



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:42 PM UTC

PDB ID : 1GTT / pdb_00001gtt
Title : CRYSTAL STRUCTURE OF HPCE
Authors : Tame, J.R.H.; Namba, K.; Dodson, E.J.; Roper, D.I.
Deposited on : 2002-01-18
Resolution : 1.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

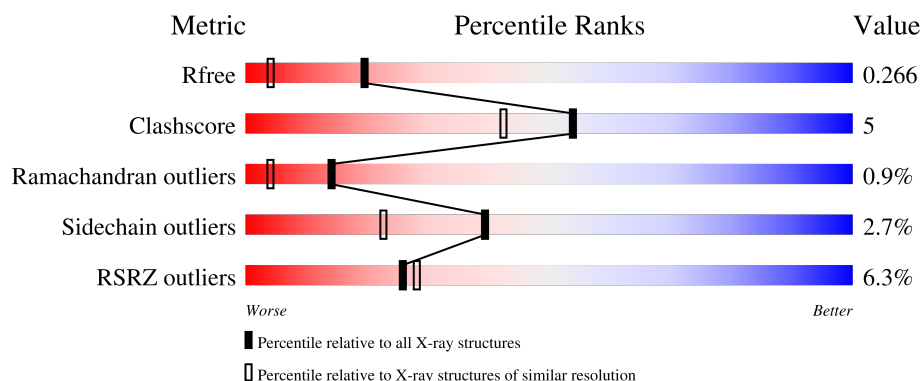
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	429	
1	B	429	
1	C	429	
1	D	429	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14274 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-HYDROXYPHENYLACETATE DEGRADATION BI-FUNCTIONAL ISOMERASE/DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	24	4	0
			3263	2067	556	629	11			
1	B	421	Total	C	N	O	S	29	4	0
			3264	2068	556	629	11			
1	C	421	Total	C	N	O	S	31	3	0
			3260	2066	555	628	11			
1	D	421	Total	C	N	O	S	30	4	0
			3266	2069	557	629	11			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

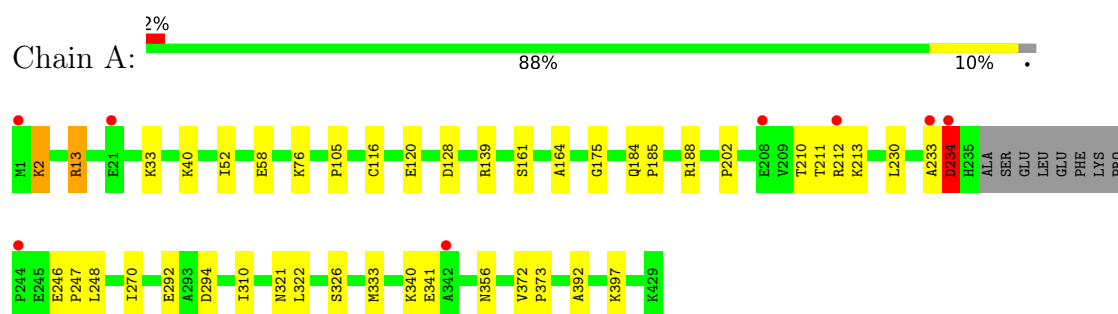
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	316	Total	O	0	0
			316	316		
3	B	306	Total	O	0	0
			306	306		
3	C	322	Total	O	0	0
			322	322		
3	D	273	Total	O	0	0
			273	273		

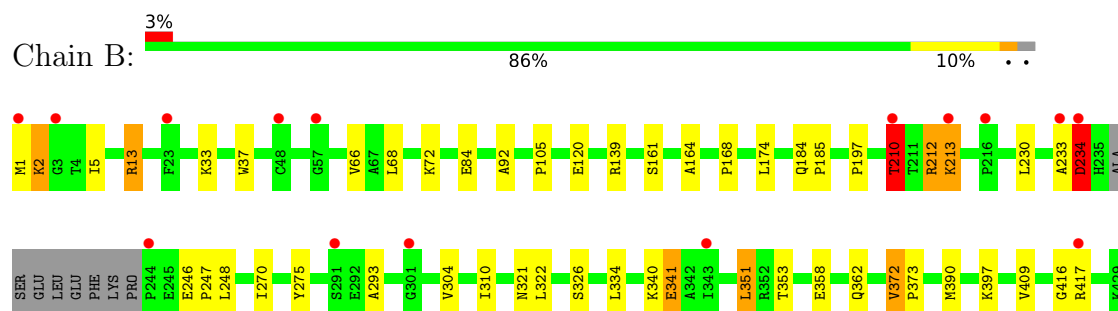
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

