



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:50 AM UTC

PDB ID : 1I7O / pdb_00001i7o
Title : CRYSTAL STRUCTURE OF HPCE
Authors : Tame, J.R.H.; Namba, K.; Dodson, E.J.; Roper, D.I.
Deposited on : 2001-03-10
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

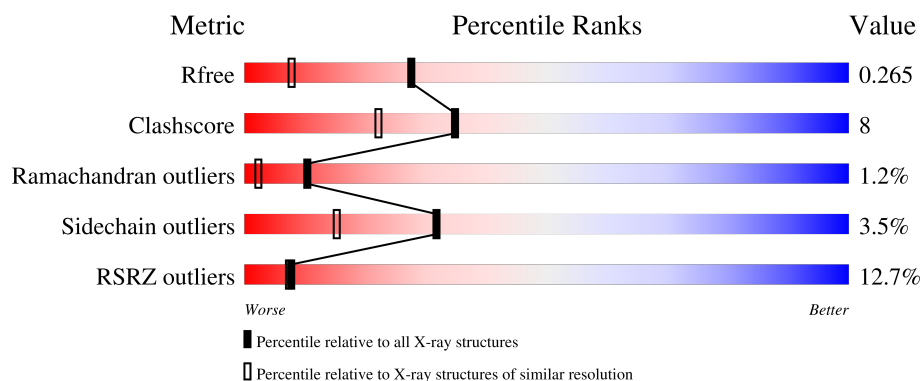
1 Overall quality at a glance

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	6% 84% 12% ...
1	B	429	8% 82% 14% ...
1	C	429	11% 80% 15% ..
1	D	429	24% 75% 20% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13619 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	11	1	0
			3237	2053	554	619	11			
1	B	421	Total	C	N	O	S	21	1	0
			3237	2053	554	619	11			
1	C	421	Total	C	N	O	S	15	1	0
			3237	2053	554	619	11			
1	D	421	Total	C	N	O	S	16	1	0
			3236	2053	554	618	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		

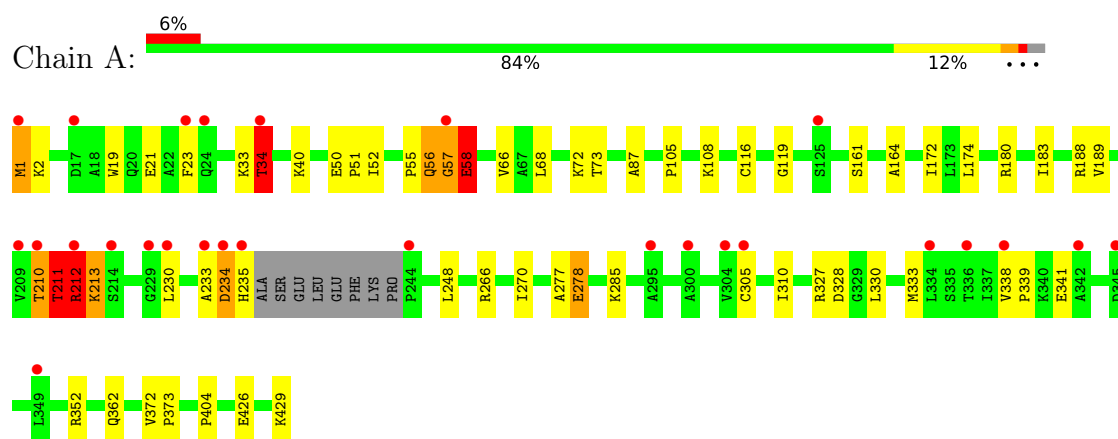
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	214	Total	O	0	0
			214	214		
3	B	174	Total	O	0	0
			174	174		
3	C	165	Total	O	0	0
			165	165		
3	D	115	Total	O	0	0
			115	115		

