



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:48 PM GMT

PDB ID : 1CJX
Title : CRYSTAL STRUCTURE OF PSEUDOMONAS FLUORESCENS HPPD
Authors : Serre, L.; Sailland, A.; Sy, D.; Boudec, P.; Rolland, A.; Pebay-Peroulla, E.;
Cohen-Addad, C.
Deposited on : 1999-04-20
Resolution : 2.40 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

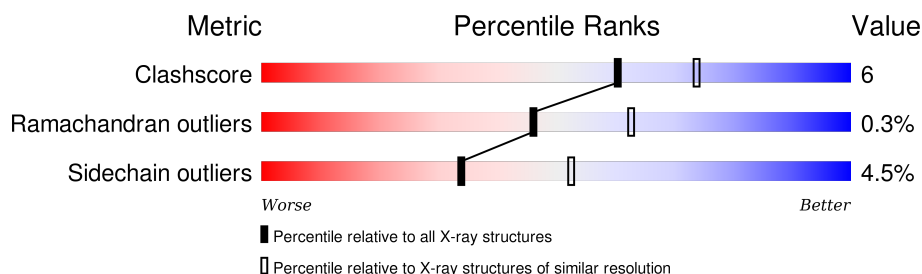
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	357	
1	B	357	
1	C	357	
1	D	357	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11821 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 4-HYDROXYPHENYLPYRUVATE DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	4	1
			2801	1791	474	522	14			
1	B	353	Total	C	N	O	S	34	4	1
			2805	1793	477	521	14			
1	C	353	Total	C	N	O	S	41	4	1
			2806	1794	477	521	14			
1	D	353	Total	C	N	O	S	40	5	1
			2810	1796	477	523	14			

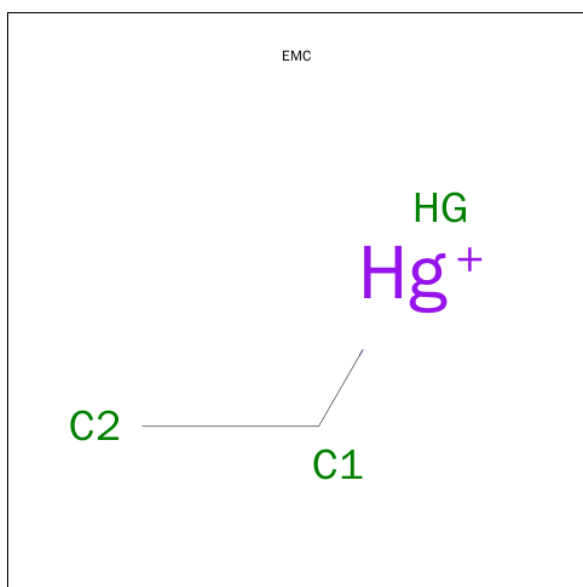
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	ALA	SER	SEE REMARK 999	UNP P80064
B	355	ALA	SER	SEE REMARK 999	UNP P80064
C	355	ALA	SER	SEE REMARK 999	UNP P80064
D	355	ALA	SER	SEE REMARK 999	UNP P80064

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

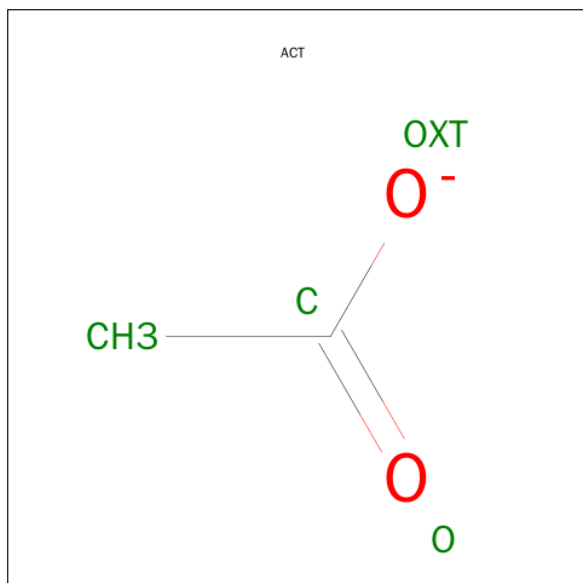
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is ETHYL MERCURY ION (three-letter code: EMC) (formula: C₂H₅Hg).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	Hg	0	0
			3	2	1		
3	B	1	Total	C	Hg	0	0
			3	2	1		
3	C	1	Total	C	Hg	0	0
			3	2	1		
3	D	1	Total	C	Hg	0	0
			3	2	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