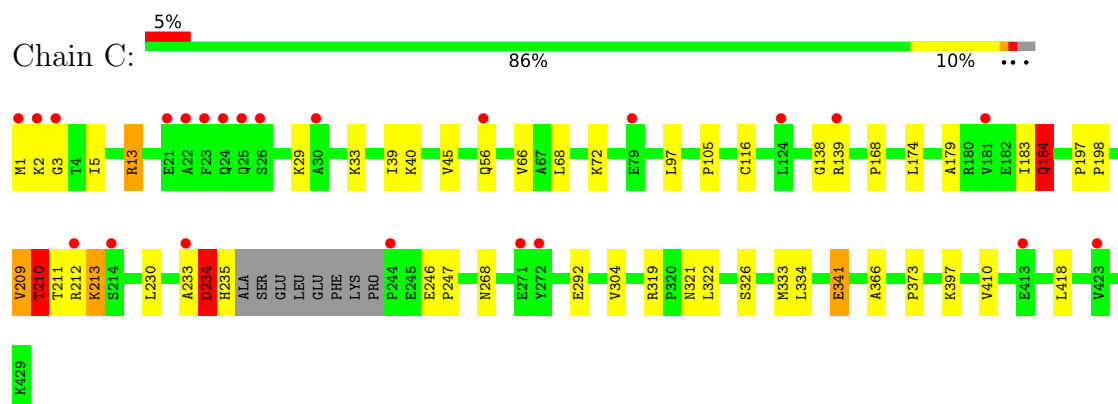
- Molecule 1: 4-HYDROXYPHENYLACETATE DEGRADATION BIFUNCTIONAL ISOMER ASE/DECARBOXYLASE



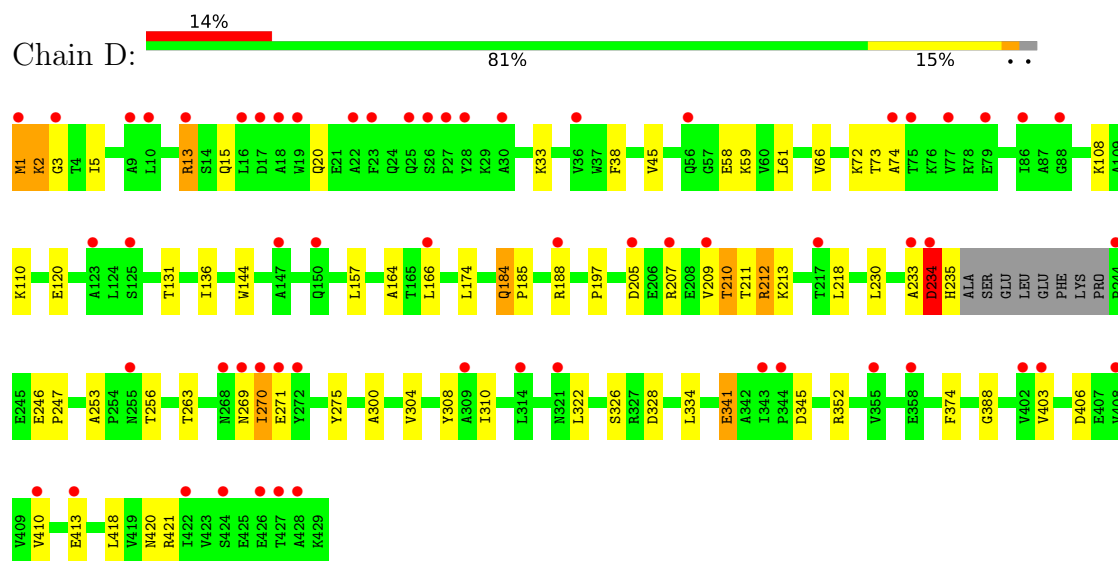
- Molecule 1: 4-HYDROXYPHENYLACETATE DEGRADATION BIFUNCTIONAL ISOMER ASE/DECARBOXYLASE



