



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:19 AM UTC

PDB ID : 1CJX / pdb_00001cjx
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

<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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

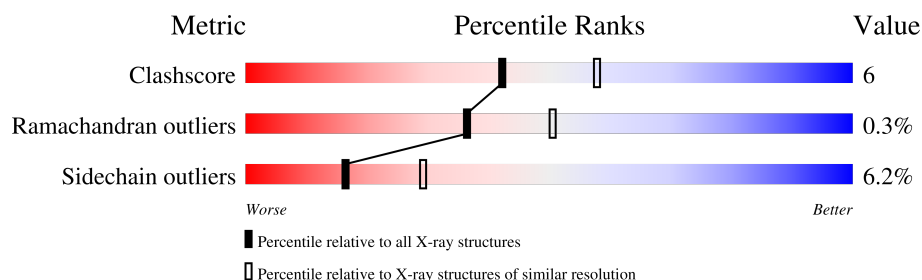
1 Overall quality at a glance

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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	357	 74% 19% 6% .
1	B	357	 76% 18% . .
1	C	357	 75% 21% . .
1	D	357	 74% 22% . .

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			

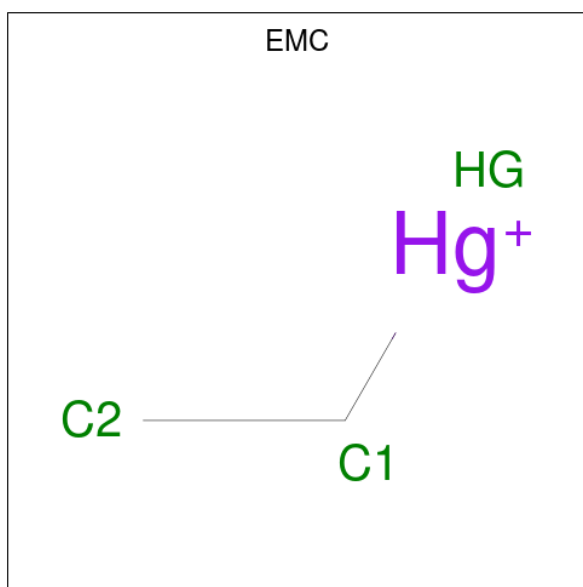
There are 4 discrepancies between the modelled and reference sequences:

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 (CCD ID: FE2) (formula: Fe).

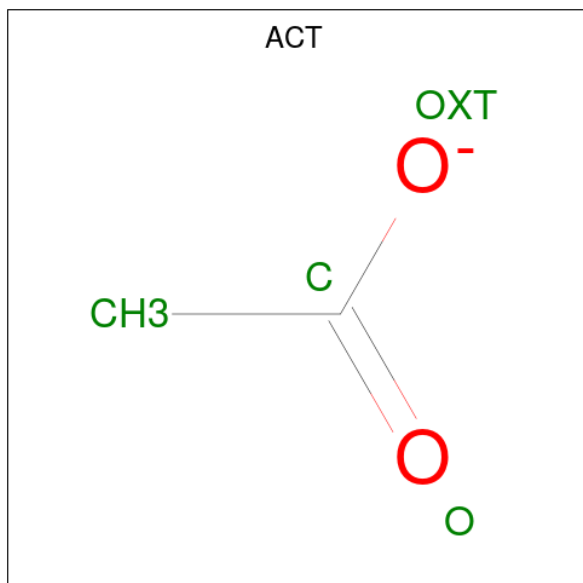
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is ETHYL MERCURY ION (CCD ID: 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 (CCD ID: 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

