Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 08:02 AM EST

PDB ID	:	1B4U
Title	:	PROTOCATECHUATE 4,5-DIOXYGENASE (LIGAB) IN COMPLEX WITH PROTOCATECHUATE (PCA)
Authors	:	Sugimoto, K.; Senda, T.; Mitsui, Y.
Deposited on	:	1998-12-29
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

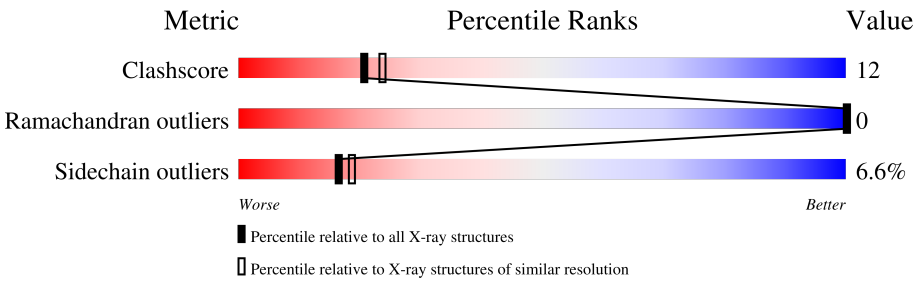
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	139	69% 22% • 5%
1	C	139	72% 17% 6% 5%
2	B	302	72% 22% • ••
2	D	302	66% 26% 6% ••

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6897 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 PROTOCATECHUATE 4,5-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	132	1029	646	177	199	7	0	0	0
1	C	132	1029	646	177	199	7	0	0	0

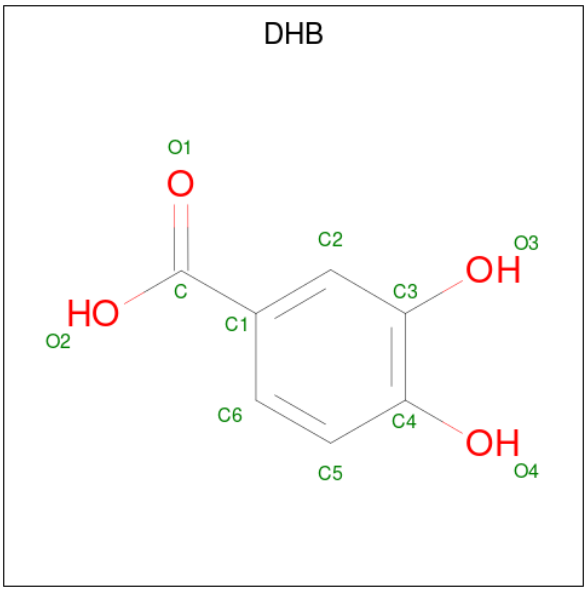
- Molecule 2 is a protein called PROTOCATECHUATE 4,5-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	298	2313	1482	385	430	16	0	0	0
2	D	298	2313	1482	385	430	16	0	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
3	B	1	1	1	0	0
3	D	1	1	1	0	0

- Molecule 4 is 3,4-DIHYDROXYBENZOIC ACID (three-letter code: DHB) (formula: $C_7H_6O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 11 7 4	0	0
4	D	1	Total C O 11 7 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	36	Total O 36 36	0	0
5	B	68	Total O 68 68	0	0
5	C	29	Total O 29 29	0	0
5	D	56	Total O 56 56	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. 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. 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: PROTOCATECHUATE 4,5-DIOXYGENASE

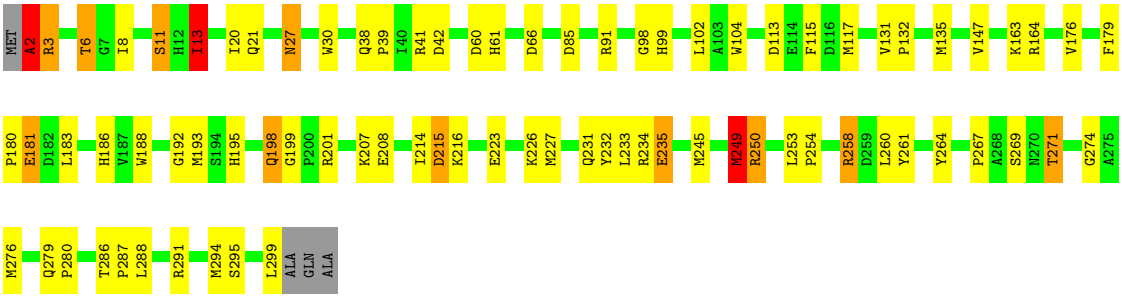
Chain A:

• Molecule 1: PROTOCATECHUATE 4,5-DIOXYGENASE

Chain C:

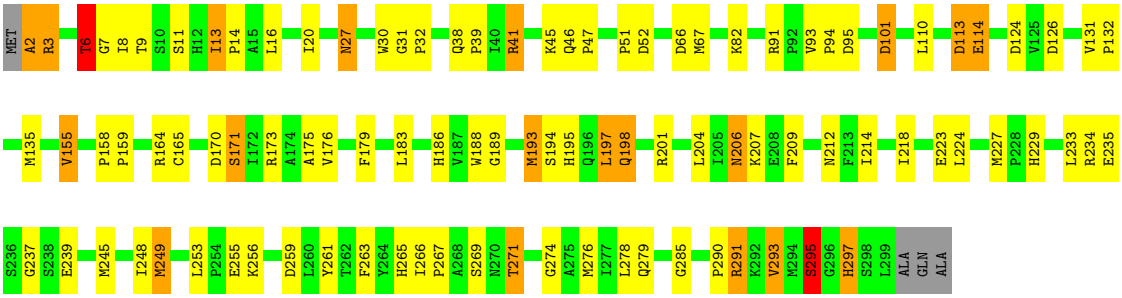
• Molecule 2: PROTOCATECHUATE 4,5-DIOXYGENASE

Chain B:



• Molecule 2: PROTOCATECHUATE 4,5-DIOXYGENASE

Chain D:


MET A2 R3 T6 G7 I8 T9 S10 S11 H12 I13 P14 A15 L16 I20 N27 W30 G31 P32 Q38 P39 I40 R41 K45 Q46 P47 P51 D52 D66 M67 K82 R91 P92 V93 P94 D95 D101 L110 D113 E114 D124 V125 D126 V131 P132
M135 V155 P158 P159 R164 C165 D170 S171 I172 R173 A174 A175 V176 F179 L183 H186 V187 W188 G189 M193 S194 H195 Q196 L197 Q198 R201 L204 I205 N206 K207 E208 F209 N212 F213 I214 I218 E223 L224 M227 P228 H229 L233 R234 E235
S236 G237 S238 E239 M245 I248 M249 L253 P254 E255 K256 D259 L260 Y261 T262 F263 Y264 H265 I266 P267 A268 S269 N270 T271 G274 A275 M276 I277 L278 Q279 G285 P290 R291 K292 V293 M294 S295 G296 H297 S298 L299 ALA GLN ALA

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.40Å 66.50Å 119.80Å 90.00° 92.50° 90.00°	Depositor
Resolution (Å)	60.00 – 2.20	Depositor
% Data completeness (in resolution range)	91.0 (60.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.161 , 0.220	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6897	wwPDB-VP
Average B, all atoms ($Å^2$)	28.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.88	0/1049	1.83	27/1408 (1.9%)
1	C	0.70	0/1049	1.61	14/1408 (1.0%)
2	B	0.88	0/2383	1.94	41/3253 (1.3%)
2	D	0.79	2/2383 (0.1%)	1.81	43/3253 (1.3%)
All	All	0.83	2/6864 (0.0%)	1.83	125/9322 (1.3%)

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
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	ARG	CD-NE	-5.84	1.36	1.46
2	D	245	MET	CG-SD	-5.68	1.66	1.81