- Molecule 1: 4-HYDROXYPHENYLACETATE DEGRADATION BIFUNCTIONAL ISOMER ASE/DECARBOXYLASE



● Molecule 1: 4-HYDROXYPHENYLACETATE DEGRADATION BIFUNCTIONAL ISOMERASE/DECARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	126.08Å 138.20Å 103.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.29 – 1.70 91.29 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (91.29-1.70) 98.6 (91.29-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.06	Depositor
R, R_{free}	0.216 , 0.252 (Not available) , 0.266	Depositor DCC
R_{free} test set	9927 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14274	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6189e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.20	7/3358 (0.2%)	1.06	2/4584 (0.0%)
1	B	1.06	5/3358 (0.1%)	1.10	9/4584 (0.2%)
1	C	1.54	8/3349 (0.2%)	1.39	14/4571 (0.3%)
1	D	1.18	5/3361 (0.1%)	1.14	9/4587 (0.2%)
All	All	1.26	25/13426 (0.2%)	1.18	34/18326 (0.2%)

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
1	B	0	3
1	C	0	4
1	D	0	1
All	All	0	10

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	210	THR	C-O	47.71	1.84	1.24
1	C	209	VAL	C-N	-40.52	0.77	1.33
1	A	234	ASP	C-N	-27.17	0.95	1.33
1	D	209	VAL	C-N	-24.91	0.98	1.33
1	D	234	ASP	C-N	-20.61	1.04	1.33
1	B	234	ASP	C-N	-14.95	1.12	1.33
1	C	210	THR	N-CA	14.09	1.64	1.46
1	C	212	ARG	C-N	13.01	1.52	1.33
1	C	210	THR	C-N	-8.91	1.20	1.33
1	D	1	MET	SD-CE	8.60	2.01	1.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	211	THR	C-N	-7.99	1.22	1.33
1	A	211	THR	C-N	-7.54	1.23	1.33
1	B	372	VAL	CA-CB	6.57	1.57	1.54
1	B	92	ALA	C-O	-6.44	1.15	1.23
1	A	333	MET	CG-SD	-6.29	1.65	1.80
1	C	179	ALA	CA-CB	6.17	1.62	1.53
1	C	211	THR	C-N	-6.01	1.25	1.33
1	B	390	MET	SD-CE	5.81	1.94	1.79
1	A	392	ALA	CA-CB	5.75	1.60	1.53
1	A	333	MET	SD-CE	5.67	1.93	1.79
1	C	333	MET	CG-SD	-5.65	1.66	1.80
1	A	321	ASN	CB-CG	5.42	1.65	1.52
1	B	353	THR	CA-C	5.40	1.59	1.52
1	D	218	LEU	N-CA	-5.10	1.41	1.45
1	A	52	ILE	N-CA	-5.06	1.42	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	VAL	O-C-N	-29.40	89.90	122.83
1	C	209	VAL	CA-C-N	26.62	172.39	121.54
1	C	209	VAL	C-N-CA	26.62	172.39	121.54
1	C	210	THR	CA-C-O	-25.00	84.76	120.51
1	C	234	ASP	O-C-N	15.19	142.79	122.59
1	B	210	THR	O-C-N	-13.95	104.03	122.59
1	D	234	ASP	O-C-N	12.88	139.72	122.59
1	C	210	THR	O-C-N	12.67	139.44	122.59
1	D	209	VAL	O-C-N	-12.29	108.58	122.83
1	B	234	ASP	O-C-N	8.33	133.67	122.59
1	D	234	ASP	CA-C-N	-7.81	107.63	121.70
1	D	234	ASP	C-N-CA	-7.81	107.63	121.70
1	B	234	ASP	CA-C-N	-7.20	108.75	121.70
1	B	234	ASP	C-N-CA	-7.20	108.75	121.70
1	C	210	THR	CA-C-N	7.08	134.11	121.66
1	C	210	THR	C-N-CA	7.08	134.11	121.66
1	B	213	LYS	N-CA-CB	-6.88	98.82	109.48
1	C	3	GLY	N-CA-C	-6.82	102.17	112.60
1	D	210	THR	N-CA-C	6.69	125.04	110.80
1	C	234	ASP	CA-C-N	-6.48	110.03	121.70
1	C	234	ASP	C-N-CA	-6.48	110.03	121.70
1	B	212	ARG	CD-NE-CZ	-6.32	115.56	124.40
1	C	97	LEU	N-CA-C	-6.15	101.09	110.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	GLY	N-CA-C	5.87	118.01	112.08
1	C	33	LYS	N-CA-C	-5.87	103.67	111.24
1	B	358	GLU	CB-CG-CD	5.65	122.20	112.60
1	B	293	ALA	N-CA-C	5.48	117.26	111.28
1	A	139	ARG	CB-CA-C	-5.41	102.66	109.31
1	B	416	GLY	N-CA-C	5.40	118.46	110.63
1	D	388	GLY	N-CA-C	-5.23	108.47	114.69
1	D	269	ASN	N-CA-C	5.12	118.65	111.74
1	C	184	GLN	CB-CG-CD	5.10	121.27	112.60
1	D	271	GLU	N-CA-C	5.04	117.88	111.69
1	D	3	GLY	N-CA-C	-5.01	103.95	112.51

