B	-7.18	111.39	127.35
2	C	401	HEC	CBB-CAB-C3B	-7.16	111.43	127.35
2	B	402	HEC	CBB-CAB-C3B	-6.91	111.98	127.35
2	C	402	HEC	CBC-CAC-C3C	-6.36	113.21	127.35
2	D	401	HEC	CMC-C2C-C1C	-6.29	117.96	128.36
2	D	402	HEC	CBC-CAC-C3C	-5.50	115.14	127.35
2	B	401	HEC	CBD-CAD-C3D	-5.06	103.46	112.53
2	A	401	HEC	CMB-C2B-C1B	-5.06	120.00	128.36
2	A	402	HEC	CBC-CAC-C3C	-4.99	116.26	127.35
2	B	401	HEC	CMC-C2C-C1C	-4.98	120.12	128.36
2	B	402	HEC	CBD-CAD-C3D	-4.62	104.25	112.53
2	C	402	HEC	CBD-CAD-C3D	-4.38	104.67	112.53
2	D	401	HEC	CBC-CAC-C3C	-4.37	117.64	127.35
2	B	401	HEC	CBC-CAC-C3C	-4.35	117.68	127.35
2	C	401	HEC	CBD-CAD-C3D	-4.33	104.77	112.53
2	D	401	HEC	CBD-CAD-C3D	-4.22	104.96	112.53
2	A	401	HEC	CBD-CAD-C3D	-4.15	105.08	112.53
2	A	402	HEC	CBD-CAD-C3D	-4.01	105.34	112.53
2	B	401	HEC	CAD-CBD-CGD	-3.96	105.48	112.75
2	C	401	HEC	CMB-C2B-C1B	-3.94	121.85	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	402	HEC	CBC-CAC-C3C	-3.88	118.73	127.35
2	D	401	HEC	CBA-CAA-C2A	-3.79	105.73	112.53
2	B	402	HEC	CAA-C2A-C1A	-3.79	122.90	127.01
2	B	401	HEC	CBA-CAA-C2A	-3.75	105.81	112.53
2	A	401	HEC	CMC-C2C-C1C	-3.72	122.20	128.36
2	C	402	HEC	CBA-CAA-C2A	-3.66	105.97	112.53
2	A	401	HEC	CBC-CAC-C3C	-3.57	119.42	127.35
2	C	401	HEC	CBA-CAA-C2A	-3.35	106.52	112.53
2	D	401	HEC	CMB-C2B-C1B	-3.16	123.13	128.36
2	B	401	HEC	CMB-C2B-C1B	-3.12	123.20	128.36
2	A	402	HEC	CBA-CAA-C2A	-3.05	107.07	112.53
2	C	402	HEC	CMB-C2B-C1B	-2.98	123.43	128.36
2	D	402	HEC	CBD-CAD-C3D	-2.89	107.35	112.53
2	B	401	HEC	CAA-C2A-C1A	-2.81	123.95	127.01
2	D	402	HEC	CMC-C2C-C1C	-2.80	123.74	128.36
2	C	402	HEC	CMC-C2C-C1C	-2.70	123.90	128.36
2	D	401	HEC	CAA-C2A-C1A	-2.59	124.19	127.01
2	C	402	HEC	CMD-C2D-C1D	-2.40	124.40	128.36
2	C	401	HEC	CAD-C3D-C2D	-2.13	122.93	129.00
2	C	402	HEC	CAA-C2A-C1A	-2.10	124.73	127.01
2	D	402	HEC	CAA-C2A-C1A	-2.08	124.75	127.01
2	A	401	HEC	CBA-CAA-C2A	-2.07	108.81	112.53
2	D	401	HEC	CAD-CBD-CGD	-2.02	109.04	112.75
2	C	402	HEC	CMD-C2D-C3D	2.19	129.82	125.24
2	B	401	HEC	CMA-C3A-C2A	2.27	129.99	125.24
2	B	402	HEC	CAA-CBA-CGA	2.40	117.14	112.75
2	C	401	HEC	CAD-C3D-C4D	4.78	132.19	127.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEC	4	0
2	A	402	HEC	1	0
2	B	401	HEC	5	0
2	B	402	HEC	1	0
2	C	401	HEC	3	0
2	C	402	HEC	4	0
2	D	401	HEC	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.