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	291	ARG	CD-NE-CZ	38.73	177.83	123.60
2	B	258	ARG	CD-NE-CZ	24.80	158.33	123.60
2	B	91	ARG	CD-NE-CZ	22.01	154.42	123.60
2	B	234	ARG	NE-CZ-NH1	21.99	131.29	120.30
1	A	133	ARG	NE-CZ-NH1	20.57	130.59	120.30
2	B	41	ARG	CD-NE-CZ	18.20	149.07	123.60
2	B	201	ARG	NE-CZ-NH2	-17.67	111.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	41	ARG	NE-CZ-NH2	-17.47	111.56	120.30
2	D	201	ARG	NE-CZ-NH2	-17.06	111.77	120.30
2	B	258	ARG	NE-CZ-NH1	16.82	128.71	120.30
2	B	258	ARG	NE-CZ-NH2	-16.59	112.00	120.30
2	D	91	ARG	CD-NE-CZ	16.21	146.29	123.60
2	B	41	ARG	NE-CZ-NH1	15.96	128.28	120.30
2	B	291	ARG	NE-CZ-NH1	-15.71	112.45	120.30
2	D	234	ARG	NE-CZ-NH2	-14.65	112.98	120.30
2	D	91	ARG	NE-CZ-NH2	-14.56	113.02	120.30
2	D	41	ARG	NE-CZ-NH1	14.24	127.42	120.30
1	A	133	ARG	NE-CZ-NH2	-14.05	113.28	120.30
1	C	133	ARG	NE-CZ-NH2	-13.88	113.36	120.30
1	C	90	TYR	CB-CG-CD2	13.73	129.24	121.00
1	C	90	TYR	CB-CG-CD1	-13.34	113.00	121.00
2	D	245	MET	CA-CB-CG	-13.04	91.14	113.30
2	D	201	ARG	CD-NE-CZ	12.97	141.76	123.60
2	B	234	ARG	NE-CZ-NH2	-12.64	113.98	120.30
2	D	41	ARG	NE-CZ-NH2	-11.86	114.37	120.30
2	B	215	ASP	CB-CG-OD1	-11.04	108.37	118.30
2	D	67	MET	CG-SD-CE	11.00	117.80	100.20
2	B	91	ARG	NE-CZ-NH1	-10.85	114.88	120.30
1	A	77	ARG	NE-CZ-NH2	-10.75	114.93	120.30
2	B	215	ASP	CB-CG-OD2	-10.64	108.73	118.30
1	C	24	ARG	NE-CZ-NH2	-10.56	115.02	120.30
2	B	215	ASP	OD1-CG-OD2	10.29	142.86	123.30
2	D	234	ARG	NE-CZ-NH1	10.10	125.35	120.30
2	B	66	ASP	CB-CG-OD1	10.01	127.31	118.30
2	D	101	ASP	CB-CG-OD1	9.86	127.18	118.30
2	B	85	ASP	CB-CG-OD1	9.71	127.04	118.30
2	B	249	MET	CG-SD-CE	9.58	115.53	100.20
2	B	245	MET	CA-CB-CG	-9.48	97.18	113.30
1	A	77	ARG	NE-CZ-NH1	9.44	125.02	120.30
2	D	66	ASP	CB-CG-OD1	8.43	125.88	118.30
1	A	50	ARG	NE-CZ-NH2	8.41	124.51	120.30
2	B	276	MET	CA-CB-CG	8.30	127.41	113.30
1	A	57	GLU	OE1-CD-OE2	-8.24	113.41	123.30
2	D	245	MET	CG-SD-CE	8.15	113.24	100.20
2	B	258	ARG	CG-CD-NE	7.92	128.42	111.80
2	B	11	SER	CB-CA-C	7.58	124.51	110.10
1	C	32	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	A	54	LYS	CD-CE-NZ	7.55	129.08	111.70
1	C	50	ARG	CD-NE-CZ	7.50	134.10	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	60	ASP	CB-CG-OD2	-7.45	111.60	118.30
2	B	42	ASP	CB-CG-OD1	7.36	124.93	118.30
1	A	56	ASP	CB-CG-OD1	7.30	124.87	118.30
2	B	235	GLU	CA-CB-CG	7.24	129.33	113.40
2	B	2	ALA	N-CA-CB	7.18	120.15	110.10
1	A	35	TYR	CB-CG-CD1	7.13	125.28	121.00
2	D	170	ASP	CB-CG-OD2	-7.04	111.97	118.30
2	D	201	ARG	NH1-CZ-NH2	6.98	127.08	119.40
1	C	127	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	A	35	TYR	CB-CG-CD2	-6.91	116.86	121.00
2	B	181	GLU	OE1-CD-OE2	-6.89	115.03	123.30
2	D	52	ASP	CB-CG-OD1	-6.78	112.19	118.30
2	B	41	ARG	CB-CG-CD	6.75	129.15	111.60
1	A	24	ARG	NE-CZ-NH1	-6.60	117.00	120.30