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	ASP	Mainchain,Peptide
1	B	210	THR	Mainchain
1	B	234	ASP	Mainchain,Peptide
1	C	209	VAL	Peptide
1	C	210	THR	Mainchain,Peptide
1	C	234	ASP	Peptide
1	D	234	ASP	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	3263	0	3216	27	1
1	B	3264	0	3221	27	2
1	C	3260	0	3215	32	3
1	D	3266	0	3224	41	2
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	316	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	306	0	0	0	0
3	C	322	0	0	5	0
3	D	273	0	0	3	0
All	All	14274	0	12876	123	4

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 5.

All (123) 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:183:ILE:O	1:C:184:GLN:NE2	1.92	1.02
1:C:304:VAL:HG12	1:C:334:LEU:HD12	1.42	0.99
1:B:184[B]:GLN:HG3	1:B:185:PRO:HD2	1.56	0.86
1:B:37:TRP:H	1:B:321:ASN:HD21	1.27	0.83
1:B:409:VAL:HG11	1:B:417:ARG:CZ	2.11	0.80
1:A:184[A]:GLN:HG3	1:A:185:PRO:HD2	1.64	0.79
1:D:184[A]:GLN:HG3	1:D:185:PRO:HD2	1.66	0.78
1:C:304:VAL:CG1	1:C:334:LEU:HD12	2.16	0.76
1:B:304:VAL:HG12	1:B:334:LEU:HD12	1.65	0.76
1:C:322:LEU:HD22	1:C:326:SER:CB	2.20	0.72
1:A:322:LEU:HD22	1:A:326:SER:CB	2.20	0.72
1:C:56:GLN:HG2	3:C:2051:HOH:O	1.90	0.71
1:C:322:LEU:HD22	1:C:326:SER:HB2	1.75	0.68
1:D:304:VAL:HG12	1:D:334:LEU:HD12	1.75	0.67
1:B:322:LEU:HD22	1:B:326:SER:HB2	1.75	0.67
1:A:322:LEU:HD22	1:A:326:SER:HB2	1.78	0.66
1:C:66:VAL:HG13	1:C:174:LEU:HD12	1.78	0.64
1:C:45:VAL:O	1:C:213:LYS:NZ	2.35	0.60
1:B:322:LEU:HD22	1:B:326:SER:CB	2.31	0.60
1:D:45:VAL:O	1:D:213:LYS:NZ	2.32	0.60
1:D:13:ARG:HH11	1:D:13:ARG:HG3	1.67	0.60
1:B:105:PRO:HD2	1:B:248:LEU:HD11	1.83	0.59
1:B:1:MET:N	1:B:5:ILE:HD11	2.18	0.59
1:D:1:MET:N	1:D:5:ILE:HD11	2.18	0.58
1:C:322:LEU:HD22	1:C:326:SER:OG	2.04	0.58
1:C:56:GLN:OE1	3:C:2051:HOH:O	2.17	0.57
1:C:1:MET:N	1:C:5:ILE:HD11	2.20	0.57
1:D:263:THR:HA	1:D:421:ARG:O	2.03	0.57
1:A:76:LYS:C	3:A:2064:HOH:O	2.48	0.57
1:A:188:ARG:NH2	1:A:202:PRO:HB3	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ILE:HD13	1:D:310:ILE:HG23	1.90	0.54
1:A:233:ALA:O	1:A:234:ASP:C	2.50	0.54