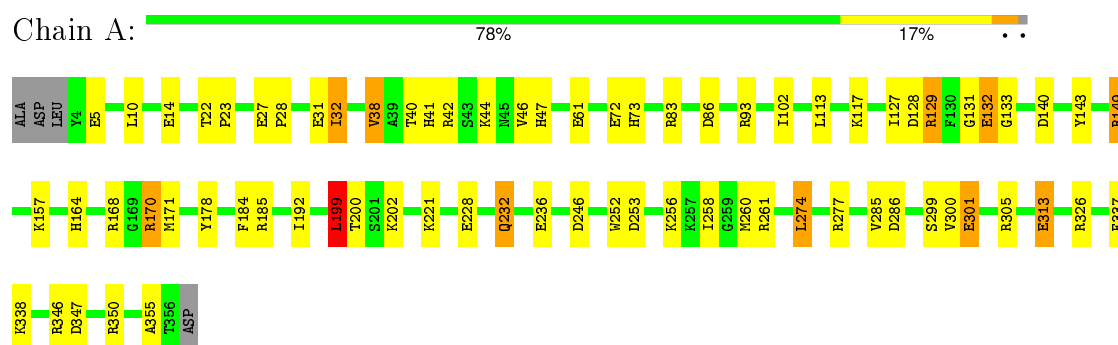
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	148	Total O 148 148	0	0
5	B	138	Total O 138 138	0	0
5	C	137	Total O 137 137	0	0
5	D	144	Total O 144 144	0	0

3 Residue-property plots [i](#)

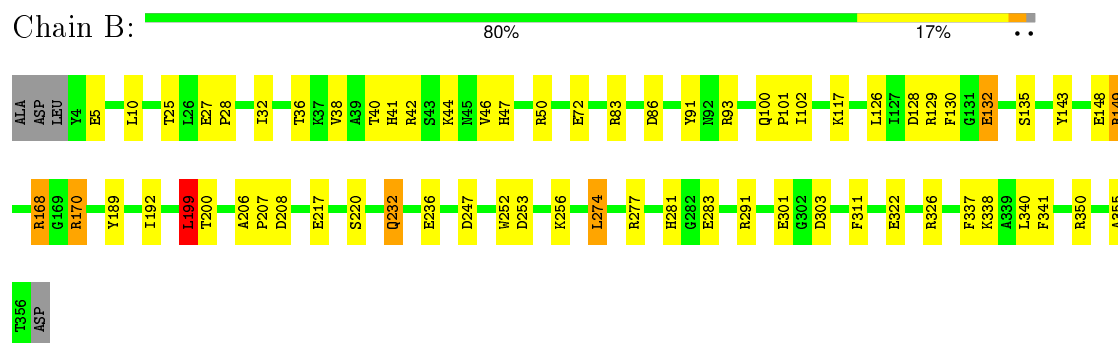
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

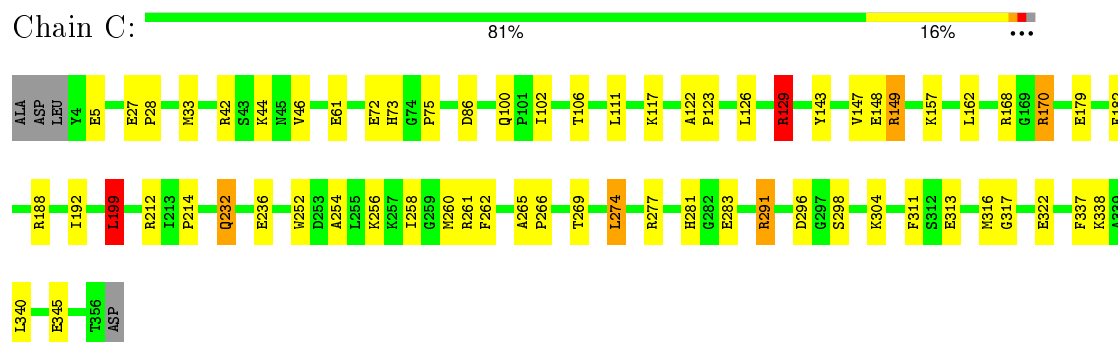
• Molecule 1: 4-HYDROXYPHENYLPYRUVATE DIOXYGENASE