2	D	234	ARG	CD-NE-CZ	6.60	132.84	123.60
2	B	3	ARG	N-CA-CB	-6.55	98.80	110.60
2	D	173	ARG	NE-CZ-NH2	-6.55	117.02	120.30
2	B	164	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	C	97	SER	N-CA-CB	6.49	120.23	110.50
1	A	62	ASP	CB-CG-OD1	6.46	124.11	118.30
2	D	114	GLU	OE1-CD-OE2	-6.30	115.75	123.30
2	B	201	ARG	CB-CG-CD	-6.29	95.26	111.60
2	D	297	HIS	CA-CB-CG	6.27	124.26	113.60
1	A	118	TYR	CB-CG-CD1	-6.27	117.24	121.00
2	D	235	GLU	OE1-CD-OE2	-6.26	115.79	123.30
2	B	11	SER	CA-CB-OG	-6.18	94.51	111.20
2	D	261	TYR	CB-CG-CD2	6.14	124.68	121.00
1	A	50	ARG	NE-CZ-NH1	-6.13	117.24	120.30
2	B	245	MET	CG-SD-CE	6.12	110.00	100.20
2	B	113	ASP	CB-CG-OD2	-6.08	112.82	118.30
2	D	124	ASP	CB-CG-OD1	6.03	123.73	118.30
2	B	91	ARG	CB-CA-C	-6.03	98.34	110.40
2	D	66	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	C	30	ARG	NE-CZ-NH1	-5.97	117.32	120.30
2	D	170	ASP	CB-CG-OD1	5.97	123.67	118.30
1	C	79	TYR	CB-CG-CD1	-5.96	117.42	121.00
2	D	3	ARG	NE-CZ-NH2	-5.93	117.34	120.30
2	B	201	ARG	NH1-CZ-NH2	5.92	125.91	119.40
2	B	91	ARG	N-CA-CB	5.91	121.24	110.60
2	D	212	ASN	OD1-CG-ND2	5.89	135.45	121.90
2	B	13	ILE	CA-CB-CG2	5.79	122.47	110.90
1	A	82	MET	CG-SD-CE	-5.78	90.96	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	ALA	N-CA-CB	5.72	118.11	110.10
1	A	90	TYR	CB-CG-CD1	-5.71	117.58	121.00
2	D	193	MET	CG-SD-CE	5.70	109.32	100.20
1	C	78	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	45	MET	CA-CB-CG	-5.66	103.68	113.30
1	C	133	ARG	CD-NE-CZ	5.65	131.51	123.60
1	A	118	TYR	CG-CD1-CE1	-5.65	116.78	121.30
1	A	9	ASP	CB-CG-OD1	5.63	123.37	118.30
2	D	95	ASP	CB-CG-OD1	5.63	123.36	118.30
2	B	91	ARG	NH1-CZ-NH2	5.60	125.56	119.40
1	C	52	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	C	133	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	D	126	ASP	CB-CG-OD1	5.57	123.31	118.30
2	D	175	ALA	N-CA-CB	-5.56	102.31	110.10
1	A	30	ARG	NE-CZ-NH1	-5.56	117.52	120.30
2	D	295	SER	N-CA-CB	5.50	118.75	110.50
2	D	155	VAL	CA-CB-CG2	5.49	119.14	110.90
2	D	255	GLU	OE1-CD-OE2	-5.49	116.71	123.30
2	D	91	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	D	293	VAL	CG1-CB-CG2	-5.41	102.25	110.90
2	D	291	ARG	NE-CZ-NH1	5.37	122.99	120.30
2	D	201	ARG	CB-CG-CD	-5.33	97.74	111.60
2	B	291	ARG	NH1-CZ-NH2	5.33	125.26	119.40
1	A	52	ARG	NE-CZ-NH1	-5.32	117.64	120.30
2	D	6	THR	CA-CB-CG2	5.32	119.85	112.40
2	D	223	GLU	OE1-CD-OE2	-5.29	116.95	123.30
2	B	250	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	A	24	ARG	NH1-CZ-NH2	5.27	125.20	119.40
2	D	3	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	24	ARG	CD-NE-CZ	5.21	130.89	123.60
1	A	24	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	52	ARG	CB-CG-CD	5.11	124.90	111.60
1	A	13	TYR	CB-CG-CD2	5.01	124.01	121.00
1	A	96	PHE	CA-CB-CG	5.01	125.93	113.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	2	ALA	Mainchain