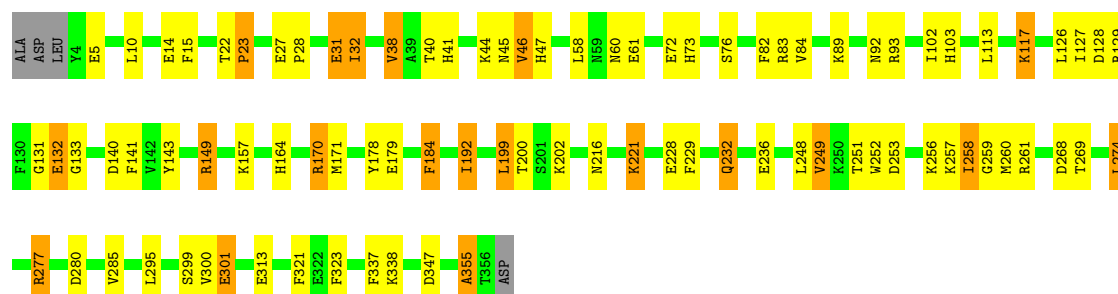
3 Residue-property plots

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.

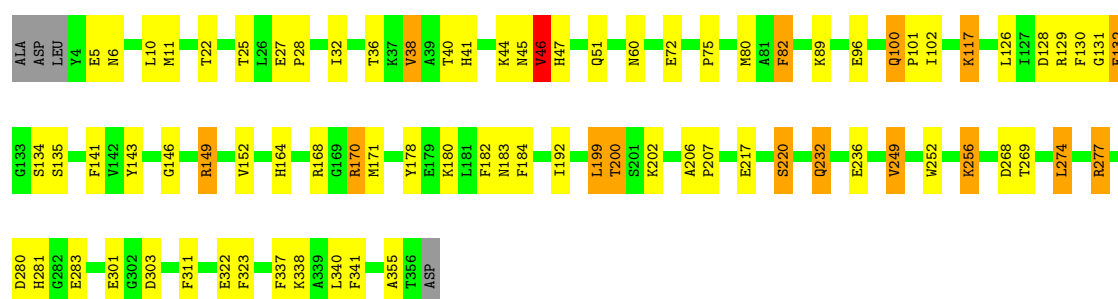
• Molecule 1: 4-HYDROXYPHENYLPYRUVATE DIOXYGENASE

Chain A: 



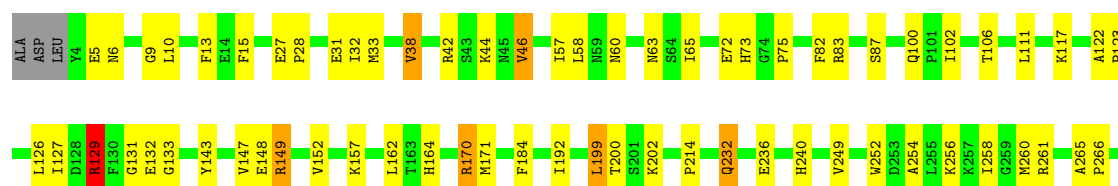
• Molecule 1: 4-HYDROXYPHENYLPYRUVATE DIOXYGENASE

Chain B: 



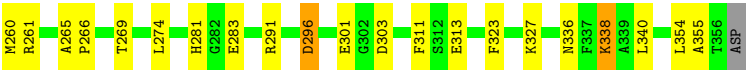
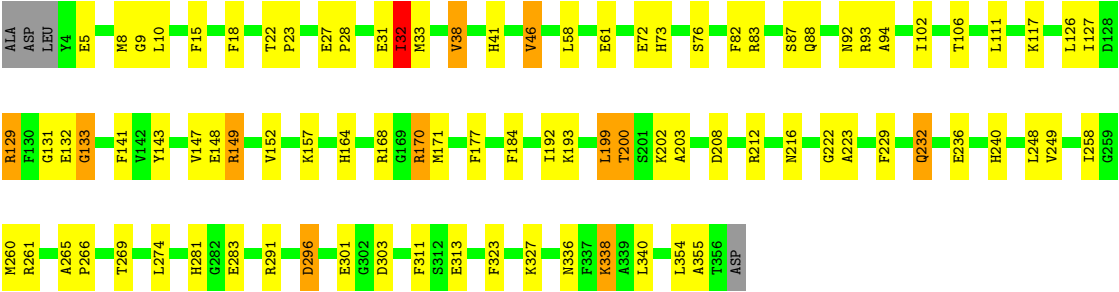
• Molecule 1: 4-HYDROXYPHENYLPYRUVATE DIOXYGENASE