1:B:304:VAL:CG1	1:B:334:LEU:HD12	2.34	0.53
1:C:13:ARG:HG2	1:C:13:ARG:HH11	1.73	0.53
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.91	0.53
1:A:246:GLU:HB2	1:A:247:PRO:HD2	1.91	0.53
1:B:233:ALA:O	1:B:234:ASP:C	2.51	0.53
1:D:108:LYS:NZ	3:D:2068:HOH:O	2.41	0.53
1:C:13:ARG:HH11	1:C:13:ARG:CG	2.21	0.53
1:C:234:ASP:HB3	1:C:397:LYS:CG	2.40	0.52
1:C:268:ASN:ND2	3:C:2219:HOH:O	2.43	0.52
1:A:322:LEU:HD22	1:A:326:SER:OG	2.10	0.52
1:A:270:ILE:HD13	1:A:310:ILE:HG23	1.90	0.52
1:A:76:LYS:HA	3:A:2064:HOH:O	2.10	0.51
1:D:410:VAL:HG23	1:D:418:LEU:HB3	1.92	0.51
1:B:409:VAL:HG11	1:B:417:ARG:NH2	2.24	0.51
1:D:13:ARG:HH11	1:D:13:ARG:CG	2.22	0.51
1:C:322:LEU:CD2	1:C:326:SER:OG	2.59	0.51
1:D:205:ASP:OD2	1:D:207:ARG:NH2	2.37	0.50
1:D:246:GLU:HB2	1:D:247:PRO:HD2	1.94	0.50
1:D:233:ALA:O	1:D:234:ASP:C	2.54	0.50
1:B:270:ILE:HD13	1:B:310:ILE:HG23	1.93	0.50
1:D:120:GLU:CD	1:D:197:PRO:HG3	2.36	0.50
1:D:341:GLU:H	1:D:341:GLU:CD	2.20	0.49
1:D:59:LYS:HE2	1:D:61:LEU:HD21	1.94	0.49
1:C:233:ALA:O	1:C:234:ASP:C	2.55	0.49
1:D:66:VAL:HG13	1:D:174:LEU:HD12	1.95	0.49
1:A:105:PRO:HD2	1:A:248:LEU:HD11	1.95	0.49
1:C:321:ASN:HB3	3:C:2255:HOH:O	2.12	0.48
1:B:161:SER:HA	1:B:164:ALA:O	2.14	0.48
1:A:128:ASP:OD2	3:A:2115:HOH:O	2.20	0.48
1:C:183:ILE:C	1:C:184:GLN:HE21	2.12	0.48
1:C:72:LYS:HA	1:C:168:PRO:HG3	1.96	0.48
1:D:322:LEU:HD22	1:D:326:SER:OG	2.14	0.47
1:C:341:GLU:CD	1:C:341:GLU:H	2.22	0.47
1:D:345:ASP:OD1	1:D:345:ASP:N	2.47	0.47
1:A:13:ARG:CG	1:A:13:ARG:HH11	2.28	0.47
1:D:308:TYR:OH	1:D:420:ASN:ND2	2.43	0.47
1:A:234:ASP:HB3	1:A:397:LYS:CG	2.45	0.47
1:B:234:ASP:HB3	1:B:397:LYS:CG	2.45	0.47
1:D:38:PHE:CE2	1:D:110:LYS:HD3	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LYS:HG3	1:B:2:LYS:O	2.15	0.47
1:B:66:VAL:HG13	1:B:174:LEU:HD12	1.98	0.46
1:A:188:ARG:HH22	1:D:188:ARG:NH1	2.13	0.46
1:C:39:ILE:HD11	1:C:322:LEU:HD21	1.96	0.46
1:C:68:LEU:C	1:C:68:LEU:HD12	2.40	0.46
1:D:2:LYS:O	1:D:2:LYS:HG3	2.16	0.46
1:B:341:GLU:H	1:B:341:GLU:CD	2.24	0.46
1:A:356:ASN:ND2	3:A:2272:HOH:O	2.48	0.45
1:C:410:VAL:CG2	1:C:418:LEU:HB3	2.46	0.45