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	1029	0	986	18	0
1	C	1029	0	986	29	0
2	B	2313	0	2252	60	0
2	D	2313	0	2252	64	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	11	0	4	3	0
4	D	11	0	4	2	0
5	A	36	0	0	0	0
5	B	68	0	0	0	0
5	C	29	0	0	1	0
5	D	56	0	0	0	0
All	All	6897	0	6484	162	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 12.

All (162) 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:249:MET:HE2	2:B:250:ARG:HA	1.40	1.01
1:C:74:VAL:HG22	1:C:82:MET:HE3	1.41	0.97
2:D:193:MET:HE3	2:D:274:GLY:HA3	1.44	0.95
1:C:114:THR:HG22	1:C:117:GLU:HG2	1.47	0.94
2:B:2:ALA:HB2	2:B:179:PHE:O	1.72	0.90
2:B:13:ILE:CD1	2:B:269:SER:HB3	2.09	0.81
2:D:193:MET:HE1	2:D:214:ILE:HD11	1.61	0.80
1:C:24:ARG:H	2:D:198:GLN:HE22	1.30	0.79
1:C:114:THR:HG22	1:C:117:GLU:H	1.48	0.79
2:D:27:ASN:ND2	2:D:30:TRP:H	1.82	0.76
2:D:7:GLY:HA3	2:D:249:MET:CE	2.15	0.76
2:D:7:GLY:HA3	2:D:249:MET:HE2	1.67	0.75
2:D:193:MET:CE	2:D:274:GLY:HA3	2.17	0.74
2:B:193:MET:CE	2:B:274:GLY:HA3	2.17	0.74
2:B:249:MET:HE2	2:B:250:ARG:CA	2.15	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:LYS:O	1:C:98:THR:HG23	1.88	0.74
1:A:24:ARG:H	2:B:198:GLN:HE22	1.37	0.70
2:B:27:ASN:ND2	2:B:30:TRP:H	1.90	0.69
2:B:193:MET:HE3	2:B:274:GLY:HA3	1.74	0.68
2:B:258:ARG:HG2	2:B:260:LEU:HD23	1.75	0.68
1:A:82:MET:CE	1:A:92:LEU:HD22	2.23	0.67
2:B:13:ILE:HD12	2:B:269:SER:HB3	1.76	0.66
2:D:197:LEU:HD22	2:D:239:GLU:HG2	1.77	0.66
2:B:99:HIS:HD2	2:B:102:LEU:H	1.45	0.64
2:B:20:ILE:HD11	2:B:135:MET:CE	2.28	0.64
2:B:216:LYS:HE3	2:B:223:GLU:OE1	1.98	0.64
2:D:271:THR:HG21	4:D:504:DHB:H2	1.80	0.64
2:D:193:MET:CE	2:D:214:ILE:HD11	2.28	0.63
2:D:6:THR:HB	2:D:279:GLN:HG2	1.81	0.62
2:B:249:MET:HE1	2:B:253:LEU:HD12	1.81	0.61
2:B:2:ALA:HA	2:B:176:VAL:O	2.01	0.61
2:B:195:HIS:HB3	2:B:271:THR:HB	1.84	0.60
2:D:20:ILE:HD11	2:D:135:MET:HE2	1.82	0.60
1:C:50:ARG:HD3	1:C:98:THR:HG22	1.84	0.60
1:A:82:MET:HE1	1:A:92:LEU:HD22	1.85	0.59
2:D:193:MET:HE3	2:D:274:GLY:CA	2.26	0.59
2:B:115:PHE:HB3	2:B:117:MET:CE	2.33	0.59
2:D:263:PHE:HD1	2:D:293:VAL:HG23	1.68	0.59
1:C:129:PRO:O	1:C:133:ARG:HD2	2.03	0.58
1:A:61:LEU:HD21	1:A:74:VAL:HG11	1.85	0.58
2:D:271:THR:HG23	4:D:504:DHB:O1	2.03	0.58
1:A:24:ARG:HH22	1:A:80:ASN:HD22	1.53	0.57
2:B:193:MET:HE2	2:B:274:GLY:HA3	1.85	0.57
1:A:82:MET:HE2	1:A:92:LEU:HD22	1.86	0.57
2:B:6:THR:HB	2:B:279:GLN:HG2	1.85	0.57
2:D:16:LEU:HB3	2:D:135:MET:CE	2.35	0.57
2:B:271:THR:HG21	4:B:503:DHB:H2	1.87	0.57
1:A:74:VAL:HG22	1:A:82:MET:HE3	1.87	0.57
2:D:13:ILE:HD12	2:D:269:SER:HB3	1.87	0.57
2:B:20:ILE:HD11	2:B:135:MET:HE2	1.87	0.56
2:B:193:MET:HE1	2:B:214:ILE:HD11	1.88	0.55