Chain C: 





● Molecule 1: 4-HYDROXYPHENYLPYRUVATE DIOXYGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.59Å 142.75Å 159.44Å 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: ACT, EMC, FE2

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	0.56	1/2892 (0.0%)	1.73	52/3901 (1.3%)
1	B	0.57	2/2895 (0.1%)	1.64	44/3904 (1.1%)
1	C	0.61	2/2895 (0.1%)	1.63	42/3904 (1.1%)
1	D	0.56	2/2904 (0.1%)	1.63	39/3917 (1.0%)
All	All	0.58	7/11586 (0.1%)	1.66	177/15626 (1.1%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	304	LYS	N-CA	-15.71	1.26	1.46
1	B	303	ASP	C-N	10.04	1.47	1.33
1	A	355	ALA	C-N	-7.09	1.23	1.33
1	D	355	ALA	C-N	-7.06	1.23	1.33
1	C	355	ALA	C-N	-7.05	1.23	1.33
1	B	355	ALA	C-N	-7.05	1.23	1.33
1	D	303	ASP	C-N	-6.08	1.24	1.33

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261[A]	ARG	CD-NE-CZ	15.19	145.66	124.40
1	A	261[B]	ARG	CD-NE-CZ	15.19	145.66	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	ARG	NE-CZ-NH2	-10.17	110.04	119.20
1	D	212	ARG	CD-NE-CZ	10.08	138.52	124.40
1	C	6	ASN	CA-CB-CG	10.06	122.66	112.60
1	A	60	ASN	CA-CB-CG	9.98	122.58	112.60
1	A	261[A]	ARG	CB-CG-CD	9.61	133.41	111.30
1	A	261[B]	ARG	CB-CG-CD	9.61	133.41	111.30
1	A	280	ASP	CA-CB-CG	9.58	122.18	112.60
1	B	82	PHE	CA-CB-CG	9.16	122.96	113.80
1	D	177	PHE	CA-CB-CG	8.80	122.60	113.80
1	A	164	HIS	CA-CB-CG	8.75	122.55	113.80
1	D	240	HIS	CA-CB-CG	8.69	122.49	113.80
1	C	261[A]	ARG	N-CA-CB	-8.69	96.93	110.65
1	C	261[B]	ARG	N-CA-CB	-8.69	96.93	110.65
1	C	164	HIS	CA-CB-CG	8.29	122.09	113.80
1	D	82	PHE	CA-CB-CG	8.11	121.91	113.80
1	B	303	ASP	CA-C-N	-8.06	111.76	123.05
1	B	303	ASP	C-N-CA	-8.06	111.76	123.05
1	A	82	PHE	CA-CB-CG	7.98	121.78	113.80
1	C	82	PHE	CA-CB-CG	7.95	121.75	113.80
1	C	240	HIS	CA-CB-CG	7.64	121.44	113.80
1	B	38	VAL	N-CA-CB	-7.63	99.83	111.57
1	B	184	PHE	CA-CB-CG	7.62	121.42	113.80
1	A	38	VAL	N-CA-CB	-7.62	99.83	111.57
1	A	133	GLY	N-CA-C	-7.53	95.91	112.17
1	C	60	ASN	CA-CB-CG	7.43	120.03	112.60
1	C	304	LYS	N-CA-C	7.35	120.71	108.73
1	D	184	PHE	CA-CB-CG	7.26	121.06	113.80
1	A	45	ASN	OD1-CG-ND2	-7.23	115.37	122.60
1	D	164	HIS	CA-CB-CG	7.19	120.99	113.80
1	D	87	SER	CA-C-O	-7.18	112.80	120.42
1	A	76	SER	N-CA-C	7.17	118.06	108.38
1	A	131	GLY	CA-C-N	-7.13	109.04	122.73
1	A	131	GLY	C-N-CA	-7.13	109.04	122.73
1	D	212	ARG	NE-CZ-NH2	-7.13	112.79	119.20
1	A	128	ASP	CA-CB-CG	7.10	119.70	112.60
1	B	141	PHE	CA-CB-CG	7.07	120.87	113.80
1	C	184	PHE	CA-CB-CG	7.04	120.83	113.80
1	A	257	LYS	CA-C-O	-6.97	113.44	120.90
1	D	141	PHE	CA-CB-CG	6.92	120.72	113.80
1	C	87	SER	CA-C-O	-6.89	113.25	120.55
1	B	164	HIS	CA-CB-CG	6.87	120.67	113.80
1	A	132	GLU	CB-CG-CD	6.85	124.25	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	88	GLN	OE1-CD-NE2	6.85	129.45	122.60