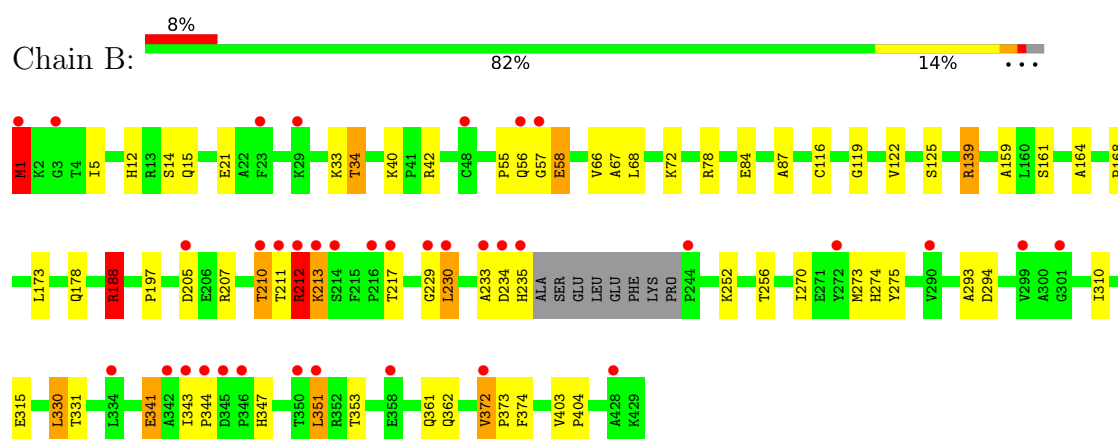
3 Residue-property plots [i](#)

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.

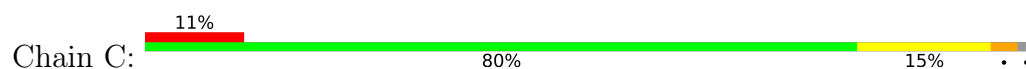
- Molecule 1: 4-HYDROXYPHENYLACETATE DEGRADATION BIFUNCTIONAL ISOMER ASE/DECARBOXYLASE

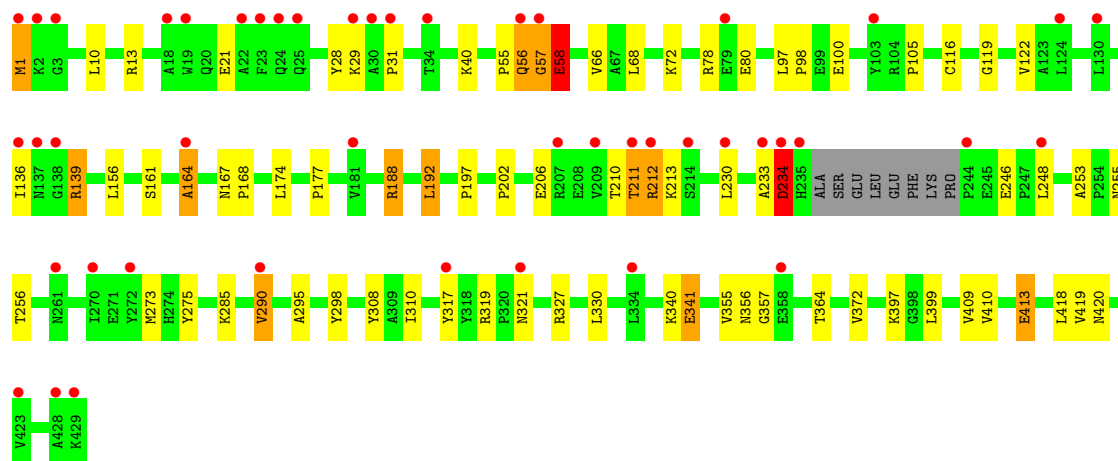


- Molecule 1: 4-HYDROXYPHENYLACETATE DEGRADATION BIFUNCTIONAL ISOMER ASE/DECARBOXYLASE

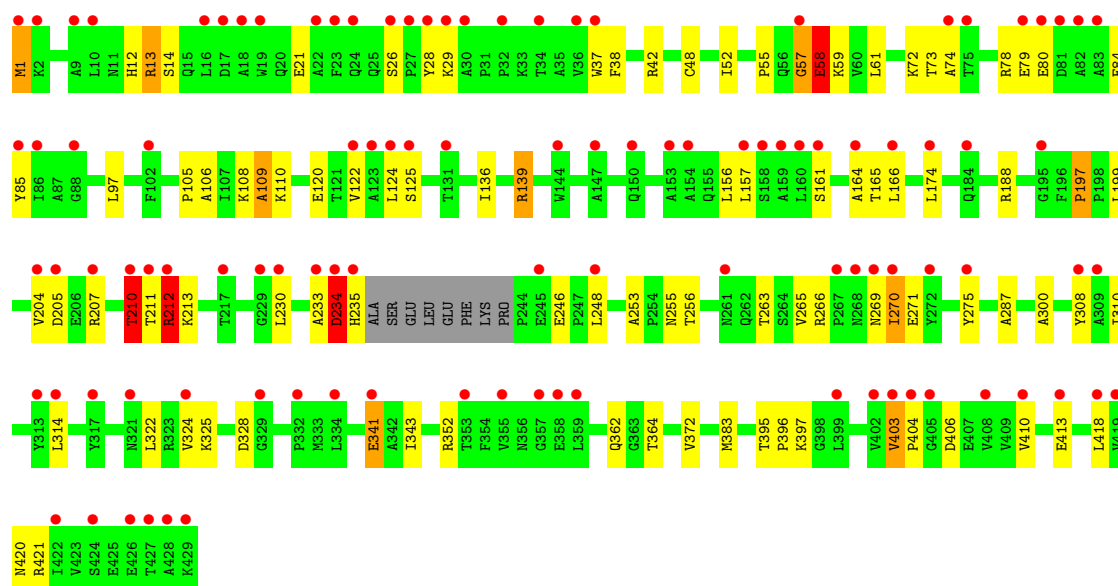
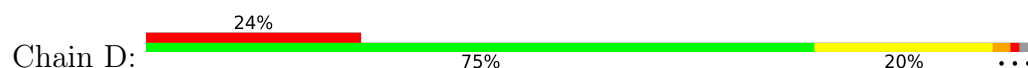