2:D:6:THR:HG23	2:D:186:HIS:NE2	2.21	0.55
2:D:16:LEU:HB3	2:D:135:MET:HE3	1.88	0.55
2:B:115:PHE:HB3	2:B:117:MET:HE2	1.88	0.55
2:D:7:GLY:HA3	2:D:249:MET:HE3	1.88	0.55
2:B:27:ASN:HD22	2:B:27:ASN:C	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:206:ASN:C	2:D:206:ASN:HD22	2.09	0.54
2:D:2:ALA:HA	2:D:176:VAL:O	2.08	0.54
1:C:114:THR:HG22	1:C:117:GLU:CG	2.28	0.54
2:D:46:GLN:HB3	2:D:47:PRO:CD	2.38	0.53
2:D:51:PRO:HB3	2:D:186:HIS:CD2	2.44	0.53
2:D:276:MET:CE	2:D:278:LEU:HD21	2.39	0.53
2:B:193:MET:CE	2:B:214:ILE:HD11	2.38	0.53
2:B:249:MET:HE1	2:B:253:LEU:CD1	2.39	0.53
2:B:20:ILE:HD11	2:B:135:MET:HE1	1.91	0.52
2:D:206:ASN:ND2	2:D:209:PHE:H	2.07	0.52
1:A:90:TYR:CE1	2:B:61:HIS:HD2	2.28	0.52
2:B:249:MET:O	2:B:249:MET:HE3	2.11	0.50
2:D:27:ASN:HD21	2:D:30:TRP:H	1.55	0.50
2:B:2:ALA:HB3	2:B:181:GLU:O	2.11	0.50
1:C:82:MET:CE	1:C:92:LEU:HD22	2.41	0.50
2:B:131:VAL:HB	2:B:132:PRO:HD3	1.94	0.50
2:D:41:ARG:HD2	2:D:135:MET:O	2.12	0.49
1:C:88:ASN:ND2	1:C:90:TYR:HB2	2.27	0.49
2:D:93:VAL:HB	2:D:94:PRO:HD2	1.93	0.49
2:D:207:LYS:HE2	2:D:207:LYS:HB3	1.68	0.48
1:C:114:THR:CG2	1:C:117:GLU:HG2	2.33	0.48
2:B:98:GLY:HA2	2:B:147:VAL:O	2.13	0.48
2:D:13:ILE:HG12	2:D:16:LEU:HG	1.95	0.48
2:D:249:MET:CE	2:D:253:LEU:HD11	2.44	0.48
2:B:193:MET:HE3	2:B:274:GLY:CA	2.41	0.48
2:B:271:THR:HG23	4:B:503:DHB:O1	2.13	0.48
1:C:93:SER:HA	1:C:96:PHE:CE2	2.49	0.48
1:C:44:LEU:HB3	1:C:98:THR:HG21	1.96	0.47
2:B:27:ASN:HD21	2:B:30:TRP:H	1.60	0.47
2:B:286:THR:HG22	2:B:287:PRO:O	2.14	0.47
1:C:13:TYR:OH	2:D:229:HIS:HD2	1.98	0.47
2:D:6:THR:HG23	2:D:186:HIS:CD2	2.50	0.47
1:C:24:ARG:H	2:D:198:GLN:NE2	2.06	0.46
1:C:93:SER:HA	1:C:96:PHE:CZ	2.51	0.46
2:B:271:THR:CG2	4:B:503:DHB:O1	2.63	0.46
1:A:93:SER:HA	1:A:96:PHE:CZ	2.51	0.46
2:D:9:THR:HA	2:D:189:GLY:O	2.16	0.46
1:A:32:ARG:NH2	2:D:101:ASP:OD1	2.47	0.46
1:C:114:THR:H	1:C:117:GLU:CG	2.29	0.45
2:D:131:VAL:HB	2:D:132:PRO:HD3	1.99	0.45
2:B:249:MET:HE2	2:B:250:ARG:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:MET:HB3	2:B:294:MET:HE3	1.80	0.45
2:B:295:SER:O	2:B:299:LEU:HD12	2.17	0.45
1:C:88:ASN:HD21	1:C:90:TYR:HB2	1.81	0.45
2:B:13:ILE:HD11	2:B:269:SER:HB3	1.97	0.45
2:D:2:ALA:HB2	2:D:179:PHE:O	2.17	0.45
2:D:194:SER:O	2:D:195:HIS:HB3	2.16	0.45
1:C:114:THR:N	1:C:117:GLU:OE2	2.45	0.45
2:B:6:THR:HG23	2:B:186:HIS:NE2	2.32	0.45
1:A:88:ASN:ND2	1:A:90:TYR:H	2.14	0.45
2:D:8:ILE:O	2:D:188:TRP:HA	2.17	0.45
2:D:110:LEU:CD2	2:D:171:SER:HB3	2.47	0.45
2:B:227:MET:HG3	2:B:231:GLN:OE1	2.17	0.45
2:B:99:HIS:CD2	2:B:102:LEU:H	2.30	0.44
2:B:261:TYR:HB2	2:B:288:LEU:HD12	1.99	0.44
2:D:276:MET:HE2	2:D:278:LEU:HD21	1.99	0.44
1:C:74:VAL:HG22	1:C:82:MET:CE	2.31	0.44