1	D	38	VAL	N-CA-CB	-6.78	102.97	112.12
1	A	132	GLU	N-CA-C	6.75	120.54	109.94
1	A	184	PHE	CA-CB-CG	6.74	120.53	113.80
1	B	89	LYS	CA-C-O	-6.72	113.77	120.82
1	A	89	LYS	CA-C-O	-6.68	113.82	120.70
1	A	92	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	B	277	ARG	N-CA-C	6.65	119.36	111.71
1	D	296	ASP	CA-CB-CG	6.60	119.20	112.60
1	B	51	GLN	OE1-CD-NE2	-6.58	116.02	122.60
1	D	203	ALA	CA-C-O	-6.54	113.91	120.98
1	A	140	ASP	CA-CB-CG	6.50	119.10	112.60
1	C	170	ARG	NH1-CZ-NH2	6.48	127.73	119.30
1	A	93	ARG	NE-CZ-NH2	-6.46	113.39	119.20
1	B	323	PHE	CA-CB-CG	-6.41	107.39	113.80
1	A	259	GLY	N-CA-C	6.34	124.90	115.64
1	B	60	ASN	CA-CB-CG	6.34	118.94	112.60
1	D	216	ASN	CA-CB-CG	6.32	118.92	112.60
1	D	258	ILE	CA-C-O	-6.31	112.90	120.78
1	C	13	PHE	CA-CB-CG	6.28	120.08	113.80
1	C	170	ARG	CD-NE-CZ	6.25	133.15	124.40
1	C	133	GLY	N-CA-C	-6.24	100.64	111.50
1	C	127	ILE	CA-C-O	-6.23	113.88	120.48
1	B	337	PHE	CA-CB-CG	6.22	120.02	113.80
1	B	22	THR	CB-CA-C	-6.20	103.02	110.15
1	D	133	GLY	N-CA-C	-6.19	98.51	113.18
1	A	337	PHE	CA-CB-CG	6.18	119.98	113.80
1	A	179	GLU	CA-C-O	6.18	127.07	120.70
1	A	132	GLU	CA-CB-CG	-6.13	101.83	114.10
1	D	131	GLY	O-C-N	-6.12	115.69	122.61
1	D	168	ARG	CD-NE-CZ	6.11	132.95	124.40
1	A	228	GLU	CA-C-O	-6.07	113.99	120.42
1	D	92	ASN	O-C-N	-6.02	115.87	122.07
1	D	76	SER	N-CA-C	6.01	116.49	108.38
1	C	261[A]	ARG	CB-CA-C	5.99	120.39	110.74
1	C	261[B]	ARG	CB-CA-C	5.99	120.39	110.74
1	C	129	ARG	CD-NE-CZ	5.95	132.72	124.40
1	A	249	VAL	N-CA-CB	5.92	119.47	110.58
1	D	93	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	D	31	GLU	CB-CG-CD	5.91	122.64	112.60
1	A	31	GLU	O-C-N	-5.90	115.86	122.12
1	A	141	PHE	CA-CB-CG	5.90	119.70	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	15	PHE	CA-CB-CG	5.89	119.69	113.80
1	B	220	SER	CA-C-N	5.87	128.14	120.28
1	B	220	SER	C-N-CA	5.87	128.14	120.28
1	B	117	LYS	CA-C-O	-5.86	114.07	120.81
1	B	6	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	B	128	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	249	VAL	N-CA-CB	5.85	119.35	110.58
1	A	23	PRO	CA-C-O	-5.83	114.80	121.56
1	A	221	LYS	CA-CB-CG	-5.81	102.47	114.10
1	C	131	GLY	CA-C-N	-5.76	112.13	122.15
1	C	131	GLY	C-N-CA	-5.76	112.13	122.15
1	A	170	ARG	CD-NE-CZ	5.75	132.45	124.40
1	B	146	GLY	N-CA-C	5.71	123.13	115.59
1	C	38	VAL	N-CA-CB	-5.71	104.41	112.12
1	C	15	PHE	CA-CB-CG	5.70	119.50	113.80
1	D	83	ARG	CA-C-O	-5.68	114.39	120.92
1	B	100	GLN	CB-CA-C	5.68	116.32	109.85
1	D	18	PHE	CA-CB-CG	5.67	119.47	113.80
1	B	100	GLN	CA-C-O	5.66	125.66	119.32
1	B	89	LYS	O-C-N	5.65	127.89	122.07
1	B	46	VAL	CA-C-O	5.65	126.35	120.36
1	C	31	GLU	CB-CG-CD	5.65	122.20	112.60
1	A	15	PHE	CA-CB-CG	5.64	119.44	113.80
1	D	291	ARG	NE-CZ-NH2	-5.64	114.13	119.20