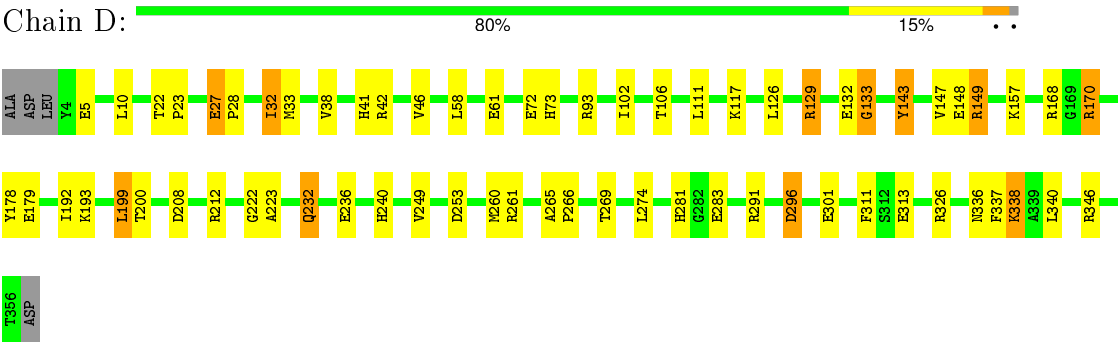
• Molecule 1: 4-HYDROXYPHENYLPYRUVATE DIOXYGENASE



• Molecule 1: 4-HYDROXYPHENYLPYRUVATE DIOXYGENASE



● Molecule 1: 4-HYDROXYPHENYLPYRUVATE DIOXYGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.59 Å 142.75 Å 159.44 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	79.8 (20.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	8.00	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.219 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11821	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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: FE2, EMC, ACT

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	6.72	6/2892 (0.2%)	2.08	41/3901 (1.1%)
1	B	0.47	1/2895 (0.0%)	1.46	33/3904 (0.8%)
1	C	0.50	1/2895 (0.0%)	1.36	23/3904 (0.6%)
1	D	0.49	0/2904	1.37	27/3917 (0.7%)
All	All	3.39	8/11586 (0.1%)	1.60	124/15626 (0.8%)

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	A	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313[A]	GLU	CD-OE1	233.44	3.82	1.25
1	A	313[B]	GLU	CD-OE1	233.44	3.82	1.25
1	A	313[A]	GLU	CD-OE2	84.97	2.19	1.25
1	A	313[B]	GLU	CD-OE2	84.97	2.19	1.25
1	A	313[A]	GLU	CG-CD	57.69	2.38	1.51
1	A	313[B]	GLU	CG-CD	57.69	2.38	1.51
1	C	304	LYS	N-CA	-9.75	1.26	1.46
1	B	303	ASP	C-N	5.85	1.47	1.34