1:C:366:ALA:O	3:C:2286:HOH:O	2.21	0.45
1:B:120:GLU:HB3	1:B:197:PRO:HG2	1.98	0.45
1:D:184[B]:GLN:CD	1:D:185:PRO:HD2	2.42	0.45
1:C:105:PRO:HD3	1:C:319:ARG:O	2.17	0.44
1:D:15:GLN:NE2	3:D:2012:HOH:O	2.50	0.44
1:D:213:LYS:HB3	1:D:213:LYS:HE3	1.72	0.44
1:C:40:LYS:HE3	1:C:116:CYS:HB2	2.00	0.44
1:D:74:ALA:HB3	1:D:166:LEU:HB2	1.99	0.44
1:A:188:ARG:HH22	1:D:188:ARG:HH12	1.66	0.43
1:B:72:LYS:HA	1:B:168:PRO:HG3	2.00	0.43
1:B:321:ASN:CG	1:B:322:LEU:H	2.26	0.43
1:A:188:ARG:NH1	1:D:188:ARG:NH2	2.67	0.43
1:A:322:LEU:HD23	3:A:2258:HOH:O	2.17	0.43
1:D:275:TYR:HA	1:D:308:TYR:CD1	2.53	0.43
1:D:164:ALA:HA	1:D:328:ASP:OD1	2.18	0.42
1:A:184[B]:GLN:HG2	1:A:185:PRO:HD2	2.00	0.42
1:A:292:GLU:O	3:A:2237:HOH:O	2.20	0.42
1:D:157:LEU:HD12	1:D:166:LEU:HD13	2.01	0.42
1:B:246:GLU:HB2	1:B:247:PRO:HD2	2.00	0.42
1:B:68:LEU:C	1:B:68:LEU:HD12	2.44	0.42
1:B:275:TYR:CD1	1:B:275:TYR:C	2.98	0.42
1:D:253:ALA:O	1:D:256:THR:HG22	2.20	0.42
1:D:403:VAL:O	1:D:406:ASP:HB2	2.19	0.42
1:D:131:THR:HA	1:D:144:TRP:O	2.20	0.42
1:A:161:SER:HA	1:A:164:ALA:O	2.19	0.42
1:A:292:GLU:HG3	1:A:373:PRO:HB2	2.02	0.41
1:D:304:VAL:CG1	1:D:334:LEU:HD12	2.45	0.41
1:B:351:LEU:O	1:B:362:GLN:HA	2.21	0.41
1:D:2:LYS:O	1:D:2:LYS:CG	2.68	0.41
1:C:410:VAL:HG23	1:C:418:LEU:HB3	2.03	0.41
1:A:120:GLU:OE2	3:A:2103:HOH:O	2.22	0.41
1:C:246:GLU:HB2	1:C:247:PRO:HD2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LYS:HE3	1:A:116:CYS:HB2	2.02	0.41
1:B:66:VAL:CG1	1:B:174:LEU:HD12	2.50	0.41
1:A:322:LEU:CD2	1:A:326:SER:OG	2.70	0.40
1:B:210:THR:HG21	1:C:138:GLY:HA3	2.02	0.40
1:D:300:ALA:O	3:D:2197:HOH:O	2.22	0.40
1:D:72:LYS:O	1:D:73:THR:C	2.65	0.40
1:C:197:PRO:HA	1:C:198:PRO:HD3	1.90	0.40
1:D:322:LEU:HD22	1:D:326:SER:CB	2.51	0.40
1:A:372:VAL:HB	1:A:373:PRO:HD3	2.03	0.40
1:C:292:GLU:HG3	1:C:373:PRO:HB2	2.03	0.40
1:D:374:PHE:CD1	1:D:374:PHE:C	2.99	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ARG:NH1	1:C:235:HIS:NE2[4_546]	1.74	0.46
1:B:13:ARG:NH1	1:C:235:HIS:CE1[4_546]	1.79	0.41
1:A:13:ARG:NH1	1:D:235:HIS:NE2[4_545]	2.04	0.16
1:C:139:ARG:NH2	1:D:136:ILE:O[2_555]	2.07	0.13