1	B	180	LYS	N-CA-C	5.62	117.09	111.07
1	A	323	PHE	CA-CB-CG	-5.59	108.21	113.80
1	C	9	GLY	CA-C-O	5.58	126.18	119.82
1	A	321	PHE	CA-CB-CG	-5.55	108.25	113.80
1	B	280	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	134	SER	N-CA-C	5.52	117.69	108.02
1	B	100	GLN	CA-C-N	5.50	125.26	119.76
1	B	100	GLN	C-N-CA	5.50	125.26	119.76
1	D	61[A]	GLU	CA-C-O	5.50	124.65	119.76
1	D	61[B]	GLU	CA-C-O	5.50	124.65	119.76
1	C	65	ILE	CA-C-O	5.49	126.98	121.27
1	B	131	GLY	CA-C-N	5.48	132.01	121.54
1	B	131	GLY	C-N-CA	5.48	132.01	121.54
1	A	149	ARG	CB-CG-CD	5.48	123.90	111.30
1	C	83	ARG	CA-C-O	-5.48	114.81	121.05
1	D	127	ILE	N-CA-C	5.44	115.69	107.80
1	C	296	ASP	CA-CB-CG	5.43	118.03	112.60
1	B	184	PHE	CA-C-O	-5.43	115.80	121.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	A	216	ASN	CA-CB-CG	5.41	118.01	112.60
1	B	170	ARG	CD-NE-CZ	5.40	131.96	124.40
1	B	178	TYR	CA-C-O	-5.40	114.25	120.24
1	A	164	HIS	N-CA-CB	5.39	119.24	110.77
1	A	277	ARG	N-CA-C	5.36	117.88	111.71
1	B	11	MET	CA-C-O	-5.32	115.66	121.20
1	D	170	ARG	NE-CZ-NH2	-5.30	114.43	119.20
1	B	75	PRO	CA-C-O	-5.27	115.58	121.32
1	C	323	PHE	CA-CB-CG	-5.25	108.55	113.80
1	A	132	GLU	CA-C-O	-5.25	114.93	121.55
1	C	63	ASN	CA-CB-CG	-5.25	107.35	112.60
1	D	291	ARG	NH1-CZ-NH2	5.25	126.12	119.30
1	B	268	ASP	N-CA-C	5.24	118.46	111.75
1	C	6	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	D	164	HIS	N-CA-CB	5.24	119.00	110.77
1	D	208	ASP	CA-C-O	5.24	125.82	119.11
1	D	248	LEU	CA-C-O	-5.24	114.87	120.42
1	D	354	LEU	CA-C-O	5.23	125.90	120.30
1	B	183	ASN	CA-C-O	-5.22	115.54	121.65
1	D	32	ILE	CA-CB-CG2	5.21	119.36	110.50
1	D	323	PHE	CA-CB-CG	-5.19	108.61	113.80
1	A	248	LEU	CA-C-O	-5.19	114.92	120.42
1	C	6	ASN	CA-C-N	5.18	124.84	119.56
1	C	6	ASN	C-N-CA	5.18	124.84	119.56
1	A	117	LYS	CA-C-O	-5.17	114.79	120.69
1	A	253	ASP	CA-C-O	-5.17	115.07	120.55
1	C	132	GLU	N-CA-C	5.17	116.64	109.31
1	B	96	GLU	CA-C-O	-5.16	114.03	119.97
1	A	268	ASP	CA-C-N	5.12	127.40	120.38
1	A	268	ASP	C-N-CA	5.12	127.40	120.38
1	B	355	ALA	N-CA-CB	5.12	118.08	110.40
1	A	84	VAL	CA-C-O	5.12	127.04	121.67
1	D	149	ARG	CB-CG-CD	5.12	123.07	111.30
1	C	313[A]	GLU	N-CA-C	-5.10	103.95	110.53
1	C	313[B]	GLU	N-CA-C	-5.10	103.95	110.53
1	A	192	ILE	N-CA-C	5.09	115.64	108.36
1	C	42	ARG	CD-NE-CZ	5.09	131.52	124.40
1	C	354	LEU	CA-C-N	5.09	130.85	121.70
1	C	354	LEU	C-N-CA	5.09	130.85	121.70
1	C	57	ILE	CA-C-O	5.08	125.87	120.48
1	B	182	PHE	CA-C-O	-5.08	113.18	119.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	9	GLY	CA-C-O	5.08	125.61	119.82
1	C	298	SER	O-C-N	5.04	129.27	123.17
1	C	149	ARG	CG-CD-NE	5.04	123.08	112.00
1	A	258	ILE	CA-C-N	5.02	129.78	122.10
1	A	258	ILE	C-N-CA	5.02	129.78	122.10
1	B	164	HIS	N-CA-CB	5.02	118.65	110.77
1	A	295	LEU	CA-C-O	-5.01	114.95	120.36