- Molecule 1: 4-HYDROXYPHENYLACETATE DEGRADATION BIFUNCTIONAL ISOMER ASE/DECARBOXYLASE





● Molecule 1: 4-HYDROXYPHENYLACETATE DEGRADATION BIFUNCTIONAL ISOMER ASE/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)	15.00 – 1.70 15.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (15.00-1.70) 98.6 (15.00-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.251 , 0.278 0.234 , 0.265	Depositor DCC
R_{free} test set	9927 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.5	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	0.95	EDS
Total number of atoms	13619	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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 2.6190e-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	1.15	7/3316 (0.2%)	1.21	13/4525 (0.3%)
1	B	1.09	6/3316 (0.2%)	1.19	12/4525 (0.3%)
1	C	1.07	5/3316 (0.2%)	1.23	14/4525 (0.3%)
1	D	1.03	5/3315 (0.2%)	1.22	18/4523 (0.4%)
All	All	1.08	23/13263 (0.2%)	1.21	57/18098 (0.3%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	139	ARG	CB-CG	-14.81	1.08	1.52
1	A	212	ARG	CG-CD	-14.54	1.08	1.52
1	B	139	ARG	CG-CD	14.39	1.95	1.52
1	C	212	ARG	CG-CD	13.95	1.94	1.52
1	C	188	ARG	CG-CD	-9.48	1.24	1.52
1	B	1	MET	SD-CE	9.13	2.02	1.79
1	D	372	VAL	CA-CB	7.92	1.58	1.54
1	C	372	VAL	CA-CB	7.70	1.57	1.54
1	C	1	MET	SD-CE	6.77	1.96	1.79
1	A	277	ALA	CA-CB	6.70	1.63	1.53
1	A	333	MET	CG-SD	-6.45	1.64	1.80
1	B	188	ARG	CG-CD	6.29	1.71	1.52
1	D	383	MET	SD-CE	6.09	1.94	1.79
1	A	52	ILE	N-CA	-5.68	1.42	1.46
1	B	372	VAL	CA-C	5.49	1.58	1.52
1	D	109	ALA	CA-CB	5.42	1.61	1.53
1	B	159	ALA	CA-CB	5.37	1.61	1.53
1	A	333	MET	SD-CE	5.30	1.92	1.79
1	A	1	MET	SD-CE	5.25	1.92	1.79
1	D	52	ILE	CA-CB	-5.25	1.48	1.53
1	C	321	ASN	C-O	-5.12	1.17	1.23
1	B	87	ALA	CA-CB	-5.09	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	ALA	CA-CB	5.09	1.61	1.53