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313[A]	GLU	CG-CD-OE1	-43.26	31.79	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313[B]	GLU	CG-CD-OE1	-43.26	31.79	118.30
1	A	313[A]	GLU	OE1-CD-OE2	-41.84	73.09	123.30
1	A	313[B]	GLU	OE1-CD-OE2	-41.84	73.09	123.30
1	A	313[A]	GLU	CG-CD-OE2	-27.68	62.94	118.30
1	A	313[B]	GLU	CG-CD-OE2	-27.68	62.94	118.30
1	B	350[A]	ARG	NE-CZ-NH1	22.81	131.71	120.30
1	B	350[B]	ARG	NE-CZ-NH1	22.81	131.71	120.30
1	C	170	ARG	NE-CZ-NH2	-20.51	110.04	120.30
1	A	261[A]	ARG	CD-NE-CZ	15.76	145.66	123.60
1	A	261[B]	ARG	CD-NE-CZ	15.76	145.66	123.60
1	D	212	ARG	NE-CZ-NH2	-15.03	112.79	120.30
1	A	93	ARG	NE-CZ-NH2	-13.82	113.39	120.30
1	D	291	ARG	NE-CZ-NH2	-12.35	114.13	120.30
1	B	86	ASP	CB-CG-OD1	12.34	129.41	118.30
1	D	170	ARG	NE-CZ-NH2	-11.74	114.43	120.30
1	D	212	ARG	NE-CZ-NH1	11.70	126.15	120.30
1	B	291	ARG	NE-CZ-NH1	11.37	125.99	120.30
1	B	50	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	C	149	ARG	NE-CZ-NH1	10.83	125.72	120.30
1	D	253	ASP	CB-CG-OD1	10.67	127.90	118.30
1	D	212	ARG	CD-NE-CZ	10.65	138.52	123.60
1	C	212	ARG	NE-CZ-NH2	-10.57	115.02	120.30
1	B	350[A]	ARG	CD-NE-CZ	10.52	138.33	123.60
1	B	350[B]	ARG	CD-NE-CZ	10.52	138.33	123.60
1	A	326	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	B	350[A]	ARG	NE-CZ-NH2	-9.47	115.56	120.30
1	B	350[B]	ARG	NE-CZ-NH2	-9.47	115.56	120.30
1	B	170	ARG	NE-CZ-NH1	9.27	124.93	120.30
1	A	313[A]	GLU	CB-CG-CD	-9.02	89.84	114.20
1	A	313[B]	GLU	CB-CG-CD	-9.02	89.84	114.20
1	D	253	ASP	CB-CG-OD2	-8.90	110.29	118.30
1	A	350	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	A	140	ASP	CB-CG-OD1	8.83	126.25	118.30
1	D	27	GLU	OE1-CD-OE2	-8.80	112.74	123.30
1	A	346	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	D	93	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	A	261[A]	ARG	CB-CG-CD	8.39	133.41	111.60
1	A	261[B]	ARG	CB-CG-CD	8.39	133.41	111.60
1	A	128	ASP	CB-CG-OD1	8.37	125.84	118.30
1	D	149	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	A	253	ASP	CB-CG-OD2	7.96	125.47	118.30
1	B	253	ASP	CB-CG-OD2	7.90	125.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	A	185	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	C	261[A]	ARG	N-CA-CB	-7.60	96.93	110.60
1	C	261[B]	ARG	N-CA-CB	-7.60	96.93	110.60
1	C	170	ARG	NH1-CZ-NH2	7.57	127.73	119.40
1	B	326	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	A	86	ASP	CB-CG-OD1	7.44	125.00	118.30
1	B	93	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	A	305	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	B	128	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	170	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	A	149	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	D	178	TYR	CB-CG-CD1	7.05	125.23	121.00
1	C	199	LEU	CA-CB-CG	7.03	131.47	115.30
1	A	133	GLY	N-CA-C	-6.88	95.91	113.10
1	B	50	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	C	170	ARG	CD-NE-CZ	6.82	133.15	123.60
1	C	291	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	C	168	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	D	168	ARG	CD-NE-CZ	6.68	132.95	123.60
1	D	178	TYR	CB-CG-CD2	-6.67	117.00	121.00
1	C	179	GLU	OE1-CD-OE2	-6.64	115.33	123.30
1	A	42	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	B	83	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	B	189	TYR	CB-CG-CD2	6.56	124.93	121.00
1	C	129	ARG	CD-NE-CZ	6.52	132.72	123.60
1	C	86	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	A	170	ARG	CD-NE-CZ	6.32	132.45	123.60
1	A	228	GLU	OE1-CD-OE2	-6.26	115.79	123.30
1	B	189	TYR	CB-CG-CD1	-6.14	117.32	121.00
1	D	326	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	D	291	ARG	NH1-CZ-NH2	6.11	126.12	119.40
1	B	350[A]	ARG	NH1-CZ-NH2	-6.07	112.72	119.40
1	B	350[B]	ARG	NH1-CZ-NH2	-6.07	112.72	119.40
1	B	247	ASP	CB-CG-OD1	6.02	123.72	118.30
1	C	188	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	170	ARG	CD-NE-CZ	5.97	131.96	123.60
1	D	42	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	C	262	PHE	CB-CG-CD2	5.88	124.92	120.80
1	C	42	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	D	133	GLY	N-CA-C	-5.84	98.51	113.10
1	D	170	ARG	NH1-CZ-NH2	5.73	125.70	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355	ALA	N-CA-CB	5.70	118.08	110.10
1	B	291	ARG	NH1-CZ-NH2	-5.69	113.14	119.40
1	A	42	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	345	GLU	OE1-CD-OE2	-5.67	116.49	123.30
1	C	42	ARG	CD-NE-CZ	5.66	131.52	123.60
1	C	188	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	D	208	ASP	CB-CG-OD1	5.62	123.35	118.30
1	A	326	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	86	ASP	OD1-CG-OD2	-5.55	112.76	123.30
1	D	346	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	B	199	LEU	CA-CB-CG	5.38	127.68	115.30
1	C	149	ARG	CG-CD-NE	5.37	123.08	111.80
1	B	149	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	D	179	GLU	OE1-CD-OE2	-5.33	116.91	123.30
1	B	38	VAL	N-CA-CB	-5.31	99.83	111.50
1	A	38	VAL	N-CA-CB	-5.30	99.83	111.50
1	A	93	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	91	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	A	164	HIS	CA-CB-CG	5.26	122.55	113.60
1	A	132	GLU	CA-CB-CG	-5.26	101.83	113.40
1	A	199	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	168	ARG	CD-NE-CZ	5.24	130.94	123.60
1	B	42	ARG	CD-NE-CZ	5.24	130.93	123.60
1	D	240	HIS	CA-CB-CG	5.23	122.49	113.60
1	B	148	GLU	OE1-CD-OE2	-5.22	117.04	123.30
1	D	296	ASP	CB-CG-OD2	5.20	122.97	118.30
1	A	129	ARG	CD-NE-CZ	5.18	130.86	123.60
1	D	143	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	A	286	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	246	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	208	ASP	CB-CG-OD1	5.12	122.91	118.30
1	D	61[A]	GLU	CB-CG-CD	-5.11	100.42	114.20
1	D	61[B]	GLU	CB-CG-CD	-5.11	100.42	114.20
1	C	296	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	149	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	182	PHE	CB-CG-CD2	-5.08	117.25	120.80
1	B	168	ARG	CD-NE-CZ	5.07	130.70	123.60
1	A	131	GLY	C-N-CA	-5.06	109.04	121.70
1	C	61	GLU	OE1-CD-OE2	-5.01	117.29	123.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	GLU	Mainchain
1	A	31	GLU	Mainchain