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	216/429 (50%)	210 (97%)	4 (2%)	2 (1%)	14	4
1	B	421/429 (98%)	405 (96%)	13 (3%)	3 (1%)	18	7
1	C	420/429 (98%)	403 (96%)	14 (3%)	3 (1%)	18	7
1	D	421/429 (98%)	407 (97%)	9 (2%)	5 (1%)	10	2
All	All	1478/1716 (86%)	1425 (96%)	40 (3%)	13 (1%)	14	4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	210	THR
1	B	234	ASP
1	C	210	THR
1	C	234	ASP
1	D	234	ASP
1	A	234	ASP
1	D	210	THR
1	D	230	LEU
1	A	2	LYS
1	D	413	GLU
1	C	230	LEU
1	D	212	ARG
1	B	212	ARG

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	355/360 (99%)	344 (97%)	11 (3%)	35	18
1	B	355/360 (99%)	345 (97%)	10 (3%)	38	21
1	C	354/360 (98%)	347 (98%)	7 (2%)	48	32
1	D	356/360 (99%)	345 (97%)	11 (3%)	35	18
All	All	1420/1440 (99%)	1381 (97%)	39 (3%)	39	23

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	13	ARG
1	A	33	LYS
1	A	58	GLU
1	A	210	THR
1	A	212	ARG
1	A	213	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	230	LEU
1	A	294	ASP
1	A	340	LYS
1	A	341	GLU
1	B	2	LYS
1	B	13	ARG
1	B	33	LYS
1	B	84	GLU
1	B	139	ARG
1	B	213	LYS
1	B	230	LEU
1	B	340	LYS
1	B	341	GLU
1	B	351	LEU
1	C	2	LYS
1	C	13	ARG
1	C	29	LYS
1	C	184	GLN
1	C	210	THR
1	C	213	LYS
1	C	341	GLU
1	D	2	LYS
1	D	13	ARG
1	D	20	GLN
1	D	33	LYS
1	D	58	GLU
1	D	184[A]	GLN
1	D	184[B]	GLN
1	D	212	ARG
1	D	270	ILE
1	D	341	GLU
1	D	352	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	129	ASN
1	A	201	ASN
1	A	268	ASN
1	A	274	HIS
1	A	286	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	289	ASN
1	A	348	ASN
1	A	386	ASN
1	A	420	ASN
1	B	25	GLN
1	B	129	ASN
1	B	269	ASN
1	B	286	GLN
1	B	321	ASN
1	B	348	ASN
1	B	386	ASN
1	B	420	ASN
1	C	15	GLN
1	C	25	GLN
1	C	150	GLN
1	C	201	ASN
1	C	362	GLN
1	C	420	ASN
1	D	25	GLN
1	D	129	ASN
1	D	201	ASN
1	D	289	ASN
1	D	362	GLN
1	D	420	ASN

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2
1	D	2
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	210:THR	C	211:THR	N	1.19
1	B	234:ASP	C	235:HIS	N	1.12
1	D	234:ASP	C	235:HIS	N	1.04
1	D	209:VAL	C	210:THR	N	0.98
1	A	234:ASP	C	235:HIS	N	0.95
1	C	209:VAL	C	210:THR	N	0.77