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	188	ARG	CB-CG-CD	11.77	138.36	111.30
1	C	212	ARG	CG-CD-NE	-11.39	86.94	112.00
1	C	212	ARG	CB-CG-CD	-10.14	87.97	111.30
1	D	139	ARG	CA-CB-CG	9.11	132.33	114.10
1	A	212	ARG	CB-CG-CD	8.74	131.40	111.30
1	B	188	ARG	CG-CD-NE	7.95	129.50	112.00
1	C	321	ASN	N-CA-C	7.89	121.24	110.35
1	B	33	LYS	CB-CG-CD	7.72	129.06	111.30
1	A	278	GLU	N-CA-C	7.49	120.84	109.23
1	B	139	ARG	CB-CG-CD	-7.38	94.31	111.30
1	A	55	PRO	CA-C-N	-7.28	109.51	120.94
1	A	55	PRO	C-N-CA	-7.28	109.51	120.94
1	A	211	THR	N-CA-C	7.03	121.95	113.23
1	D	197	PRO	N-CA-C	-6.98	102.18	110.70
1	A	2	LYS	N-CA-C	-6.95	104.37	112.92
1	B	293	ALA	N-CA-C	6.78	118.67	111.28
1	B	210	THR	N-CA-C	6.66	124.98	110.80
1	D	210	THR	N-CA-C	6.61	124.87	110.80
1	A	57	GLY	CA-C-N	6.41	133.24	121.70
1	A	57	GLY	C-N-CA	6.41	133.24	121.70
1	D	212	ARG	CG-CD-NE	-6.32	98.09	112.00
1	D	271	GLU	N-CA-C	6.28	119.06	111.40
1	D	57	GLY	CA-C-N	6.24	132.93	121.70
1	D	57	GLY	C-N-CA	6.24	132.93	121.70
1	C	188	ARG	CG-CD-NE	6.23	125.72	112.00
1	A	234	ASP	N-CA-C	6.23	124.06	110.80
1	A	210	THR	N-CA-C	6.16	123.91	110.80
1	C	233	ALA	N-CA-C	-6.15	104.26	110.97
1	C	139	ARG	CB-CG-CD	-6.14	97.18	111.30
1	B	212	ARG	CG-CD-NE	-6.13	98.51	112.00
1	C	290	VAL	N-CA-CB	-6.00	104.18	110.72
1	D	325	LYS	N-CA-C	5.94	120.69	113.38
1	D	266	ARG	N-CA-C	-5.91	102.33	109.72
1	D	234	ASP	N-CA-C	5.84	123.25	110.80
1	C	97	LEU	N-CA-C	-5.83	100.49	109.41
1	B	5	ILE	N-CA-C	5.79	115.68	106.88
1	D	287	ALA	N-CA-C	5.77	118.31	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	265	VAL	CB-CA-C	-5.74	104.37	111.08
1	A	34	THR	N-CA-CB	-5.72	102.65	111.46
1	A	56	GLN	N-CA-CB	5.62	118.26	110.17
1	B	212	ARG	CB-CG-CD	-5.58	98.48	111.30
1	B	42	ARG	N-CA-C	5.50	117.28	111.28
1	C	295	ALA	N-CA-C	5.41	117.18	111.28
1	A	266	ARG	N-CA-C	-5.40	101.79	109.62
1	C	164	ALA	CA-C-N	5.37	128.46	120.95
1	C	164	ALA	C-N-CA	5.37	128.46	120.95
1	D	403	VAL	N-CA-C	5.32	114.83	108.45
1	D	300	ALA	N-CA-C	-5.28	105.11	112.45
1	B	330	LEU	CA-C-N	-5.27	117.16	122.74
1	B	330	LEU	C-N-CA	-5.27	117.16	122.74
1	B	294	ASP	N-CA-C	5.21	119.74	113.17
1	D	265	VAL	N-CA-C	5.17	116.19	108.54
1	D	97	LEU	N-CA-C	-5.16	102.54	110.07
1	D	42	ARG	N-CA-C	5.09	117.50	111.33
1	D	269	ASN	N-CA-C	5.08	118.41	111.39
1	C	57	GLY	CA-C-N	5.02	130.73	121.70
1	C	57	GLY	C-N-CA	5.02	130.73	121.70

There are no chirality outliers.

There are no planarity outliers.

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	3237	0	3193	35	3
1	B	3237	0	3195	46	16
1	C	3237	0	3195	47	5
1	D	3236	0	3193	65	22
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	214	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	174	0	0	1	0
3	C	165	0	0	3	0
3	D	115	0	0	3	0
All	All	13619	0	12776	192	23

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 8.