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	2801	0	2725	31	0
1	B	2805	0	2736	26	0
1	C	2806	0	2740	35	0
1	D	2810	0	2742	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
4	D	4	0	3	0	0
5	A	148	0	0	4	0
5	B	138	0	0	4	0
5	C	137	0	0	4	0
5	D	144	0	0	3	0
All	All	11821	0	10955	124	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 (124) 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:D:261[B]:ARG:NH1	1:D:313[B]:GLU:OE2	1.90	1.04
1:A:313[A]:GLU:CD	1:A:313[A]:GLU:CG	2.38	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ILE:HD11	1:A:117:LYS:HG2	1.53	0.90
1:D:281:HIS:HD2	1:D:283:GLU:H	1.22	0.85
1:A:313[A]:GLU:CD	1:A:313[A]:GLU:OE2	2.19	0.81
1:B:281:HIS:HD2	1:B:283:GLU:H	1.29	0.80
1:D:102:ILE:HD11	1:D:117:LYS:HG2	1.69	0.76
1:C:281:HIS:HD2	1:C:283:GLU:H	1.34	0.75
1:A:300:VAL:HG12	1:A:301:GLU:HG3	1.71	0.73
1:A:232:GLN:HE21	1:A:232:GLN:HA	1.52	0.73
1:D:132:GLU:O	1:D:133:GLY:C	2.25	0.73
1:A:313[A]:GLU:OE2	1:A:313[A]:GLU:CG	2.39	0.71
1:C:102:ILE:HD11	1:C:117:LYS:HG2	1.73	0.70
1:D:261[B]:ARG:HD2	1:D:313[B]:GLU:OE2	1.91	0.70
1:C:232:GLN:HE21	1:C:232:GLN:HA	1.59	0.68
1:D:41:HIS:HB2	1:D:46:VAL:HG22	1.77	0.66
1:B:232:GLN:HA	1:B:232:GLN:HE21	1.60	0.66
1:C:252:TRP:CD2	1:C:291:ARG:HG2	2.32	0.65
1:B:102:ILE:HD11	1:B:117:LYS:HG2	1.79	0.64
1:D:199:LEU:C	1:D:199:LEU:HD23	2.19	0.63
1:B:281:HIS:CD2	1:B:283:GLU:H	2.15	0.63
1:A:285:VAL:HG21	5:A:766:HOH:O	1.98	0.63
1:B:192:ILE:HB	1:B:199:LEU:HD22	1.82	0.62
1:D:281:HIS:CD2	1:D:283:GLU:H	2.12	0.61
1:A:72:GLU:HG2	1:A:73:HIS:CE1	2.37	0.60
1:C:281:HIS:CD2	1:C:283:GLU:H	2.20	0.59
1:C:27:GLU:HB2	1:C:28:PRO:HD3	1.83	0.59
1:A:170:ARG:HD3	1:A:236:GLU:OE2	2.02	0.59
1:A:199:LEU:HD23	1:A:199:LEU:C	2.23	0.59
1:B:252:TRP:CZ3	1:B:256:LYS:HG3	2.39	0.57
1:A:192:ILE:HB	1:A:199:LEU:HD22	1.86	0.57
1:A:313[A]:GLU:CD	5:A:763:HOH:O	2.42	0.57
1:A:252:TRP:CZ3	1:A:256:LYS:HG3	2.39	0.57
1:A:300:VAL:HG12	1:A:301:GLU:CG	2.34	0.56
1:D:281:HIS:HD2	1:D:283:GLU:N	2.00	0.54
1:C:199:LEU:C	1:C:199:LEU:HD23	2.27	0.54
1:D:33:MET:HG2	1:D:260:MET:CE	2.39	0.53
1:A:27:GLU:N	1:A:28:PRO:HD2	2.23	0.53
1:C:143:TYR:CD1	1:C:149:ARG:HG2	2.43	0.53
1:C:192:ILE:HB	1:C:199:LEU:HD22	1.92	0.52
1:C:33:MET:HG2	1:C:260:MET:HE1	1.92	0.52
1:C:129:ARG:HB2	5:C:701:HOH:O	2.10	0.51
1:A:171:MET:HE2	1:A:202:LYS:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:HIS:HB2	1:B:46:VAL:HG22	1.92	0.51
1:B:72:GLU:OE2	1:D:170:ARG:NH2	2.42	0.51
1:C:72:GLU:HG2	1:C:73:HIS:CE1	2.46	0.51
1:B:130:PHE:HA	5:B:733:HOH:O	2.11	0.51
1:C:33:MET:HG2	1:C:260:MET:CE	2.40	0.50
1:C:170:ARG:HD3	1:C:236:GLU:OE2	2.11	0.50
1:D:132:GLU:C	1:D:133:GLY:O	2.46	0.50
1:B:170:ARG:HD3	1:B:236:GLU:OE2	2.12	0.49
1:C:157[A]:LYS:HE2	5:C:670:HOH:O	2.12	0.49
1:C:75:PRO:HB2	1:C:316:MET:HB3	1.93	0.49
1:B:199:LEU:C	1:B:199:LEU:HD23	2.33	0.49
1:C:313[A]:GLU:HB3	5:C:763:HOH:O	2.12	0.48
1:A:14:GLU:HB2	1:A:83:ARG:HG3	1.95	0.48
1:A:32:ILE:HG23	1:A:260:MET:HE2	1.93	0.48
1:D:143:TYR:CD1	1:D:149:ARG:HG2	2.48	0.48
1:A:44:LYS:HG2	1:A:61[A]:GLU:OE2	2.14	0.47