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	418/429 (97%)	0.07	8 (1%) 66 71	24, 31, 48, 64	4 (0%)
1	B	418/429 (97%)	0.30	15 (3%) 46 50	25, 35, 54, 70	5 (1%)
1	C	418/429 (97%)	0.40	23 (5%) 30 34	24, 35, 53, 70	5 (1%)
1	D	418/429 (97%)	0.94	60 (14%) 6 5	24, 39, 61, 76	5 (1%)
All	All	1672/1716 (97%)	0.43	106 (6%) 26 28	24, 35, 55, 76	19 (1%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	244	PRO	5.5
1	D	1	MET	5.3
1	D	74	ALA	5.1
1	D	428	ALA	4.9
1	C	233	ALA	4.8
1	D	147	ALA	4.4
1	D	272	TYR	4.3
1	D	30	ALA	4.2
1	C	413	GLU	4.1
1	B	244	PRO	4.0
1	B	1	MET	4.0
1	C	1	MET	3.9
1	B	210	THR	3.9
1	D	270	ILE	3.7
1	D	18	ALA	3.7
1	D	413	GLU	3.5
1	D	150	GLN	3.4
1	D	233	ALA	3.4
1	D	344	PRO	3.3
1	D	56	GLN	3.3
1	D	422	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	22	ALA	3.2
1	D	410	VAL	3.2
1	D	28	TYR	3.1
1	D	309	ALA	3.1
1	D	22	ALA	3.1
1	D	19	TRP	3.0
1	A	212	ARG	3.0
1	D	269	ASN	3.0
1	D	403	VAL	3.0
1	D	408	VAL	3.0
1	C	56	GLN	3.0
1	D	207	ARG	3.0
1	D	79	GLU	3.0
1	C	23	PHE	3.0
1	C	214	SER	2.9
1	C	2	LYS	2.9
1	D	271	GLU	2.9
1	A	233	ALA	2.8
1	A	1	MET	2.8
1	C	272	TYR	2.8
1	A	234	ASP	2.8
1	D	16	LEU	2.7
1	D	3	GLY	2.7
1	D	355	VAL	2.7
1	C	21	GLU	2.6
1	B	23	PHE	2.6
1	D	402	VAL	2.6
1	D	13	ARG	2.6
1	D	36	VAL	2.6
1	B	233	ALA	2.6
1	D	424	SER	2.6
1	A	342	ALA	2.6
1	D	358	GLU	2.5
1	D	244	PRO	2.5
1	B	301	GLY	2.5
1	C	181	VAL	2.5
1	D	205	ASP	2.5
1	D	427	THR	2.5
1	D	209	VAL	2.5
1	C	139	ARG	2.5
1	D	125	SER	2.5
1	B	234	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	234	ASP	2.4
1	B	48[A]	CYS	2.4
1	D	123	ALA	2.4
1	B	417	ARG	2.4
1	D	188	ARG	2.4
1	A	21	GLU	2.4
1	A	208	GLU	2.4
1	C	3	GLY	2.4
1	D	75	THR	2.4
1	B	213	LYS	2.4
1	C	423	VAL	2.3
1	D	426	GLU	2.3
1	D	17	ASP	2.3
1	B	343	ILE	2.3
1	A	244	PRO	2.3
1	C	24	GLN	2.3
1	C	30	ALA	2.3
1	C	124	LEU	2.3
1	D	88	GLY	2.3
1	C	25	GLN	2.2
1	B	291	SER	2.2
1	D	27	PRO	2.2
1	C	212	ARG	2.2
1	D	10	LEU	2.2
1	C	79	GLU	2.2
1	D	86	ILE	2.2
1	D	26	SER	2.2
1	D	314	LEU	2.2
1	D	217	THR	2.2
1	B	57	GLY	2.1
1	B	216	PRO	2.1
1	D	9	ALA	2.1
1	D	77	VAL	2.1
1	D	268	ASN	2.1
1	D	25	GLN	2.1
1	D	343	ILE	2.1
1	B	3	GLY	2.0
1	C	271	GLU	2.0
1	C	26	SER	2.0
1	D	166	LEU	2.0
1	D	255	ASN	2.0
1	D	321	ASN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	23	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	D	1430	1/1	0.94	0.07	36,36,36,36	0
2	CA	B	1430	1/1	0.99	0.02	31,31,31,31	0
2	CA	C	1430	1/1	0.99	0.03	32,32,32,32	0
2	CA	A	1430	1/1	0.99	0.02	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.