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	34	0
1	B	2805	0	2736	29	0
1	C	2806	0	2740	38	0
1	D	2810	0	2742	38	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	137	0	0	4	0
5	D	144	0	0	3	0
All	All	11821	0	10955	138	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 (138) 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	0.96
1:A:102:ILE:HD11	1:A:117:LYS:HG2	1.53	0.90
1:A:313[A]:GLU:CD	1:A:313[A]:GLU:OE2	2.19	0.86
1:D:281:HIS:HD2	1:D:283:GLU:H	1.22	0.85
1:B:281:HIS:HD2	1:B:283:GLU:H	1.29	0.80
1:D:132:GLU:O	1:D:133:GLY:C	2.25	0.78
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:171:MET:HE3	1:A:202:LYS:HG3	1.69	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:A:313[A]:GLU:CG	1:A:313[A]:GLU:OE2	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:D:199:LEU:C	1:D:199:LEU:HD23	2.19	0.68
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:HE21	1:B:232:GLN:HA	1.60	0.66
1:C:33:MET:HG2	1:C:260:MET:HE1	1.78	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:A:199:LEU:C	1:A:199:LEU:HD23	2.23	0.64
1:A:285:VAL:HG21	5:A:766:HOH:O	1.98	0.63
1:B:281:HIS:CD2	1:B:283:GLU:H	2.15	0.63
1:B:192:ILE:HB	1:B:199:LEU:HD22	1.82	0.62
1:A:313[A]:GLU:CD	5:A:763:HOH:O	2.42	0.61
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:27:GLU:HB2	1:C:28:PRO:HD3	1.83	0.59
1:C:281:HIS:CD2	1:C:283:GLU:H	2.20	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ARG:HD3	1:A:236:GLU:OE2	2.02	0.59
1:C:199:LEU:C	1:C:199:LEU:HD23	2.27	0.59
1:B:252:TRP:CZ3	1:B:256:LYS:HG3	2.39	0.57
1:C:171:MET:HE3	1:C:202:LYS:HE3	1.86	0.57
1:A:192:ILE:HB	1:A:199:LEU:HD22	1.86	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:171:MET:HE3	1:D:202:LYS:HG3	1.88	0.55
1:D:132:GLU:C	1:D:133:GLY:O	2.46	0.54
1:D:281:HIS:HD2	1:D:283:GLU:N	2.00	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:B:199:LEU:C	1:B:199:LEU:HD23	2.33	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:129:ARG:HB2	5:C:701:HOH:O	2.10	0.51
1:B:41:HIS:HB2	1:B:46:VAL:HG22	1.92	0.51
1:D:8:MET:HE1	1:D:94:ALA:HB2	1.93	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:170:ARG:HD3	1:C:236:GLU:OE2	2.11	0.50
1:C:33:MET:HG2	1:C:260:MET:CE	2.40	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: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:D:143:TYR:CD1	1:D:149:ARG:HG2	2.48	0.48
1:D:199:LEU:C	1:D:199:LEU:CD2	2.86	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:A:199:LEU:C	1:A:199:LEU:CD2	2.87	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: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:C:199:LEU:C	1:C:199:LEU:CD2	2.89	0.46