All (192) 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:B:1:MET:CE	1:B:1:MET:SD	2.02	1.45
1:B:57:GLY:HA3	1:B:58:GLU:HB2	1.25	1.18
1:D:1:MET:N	1:D:1:MET:HE3	1.59	1.15
1:D:205:ASP:OD2	1:D:207:ARG:NH2	1.89	1.06
1:C:57:GLY:HA3	1:C:58:GLU:HB2	1.10	1.05
1:A:57:GLY:HA3	1:A:58:GLU:HB2	1.38	1.03
1:D:57:GLY:HA3	1:D:58:GLU:HB2	1.38	1.00
1:C:57:GLY:CA	1:C:58:GLU:HB2	1.92	0.99
1:B:57:GLY:CA	1:B:58:GLU:HB2	1.92	0.98
1:D:1:MET:HE3	1:D:1:MET:H2	1.29	0.94
1:C:308:TYR:OH	1:C:420:ASN:ND2	2.05	0.89
1:D:157:LEU:CD1	1:D:166:LEU:HD13	2.04	0.88
1:A:57:GLY:CA	1:A:58:GLU:HB2	2.05	0.85
1:D:57:GLY:CA	1:D:58:GLU:HB2	2.08	0.82
1:D:74:ALA:HB3	1:D:166:LEU:HB2	1.59	0.82
1:B:122:VAL:HG21	1:B:197:PRO:HD3	1.63	0.80
1:D:1:MET:HE3	1:D:1:MET:H1	1.47	0.80
1:D:13:ARG:HH11	1:D:13:ARG:HG3	1.46	0.78
1:A:56:GLN:HG3	1:A:57:GLY:H	1.47	0.78
1:A:56:GLN:HG3	1:A:57:GLY:N	1.99	0.77
1:A:352:ARG:NE	1:A:362:GLN:OE1	2.11	0.77
1:B:233:ALA:O	1:B:235:HIS:N	2.17	0.77
1:D:13:ARG:HH11	1:D:13:ARG:CG	1.98	0.77
1:B:211:THR:O	1:B:212:ARG:HB2	1.84	0.76
1:C:122:VAL:HG21	1:C:197:PRO:HD3	1.67	0.75
1:B:347:HIS:NE2	1:B:372:VAL:HG23	2.01	0.75
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.68	0.74
1:D:157:LEU:HD11	1:D:166:LEU:HD13	1.68	0.74
1:C:56:GLN:HE21	1:C:57:GLY:H	1.33	0.73
1:B:252:LYS:NZ	1:B:331:THR:OG1	2.14	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:THR:O	1:A:212:ARG:HB2	1.90	0.72
1:B:122:VAL:HG21	1:B:197:PRO:CD	2.21	0.70
1:C:410:VAL:CG2	1:C:418:LEU:HB3	2.21	0.70
1:D:210:THR:HB	1:D:211:THR:HG23	1.74	0.70
1:D:410:VAL:HG23	1:D:418:LEU:HB3	1.74	0.69
1:D:13:ARG:HG3	1:D:13:ARG:NH1	2.04	0.68
1:D:72:LYS:HG3	1:D:85:TYR:CD2	2.29	0.68
1:D:1:MET:N	1:D:1:MET:CE	2.50	0.68
1:C:13:ARG:HG2	1:C:13:ARG:HH11	1.59	0.67
1:A:1:MET:HE3	1:A:119:GLY:O	1.95	0.67
1:A:278:GLU:HB2	1:A:305:CYS:SG	2.35	0.67
1:B:205:ASP:OD2	1:B:207:ARG:NH2	2.24	0.65
1:D:1:MET:HE3	1:D:1:MET:CA	2.28	0.64
1:C:410:VAL:HG23	1:C:418:LEU:HB3	1.80	0.64
1:C:57:GLY:HA3	1:C:58:GLU:CB	2.05	0.64
1:D:156:LEU:HD12	1:D:174:LEU:HD22	1.80	0.62
1:C:1:MET:HE3	1:C:119:GLY:O	2.00	0.61
1:C:234:ASP:HB3	1:C:397:LYS:CG	2.30	0.61
1:A:183:ILE:HG21	1:A:189:VAL:HG21	1.83	0.61
1:D:308:TYR:OH	1:D:420:ASN:ND2	2.33	0.61
1:C:161:SER:HA	1:C:164:ALA:O	2.00	0.60
1:C:56:GLN:NE2	1:C:57:GLY:H	2.00	0.59
1:D:234:ASP:HB3	1:D:397:LYS:CG	2.34	0.58
1:D:1:MET:CE	1:D:1:MET:CA	2.83	0.57
1:D:12:HIS:HD2	1:D:14:SER:OG	1.87	0.57
1:D:403:VAL:O	1:D:406:ASP:HB2	2.04	0.57
1:A:34:THR:HG21	3:A:1187:HOH:O	2.04	0.56
1:A:66:VAL:HG13	1:A:174:LEU:HD12	1.87	0.56
1:B:270:ILE:HD13	1:B:310:ILE:HG23	1.87	0.56
1:D:72:LYS:HG3	1:D:85:TYR:HD2	1.68	0.56
1:C:40:LYS:HE3	1:C:116:CYS:HB2	1.87	0.55
1:C:413:GLU:HG3	3:C:1123:HOH:O	2.06	0.55
1:D:106:ALA:HB1	1:D:109:ALA:HB3	1.89	0.55