1:D:265:ALA:HB1	1:D:266:PRO:HD2	1.97	0.47
1:A:32:ILE:HG13	1:A:258:ILE:O	2.15	0.47
1:B:217:GLU:HG3	5:B:726:HOH:O	2.14	0.47
1:C:274:LEU:HD12	1:C:277:ARG:NH1	2.30	0.46
1:D:33:MET:HG2	1:D:260:MET:HE3	1.97	0.46
1:B:199:LEU:HD13	1:B:341:PHE:CD2	2.50	0.46
1:A:143:TYR:CD1	1:A:149:ARG:HG2	2.51	0.46
1:A:113:LEU:HD22	1:A:127:ILE:HD12	1.97	0.46
1:C:147:VAL:HG12	1:C:148:GLU:O	2.16	0.46
1:B:311:PHE:CD2	1:B:340:LEU:HD13	2.51	0.45
1:A:274:LEU:HD12	1:A:277:ARG:NH1	2.31	0.45
1:D:192:ILE:HB	1:D:199:LEU:HD22	1.99	0.45
1:D:170:ARG:HD3	1:D:236:GLU:OE2	2.16	0.45
1:D:27:GLU:HB2	1:D:28:PRO:HD3	1.98	0.45
1:C:254:ALA:O	1:C:258:ILE:HG12	2.18	0.44
1:D:311:PHE:CD2	1:D:340:LEU:HD13	2.52	0.44
1:C:44:LYS:HB2	1:C:46:VAL:HG13	1.98	0.44
1:B:168:ARG:HG3	1:B:168:ARG:HH11	1.83	0.44
1:C:252:TRP:CE3	1:C:291:ARG:HG2	2.52	0.44
1:B:143:TYR:CD1	1:B:149:ARG:HG2	2.52	0.44
1:D:32:ILE:HG23	1:D:260:MET:HE2	1.99	0.44
1:C:311:PHE:CZ	1:C:340:LEU:HD22	2.53	0.44
1:D:199:LEU:HD23	1:D:200:THR:N	2.33	0.44
1:D:157[A]:LYS:HE2	5:D:672:HOH:O	2.17	0.44
1:B:27:GLU:N	1:B:28:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ALA:HB1	1:B:207:PRO:HD2	1.99	0.43
1:D:129:ARG:HB2	5:D:704:HOH:O	2.19	0.43
1:D:106:THR:HG21	1:D:111:LEU:O	2.17	0.43
1:B:44:LYS:HB2	1:B:46:VAL:HG13	2.00	0.43
1:A:178:TYR:HB3	1:A:184:PHE:CG	2.54	0.43
1:D:296:ASP:HB2	1:D:336:ASN:OD1	2.19	0.43
1:D:222:GLY:O	1:D:223:ALA:HB3	2.18	0.42
1:D:232:GLN:HE21	1:D:232:GLN:HA	1.83	0.42
1:A:40:THR:HG23	1:A:47:HIS:CE1	2.54	0.42
1:B:40:THR:OG1	1:B:47:HIS:HD2	2.01	0.42
1:B:274:LEU:HD12	1:B:277:ARG:NH1	2.34	0.42
1:C:100:GLN:NE2	1:C:117:LYS:HE3	2.34	0.42
1:D:199:LEU:C	1:D:199:LEU:CD2	2.86	0.42
1:D:193:LYS:O	1:D:338:LYS:HE3	2.19	0.42
1:A:199:LEU:C	1:A:199:LEU:CD2	2.87	0.42
1:D:281:HIS:HE1	5:D:771:HOH:O	2.02	0.42
1:D:72:GLU:HG2	1:D:73:HIS:CE1	2.55	0.42
1:C:162:LEU:O	1:C:214:PRO:HD2	2.18	0.42
1:B:135:SER:HB2	5:B:733:HOH:O	2.19	0.42
1:D:147:VAL:HG12	1:D:148:GLU:O	2.19	0.42
1:C:106:THR:HG21	1:C:111:LEU:O	2.20	0.41
1:C:265:ALA:HB1	1:C:266:PRO:HD2	2.02	0.41
1:B:27:GLU:HB2	1:B:28:PRO:HD3	2.01	0.41
1:C:313[B]:GLU:HB3	5:C:763:HOH:O	2.19	0.41
1:C:199:LEU:C	1:C:199:LEU:CD2	2.89	0.41
1:C:260:MET:HE2	1:C:260:MET:HB2	1.94	0.41
1:C:316:MET:O	1:C:317:GLY:C	2.59	0.41
1:A:157[A]:LYS:HE2	5:A:667:HOH:O	2.20	0.41
1:B:311:PHE:CD1	1:B:322:GLU:HB2	2.55	0.41
1:A:347:ASP:HB3	5:A:750:HOH:O	2.20	0.41
1:D:22:THR:HA	1:D:23:PRO:HD3	1.92	0.41
1:A:41:HIS:HB2	1:A:46:VAL:HG22	2.03	0.41
1:B:100:GLN:HA	1:B:101:PRO:HD2	1.91	0.40
1:C:122:ALA:HA	1:C:123:PRO:HD3	1.94	0.40
1:A:22:THR:HA	1:A:23:PRO:HD3	1.82	0.40
1:C:311:PHE:CD1	1:C:322:GLU:HB2	2.57	0.40
1:B:200:THR:HB	5:B:726:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	355/357 (99%)	339 (96%)	15 (4%)	1 (0%)	46	63
1	B	355/357 (99%)	340 (96%)	13 (4%)	2 (1%)	30	43
1	C	355/357 (99%)	343 (97%)	12 (3%)	0	100	100
1	D	356/357 (100%)	339 (95%)	16 (4%)	1 (0%)	46	63
All	All	1421/1428 (100%)	1361 (96%)	56 (4%)	4 (0%)	46	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	ALA
1	B	132	GLU
1	D	301	GLU
1	B	301	GLU