2:D:38:GLN:N	2:D:39:PRO:CD	2.80	0.44
2:B:254:PRO:HG2	2:B:280:PRO:HB3	1.99	0.44
1:A:82:MET:HE2	1:A:92:LEU:CD2	2.47	0.44
2:D:218:ILE:HD11	2:D:276:MET:CE	2.47	0.44
2:B:179:PHE:CD1	2:B:180:PRO:HD2	2.53	0.43
2:B:38:GLN:HB3	2:B:39:PRO:HD3	2.00	0.43
2:D:113:ASP:OD2	2:D:171:SER:OG	2.35	0.43
2:D:290:PRO:HG2	2:D:293:VAL:CG1	2.48	0.43
1:A:21:PRO:HG2	1:A:132:VAL:C	2.38	0.43
2:D:259:ASP:HA	2:D:278:LEU:HD23	2.01	0.43
1:C:82:MET:HE2	1:C:92:LEU:HD22	2.01	0.43
1:C:133:ARG:HD3	1:C:139:TYR:O	2.19	0.43
2:D:265:HIS:ND1	2:D:295:SER:HB2	2.34	0.43
2:D:266:ILE:HA	2:D:267:PRO:HA	1.76	0.43
2:D:276:MET:HE1	2:D:278:LEU:HD21	2.01	0.42
2:B:13:ILE:HD13	2:B:13:ILE:HG21	1.75	0.42
2:D:279:GLN:HE21	2:D:285:GLY:H	1.67	0.42
2:D:279:GLN:NE2	2:D:285:GLY:H	2.18	0.42
1:A:64:TRP:O	1:A:65:ASN:HB2	2.18	0.42
2:B:8:ILE:O	2:B:188:TRP:HA	2.20	0.42
1:A:114:THR:OG1	1:A:117:GLU:HG3	2.19	0.42
1:A:93:SER:HA	1:A:96:PHE:CE2	2.55	0.42
2:D:13:ILE:HD12	2:D:269:SER:CB	2.48	0.41
1:A:95:LEU:O	1:A:98:THR:HB	2.19	0.41
1:C:114:THR:HG23	5:C:168:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:ILE:CD1	2:D:135:MET:HE2	2.49	0.41
2:D:31:GLY:N	2:D:32:PRO:CD	2.83	0.41
1:C:114:THR:H	1:C:117:GLU:CD	2.23	0.41
2:D:249:MET:HE3	2:D:253:LEU:HD11	2.02	0.41
1:A:80:ASN:HD21	2:B:199:GLY:HA2	1.85	0.41
2:D:165:CYS:HB3	2:D:248:ILE:HG13	2.02	0.41
2:B:192:GLY:HA3	2:B:193:MET:HA	1.89	0.41
2:B:227:MET:HE3	2:B:232:TYR:CZ	2.56	0.41
2:B:104:TRP:CD1	1:C:32:ARG:HD2	2.56	0.41
1:C:111:THR:OG1	1:C:113:MET:HB2	2.21	0.41
2:D:46:GLN:CB	2:D:47:PRO:CD	2.98	0.41
2:B:223:GLU:HA	2:B:226:LYS:HD2	2.01	0.41
2:D:93:VAL:HB	2:D:94:PRO:CD	2.51	0.41
2:D:224:LEU:HD12	2:D:227:MET:HE3	2.03	0.41
2:B:193:MET:HE1	2:B:264:TYR:HD1	1.85	0.40
1:C:49:ASN:HB3	1:C:60:TYR:OH	2.21	0.40
2:B:6:THR:HG22	2:B:279:GLN:HE21	1.86	0.40
2:B:163:LYS:HD3	2:D:114:GLU:OE2	2.21	0.40
2:B:193:MET:HE1	2:B:264:TYR:CD1	2.56	0.40
1:C:25:VAL:O	1:C:30:ARG:HD2	2.22	0.40
2:B:258:ARG:HG2	2:B:260:LEU:CD2	2.47	0.40
1:C:88:ASN:ND2	1:C:90:TYR:H	2.19	0.40
2:D:158:PRO:HA	2:D:159:PRO:HD3	1.93	0.40
2:D:204:LEU:HD23	2:D:237:GLY:CA	2.52	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	130/139 (94%)	126 (97%)	4 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	130/139 (94%)	128 (98%)	2 (2%)	0	100	100
2	B	296/302 (98%)	286 (97%)	10 (3%)	0	100	100
2	D	296/302 (98%)	281 (95%)	15 (5%)	0	100	100
All	All	852/882 (97%)	821 (96%)	31 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	102/109 (94%)	98 (96%)	4 (4%)	32	41
1	C	102/109 (94%)	98 (96%)	4 (4%)	32	41
2	B	253/255 (99%)	237 (94%)	16 (6%)	18	20
2	D	253/255 (99%)	230 (91%)	23 (9%)	9	9
All	All	710/728 (98%)	663 (93%)	47 (7%)	16	19