1:A:56:GLN:HE21	1:A:57:GLY:H	1.53	0.55
1:D:28:TYR:O	1:D:29:LYS:HB3	2.06	0.55
1:D:341:GLU:H	1:D:341:GLU:CD	2.15	0.55
1:D:122:VAL:HG12	1:D:124:LEU:HG	1.89	0.54
1:B:403:VAL:HB	1:B:404:PRO:HD2	1.88	0.54
1:D:253:ALA:O	1:D:256:THR:HG22	2.08	0.54
1:D:12:HIS:CD2	1:D:14:SER:OG	2.61	0.53
1:D:37:TRP:HB2	1:D:322:LEU:HG	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ALA:HB2	1:B:173:LEU:CD2	2.39	0.53
1:B:57:GLY:CA	1:B:58:GLU:CB	2.76	0.53
1:D:343:ILE:HG22	1:D:343:ILE:O	2.09	0.53
1:D:1:MET:H2	1:D:1:MET:CE	2.10	0.52
1:D:211:THR:O	1:D:212:ARG:HB2	2.08	0.52
1:D:156:LEU:CD1	1:D:174:LEU:HD22	2.39	0.52
1:B:56:GLN:HE21	1:B:57:GLY:H	1.57	0.52
1:B:274:HIS:HE1	3:B:1116:HOH:O	1.92	0.52
1:A:56:GLN:CG	1:A:57:GLY:H	2.20	0.52
1:D:165:THR:O	1:D:255:ASN:ND2	2.35	0.52
1:B:67:ALA:HB2	1:B:173:LEU:HD23	1.92	0.51
1:C:327:ARG:HB2	3:C:1128:HOH:O	2.09	0.51
1:B:55:PRO:O	1:B:58:GLU:HB3	2.11	0.51
1:B:229:GLY:O	1:B:230:LEU:C	2.52	0.51
1:C:355:VAL:C	1:C:357:GLY:N	2.65	0.51
1:C:211:THR:O	1:C:212:ARG:HB2	2.11	0.51
1:C:275:TYR:C	1:C:275:TYR:CD1	2.87	0.51
1:A:108:LYS:NZ	3:A:1181:HOH:O	2.29	0.51
1:B:161:SER:HA	1:B:164:ALA:O	2.11	0.50
1:D:248:LEU:C	1:D:248:LEU:HD13	2.36	0.50
1:A:270:ILE:HD13	1:A:310:ILE:HG23	1.92	0.50
1:B:122:VAL:CG2	1:B:197:PRO:CD	2.88	0.50
1:B:15:GLN:HG3	1:B:178:GLN:OE1	2.11	0.49
1:C:409:VAL:HG22	1:C:419:VAL:HG22	1.93	0.49
1:A:19:TRP:CE3	1:A:23:PHE:CE1	3.00	0.49
1:B:1:MET:HE3	1:B:119:GLY:O	2.12	0.49
1:A:56:GLN:CG	1:A:57:GLY:N	2.74	0.49
1:C:55:PRO:HA	1:C:206:GLU:CD	2.37	0.49
1:B:56:GLN:NE2	1:B:57:GLY:H	2.11	0.49
1:C:28:TYR:O	1:C:29:LYS:HB3	2.13	0.49
1:D:270:ILE:HD13	1:D:310:ILE:HG23	1.94	0.49
1:A:105:PRO:HD2	1:A:248:LEU:HD21	1.94	0.48
1:C:72:LYS:HA	1:C:168:PRO:HG3	1.94	0.48
1:D:72:LYS:O	1:D:73:THR:C	2.56	0.48
1:A:330:LEU:CD1	3:A:1036:HOH:O	2.61	0.48
1:A:330:LEU:HD11	3:A:1036:HOH:O	2.13	0.48
1:B:12:HIS:HD2	1:B:14:SER:H	1.62	0.48
1:A:40:LYS:HE3	1:A:116:CYS:HB2	1.95	0.48
1:B:72:LYS:HA	1:B:168:PRO:HG3	1.96	0.48
1:C:13:ARG:HG2	1:C:13:ARG:NH1	2.28	0.47
1:D:275:TYR:HA	1:D:308:TYR:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ALA:O	1:A:235:HIS:N	2.47	0.47
1:C:327:ARG:HD3	1:C:330:LEU:HD22	1.97	0.47
1:D:72:LYS:HE3	1:D:84:GLU:HG3	1.97	0.47
1:D:263:THR:HA	1:D:421:ARG:O	2.15	0.47
1:D:410:VAL:CG2	1:D:418:LEU:HD23	2.45	0.47
1:B:213:LYS:HE3	1:B:213:LYS:HB2	1.43	0.47
1:B:273:MET:HE3	1:B:330:LEU:HD21	1.97	0.47
1:D:157:LEU:CD1	1:D:166:LEU:CD1	2.87	0.47
1:B:351:LEU:O	1:B:362:GLN:HA	2.15	0.47
1:C:98:PRO:HB2	1:C:100:GLU:HG3	1.96	0.47
1:C:192:LEU:HD12	1:C:192:LEU:N	2.30	0.47
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.97	0.46
1:C:105:PRO:HD3	1:C:319:ARG:O	2.16	0.46
1:D:410:VAL:HG21	1:D:418:LEU:HD23	1.98	0.46
1:B:34:THR:HB	1:B:315:GLU:OE2	2.16	0.46