1:C:316:MET:O	1:C:317:GLY:C	2.59	0.46
1:A:113:LEU:HD22	1:A:127:ILE:HD12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:32:ILE:HG23	1:D:260:MET:HE2	1.97	0.45
1:C:171:MET:HE3	1:C:202:LYS:HG3	1.97	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:27:GLU:HB2	1:D:28:PRO:HD3	1.98	0.45
1:D:170:ARG:HD3	1:D:236:GLU:OE2	2.16	0.45
1:C:254:ALA:O	1:C:258:ILE:HG12	2.18	0.44
1:B:80:MET:HE3	1:B:82:PHE:CE1	2.52	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:D:33:MET:HG2	1:D:260:MET:HE3	1.99	0.44
1:B:168:ARG:HH11	1:B:168:ARG:HG3	1.83	0.44
1:B:143:TYR:CD1	1:B:149:ARG:HG2	2.52	0.44
1:C:252:TRP:CE3	1:C:291:ARG:HG2	2.52	0.44
1:C:311:PHE:CZ	1:C:340:LEU:HD22	2.53	0.44
1:D:157[A]:LYS:HE2	5:D:672:HOH:O	2.17	0.44
1:D:199:LEU:HD23	1:D:200:THR:N	2.33	0.44
1:B:27:GLU:N	1:B:28:PRO:HD2	2.33	0.43
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:A:32:ILE:HG23	1:A:260:MET:HE2	1.99	0.43
1:D:106:THR:HG21	1:D:111:LEU:O	2.17	0.43
1:A:103:HIS:CD2	1:A:103:HIS:C	2.97	0.43
1:A:178:TYR:HB3	1:A:184:PHE:CG	2.54	0.43
1:B:44:LYS:HB2	1:B:46:VAL:HG13	2.00	0.43
1:A:58:LEU:C	1:A:58:LEU:HD23	2.44	0.43
1:D:296:ASP:HB2	1:D:336:ASN:OD1	2.19	0.43
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:193:LYS:O	1:D:338:LYS:HE3	2.19	0.42
1:C:162:LEU:HD12	1:C:162:LEU:C	2.45	0.42
1:D:72:GLU:HG2	1:D:73:HIS:CE1	2.55	0.42
1:D:281:HIS:HE1	5:D:771:HOH:O	2.02	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:33:MET:HG2	1:D:260:MET:HE1	2.02	0.41
1:D:222:GLY:O	1:D:223:ALA:HB3	2.18	0.41
1:B:27:GLU:HB2	1:B:28:PRO:HD3	2.01	0.41
1:B:199:LEU:C	1:B:199:LEU:CD2	2.92	0.41
1:C:313[B]:GLU:HB3	5:C:763:HOH:O	2.19	0.41
1:A:157[A]:LYS:HE2	5:A:667:HOH:O	2.20	0.41
1:B:171:MET:HE3	1:B:202:LYS:HE3	2.02	0.41
1:D:229:PHE:CD1	1:D:229:PHE:C	2.99	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:C:58:LEU:C	1:C:58:LEU:HD23	2.45	0.41
1:D:22:THR:HA	1:D:23:PRO:HD3	1.92	0.41
1:D:283:GLU:OE2	1:D:327:LYS:NZ	2.48	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:A:22:THR:HA	1:A:23:PRO:HD3	1.82	0.40
1:C:122:ALA:HA	1:C:123:PRO:HD3	1.94	0.40
1:C:311:PHE:CD1	1:C:322:GLU:HB2	2.57	0.40
1:A:229:PHE:CD1	1:A:229:PHE:C	2.99	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 [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	355/357 (99%)	339 (96%)	15 (4%)	1 (0%)	36	50
1	B	355/357 (99%)	340 (96%)	13 (4%)	2 (1%)	21	32
1	C	355/357 (99%)	343 (97%)	12 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	356/357 (100%)	339 (95%)	16 (4%)	1 (0%)	36	50
All	All	1421/1428 (100%)	1361 (96%)	56 (4%)	4 (0%)	36	50