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	94	LYS
1	A	133	ARG
1	A	136	LYS
2	B	3	ARG
2	B	6	THR
2	B	11	SER
2	B	13	ILE
2	B	21	GLN
2	B	27	ASN
2	B	183	LEU
2	B	198	GLN
2	B	207	LYS

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Mol	Chain	Res	Type
2	B	208	GLU
2	B	215	ASP
2	B	233	LEU
2	B	235	GLU
2	B	249	MET
2	B	267	PRO
2	B	271	THR
1	C	40	PHE
1	C	94	LYS
1	C	114	THR
1	C	116	GLU
2	D	3	ARG
2	D	6	THR
2	D	11	SER
2	D	13	ILE
2	D	14	PRO
2	D	27	ASN
2	D	45	LYS
2	D	82	LYS
2	D	113	ASP
2	D	155	VAL
2	D	164	ARG
2	D	171	SER
2	D	183	LEU
2	D	197	LEU
2	D	198	GLN
2	D	206	ASN
2	D	233	LEU
2	D	249	MET
2	D	256	LYS
2	D	271	THR
2	D	291	ARG
2	D	295	SER
2	D	297	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	88	ASN
1	A	104	GLN
1	A	115	GLN

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Mol	Chain	Res	Type
2	B	27	ASN
2	B	38	GLN
2	B	99	HIS
2	B	121	ASN
2	B	198	GLN
1	C	88	ASN
1	C	104	GLN
2	D	27	ASN
2	D	121	ASN
2	D	122	GLN
2	D	198	GLN
2	D	206	ASN
2	D	229	HIS
2	D	279	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	DHB	B	503	3	11,11,11	1.00	1 (9%)	15,15,15	1.96	5 (33%)
4	DHB	D	504	3	11,11,11	1.23	1 (9%)	15,15,15	1.53	3 (20%)

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	DHB	B	503	3	-	0/4/4/4	0/1/1/1
4	DHB	D	504	3	-	0/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	504	DHB	O3-C3	2.64	1.41	1.36
4	B	503	DHB	C1-C	-2.22	1.44	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	503	DHB	C6-C1-C2	3.89	123.84	119.24
4	D	504	DHB	O2-C-O1	-3.27	116.08	123.35
4	B	503	DHB	O2-C-O1	-3.11	116.44	123.35
4	B	503	DHB	C5-C4-C3	2.85	122.79	119.67
4	D	504	DHB	O2-C-C1	2.75	121.97	114.85
4	D	504	DHB	C2-C3-C4	-2.48	117.67	119.86
4	B	503	DHB	C1-C2-C3	-2.44	118.02	120.09
4	B	503	DHB	C5-C6-C1	-2.26	118.15	120.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	DHB	3	0
4	D	504	DHB	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.