1:C:285:LYS:HD2	1:C:298:TYR:CE2	2.51	0.46
1:A:161:SER:HA	1:A:164:ALA:O	2.15	0.46
1:B:229:GLY:O	1:B:230:LEU:O	2.35	0.45
1:C:341:GLU:CD	1:C:341:GLU:H	2.24	0.45
1:C:31:PRO:HA	1:C:317:TYR:OH	2.17	0.45
1:C:253:ALA:O	1:C:256:THR:HG22	2.16	0.45
1:D:161:SER:HA	1:D:164:ALA:O	2.16	0.45
1:C:210:THR:O	1:C:212:ARG:N	2.49	0.45
1:A:180:ARG:HH11	1:A:180:ARG:HD3	1.63	0.45
1:D:341:GLU:CD	1:D:341:GLU:N	2.75	0.45
1:B:1:MET:CE	1:B:1:MET:CG	2.91	0.45
1:B:403:VAL:HB	1:B:404:PRO:CD	2.46	0.44
1:C:57:GLY:CA	1:C:58:GLU:CB	2.77	0.44
1:A:338:VAL:HA	1:A:339:PRO:HD3	1.88	0.44
1:A:426:GLU:O	1:A:429:LYS:HG2	2.18	0.44
1:B:256:THR:HG23	1:B:331:THR:HB	1.99	0.44
1:C:156:LEU:HD12	1:C:174:LEU:CD2	2.48	0.44
1:D:48[B]:CYS:HB2	1:D:199:LEU:HD12	1.99	0.44
1:B:275:TYR:CD1	1:B:275:TYR:C	2.95	0.44
1:C:167:ASN:HD21	1:C:255:ASN:HD21	1.65	0.44
1:B:353:THR:HB	1:B:361:GLN:HB3	1.98	0.44
1:C:410:VAL:HG22	1:C:418:LEU:HB3	1.99	0.44
1:D:105:PRO:HD2	1:D:248:LEU:HD21	1.99	0.43
1:B:374:PHE:C	1:B:374:PHE:CD1	2.96	0.43
1:C:10:LEU:HD23	1:C:10:LEU:HA	1.81	0.43
1:C:68:LEU:C	1:C:68:LEU:HD12	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LYS:O	1:A:73:THR:C	2.61	0.43
1:D:233:ALA:O	1:D:235:HIS:N	2.52	0.43
1:D:120:GLU:HB3	1:D:197:PRO:HG2	2.01	0.42
1:B:40:LYS:HE3	1:B:116:CYS:HB2	2.00	0.42
1:D:12:HIS:HE1	3:D:1070:HOH:O	2.02	0.42
1:D:55:PRO:O	1:D:58:GLU:HB3	2.19	0.42
1:D:78:ARG:NH2	1:D:80:GLU:OE2	2.49	0.42
1:D:314:LEU:HD23	1:D:324:VAL:HG21	2.01	0.42
1:B:68:LEU:C	1:B:68:LEU:HD12	2.45	0.42
1:B:12:HIS:CD2	1:B:14:SER:H	2.38	0.42
1:C:156:LEU:HD12	1:C:174:LEU:HD22	2.00	0.42
1:D:204:VAL:HA	3:D:1106:HOH:O	2.20	0.42
1:C:355:VAL:C	1:C:357:GLY:H	2.27	0.42
1:D:72:LYS:HG2	1:D:85:TYR:HA	2.02	0.42
1:A:211:THR:O	1:A:212:ARG:CB	2.61	0.42
1:D:403:VAL:HB	1:D:404:PRO:HD2	2.02	0.42
1:B:343:ILE:HA	1:B:344:PRO:HD2	1.90	0.41
1:C:177:PRO:HD2	3:C:1017:HOH:O	2.19	0.41
1:D:108:LYS:NZ	3:D:1117:HOH:O	2.51	0.41
1:D:59:LYS:HE2	1:D:61:LEU:HD21	2.01	0.41
1:A:50:GLU:HA	1:A:51:PRO:HD3	1.94	0.41
1:A:68:LEU:HD21	1:A:172:ILE:HD12	2.02	0.41
1:C:355:VAL:O	1:C:356:ASN:C	2.64	0.41
1:B:57:GLY:N	1:B:58:GLU:HB2	2.33	0.41
1:B:40:LYS:CE	1:B:116:CYS:HB2	2.50	0.41
1:B:78:ARG:NH2	1:C:340:LYS:HD2	2.36	0.41
1:D:38:PHE:CE2	1:D:110:LYS:HD3	2.56	0.41
1:A:327:ARG:HD3	1:A:330:LEU:HD22	2.03	0.41
1:C:78:ARG:NH2	1:C:80:GLU:OE2	2.54	0.41
1:C:273:MET:HG3	1:C:310:ILE:HD13	2.02	0.40
1:D:174:LEU:HA	1:D:174:LEU:HD23	1.60	0.40
1:A:213:LYS:HB2	1:A:213:LYS:HE3	1.67	0.40
1:A:327:ARG:O	1:A:328:ASP:C	2.63	0.40
1:D:395:THR:OG1	1:D:396:PRO:HD2	2.20	0.40
1:C:122:VAL:HG21	1:C:197:PRO:CD	2.45	0.40
1:D:1:MET:CE	1:D:1:MET:HA	2.50	0.40
1:A:19:TRP:HE3	1:A:23:PHE:CE1	2.40	0.40
1:B:341:GLU:H	1:B:341:GLU:CD	2.28	0.40
1:D:164:ALA:HA	1:D:328:ASP:OD1	2.21	0.40