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	296/296 (100%)	282 (95%)	14 (5%)	32	50
1	B	296/296 (100%)	282 (95%)	14 (5%)	32	50
1	C	296/296 (100%)	285 (96%)	11 (4%)	41	62
1	D	297/296 (100%)	283 (95%)	14 (5%)	32	50
All	All	1185/1184 (100%)	1132 (96%)	53 (4%)	34	52

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	10	LEU
1	A	32	ILE
1	A	38	VAL
1	A	129	ARG
1	A	199	LEU
1	A	200	THR
1	A	221	LYS
1	A	232	GLN
1	A	274	LEU
1	A	299	SER
1	A	301	GLU
1	A	337	PHE
1	A	338	LYS
1	B	5	GLU
1	B	10	LEU
1	B	25	THR
1	B	32	ILE
1	B	36	THR
1	B	126	LEU
1	B	129	ARG
1	B	132	GLU
1	B	199	LEU
1	B	220	SER
1	B	232	GLN
1	B	274	LEU
1	B	337	PHE
1	B	338	LYS
1	C	5	GLU
1	C	126	LEU
1	C	129	ARG
1	C	199	LEU
1	C	232	GLN
1	C	256	LYS
1	C	269	THR
1	C	274	LEU
1	C	298	SER
1	C	337	PHE
1	C	338	LYS
1	D	5	GLU
1	D	10	LEU
1	D	32	ILE