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%)	278 (94%)	18 (6%)	17	30
1	B	296/296 (100%)	275 (93%)	21 (7%)	13	23
1	C	296/296 (100%)	279 (94%)	17 (6%)	18	33
1	D	297/296 (100%)	281 (95%)	16 (5%)	20	35
All	All	1185/1184 (100%)	1113 (94%)	72 (6%)	16	30

All (72) 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	46	VAL
1	A	126	LEU
1	A	129	ARG
1	A	199	LEU
1	A	200	THR
1	A	221	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	232	GLN
1	A	249	VAL
1	A	251	THR
1	A	269	THR
1	A	274	LEU
1	A	299	SER
1	A	301	GLU
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	38	VAL
1	B	46	VAL
1	B	126	LEU
1	B	129	ARG
1	B	132	GLU
1	B	149	ARG
1	B	152	VAL
1	B	199	LEU
1	B	200	THR
1	B	220	SER
1	B	232	GLN
1	B	249	VAL
1	B	256	LYS
1	B	269	THR
1	B	274	LEU
1	B	338	LYS
1	C	5	GLU
1	C	10	LEU
1	C	32	ILE
1	C	38	VAL
1	C	46	VAL
1	C	126	LEU
1	C	129	ARG
1	C	152	VAL
1	C	199	LEU
1	C	200	THR
1	C	232	GLN
1	C	249	VAL
1	C	256	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	269	THR
1	C	274	LEU
1	C	298	SER
1	C	338	LYS
1	D	5	GLU
1	D	10	LEU
1	D	32	ILE
1	D	38	VAL
1	D	46	VAL
1	D	58	LEU
1	D	126	LEU
1	D	129	ARG
1	D	152	VAL
1	D	199	LEU
1	D	200	THR
1	D	232	GLN
1	D	249	VAL
1	D	269	THR
1	D	274	LEU
1	D	338	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	92	ASN
1	A	103	HIS
1	A	216	ASN
1	A	232	GLN
1	A	289	GLN
1	B	47	HIS
1	B	92	ASN
1	B	100	GLN
1	B	232	GLN
1	B	281	HIS
1	C	47	HIS
1	C	88	GLN
1	C	92	ASN
1	C	232	GLN
1	C	281	HIS
1	D	88	GLN
1	D	92	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	103	HIS
1	D	183	ASN
1	D	216	ASN
1	D	232	GLN
1	D	281	HIS

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 oligosaccharides 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	C	630	1	1,2,2	0.42	0	-		
4	ACT	B	631	2	3,3,3	0.68	0	3,3,3	1.17	0
3	EMC	B	630	1	1,2,2	0.64	0	-		
3	EMC	A	630	1	1,2,2	0.40	0	-		
4	ACT	D	631	2	3,3,3	0.81	0	3,3,3	1.04	0
3	EMC	D	630	1	1,2,2	0.71	0	-		
4	ACT	C	631	2	3,3,3	0.87	0	3,3,3	1.30	0
4	ACT	A	631	2	3,3,3	0.75	0	3,3,3	1.36	0

There are no bond length outliers.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.