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Mol	Chain	Res	Type
1	D	38	VAL
1	D	58	LEU
1	D	126	LEU
1	D	129	ARG
1	D	199	LEU
1	D	232	GLN
1	D	249	VAL
1	D	269	THR
1	D	274	LEU
1	D	337	PHE
1	D	338	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	103	HIS
1	A	232	GLN
1	B	47	HIS
1	B	60	ASN
1	B	92	ASN
1	B	232	GLN
1	B	281	HIS
1	C	92	ASN
1	C	232	GLN
1	C	281	HIS
1	D	92	ASN
1	D	232	GLN
1	D	281	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	EMC	A	630	1	1,2,2	0.44	0	0,1,1	0.00	-
4	ACT	A	631	2	1,3,3	1.76	0	0,3,3	0.00	-
3	EMC	B	630	1	1,2,2	0.69	0	0,1,1	0.00	-
4	ACT	B	631	2	1,3,3	1.34	0	0,3,3	0.00	-
3	EMC	C	630	1	1,2,2	0.47	0	0,1,1	0.00	-
4	ACT	C	631	2	1,3,3	2.48	1 (100%)	0,3,3	0.00	-
3	EMC	D	630	1	1,2,2	0.75	0	0,1,1	0.00	-
4	ACT	D	631	2	1,3,3	2.26	1 (100%)	0,3,3	0.00	-

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	EMC	A	630	1	-	0/0/0/0	0/0/0/0
4	ACT	A	631	2	-	0/0/0/0	0/0/0/0
3	EMC	B	630	1	-	0/0/0/0	0/0/0/0
4	ACT	B	631	2	-	0/0/0/0	0/0/0/0
3	EMC	C	630	1	-	0/0/0/0	0/0/0/0
4	ACT	C	631	2	-	0/0/0/0	0/0/0/0
3	EMC	D	630	1	-	0/0/0/0	0/0/0/0
4	ACT	D	631	2	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	631	ACT	CH3-C	2.26	1.52	1.48
4	C	631	ACT	CH3-C	2.48	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 will therefore be empty.

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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