All (23) 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:139:ARG:NH1	1:D:13:ARG:CZ[2_554]	0.75	1.45
1:B:139:ARG:NH2	1:D:13:ARG:NH2[2_554]	0.75	1.45
1:B:139:ARG:CZ	1:D:13:ARG:CZ[2_554]	0.83	1.37
1:B:139:ARG:NH1	1:D:13:ARG:NE[2_554]	1.09	1.11
1:B:139:ARG:CZ	1:D:13:ARG:NH2[2_554]	1.11	1.09
1:B:139:ARG:NH1	1:D:13:ARG:NH1[2_554]	1.24	0.96
1:C:139:ARG:NH1	1:D:136:ILE:O[4_556]	1.42	0.78
1:B:139:ARG:CZ	1:D:13:ARG:NE[2_554]	1.61	0.59
1:B:139:ARG:NH2	1:D:13:ARG:CZ[2_554]	1.61	0.59
1:B:139:ARG:NH1	1:D:13:ARG:CD[2_554]	1.86	0.34
1:B:139:ARG:CZ	1:D:13:ARG:NH1[2_554]	1.88	0.32
1:B:188:ARG:NH2	1:C:202:PRO:CB[4_556]	1.90	0.30
1:B:139:ARG:NE	1:D:13:ARG:NH2[2_554]	2.04	0.16
1:A:33:LYS:CD	1:D:352:ARG:NH2[4_546]	2.05	0.15
1:B:139:ARG:NE	1:D:13:ARG:NE[2_554]	2.05	0.15
1:B:139:ARG:NH1	1:D:13:ARG:NH2[2_554]	2.07	0.13
1:B:139:ARG:NE	1:D:13:ARG:CZ[2_554]	2.07	0.13
1:C:136:ILE:CB	1:D:139:ARG:NH2[4_556]	2.07	0.13
1:A:33:LYS:CE	1:D:362:GLN:OE1[4_546]	2.10	0.10
1:C:139:ARG:NH2	1:D:136:ILE:CG2[4_556]	2.10	0.10
1:B:139:ARG:NH2	1:D:13:ARG:NH1[2_554]	2.16	0.04
1:A:33:LYS:NZ	1:D:362:GLN:OE1[4_546]	2.19	0.01
1:C:136:ILE:CG2	1:D:139:ARG:NH2[4_556]	2.19	0.01

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	418/429 (97%)	404 (97%)	9 (2%)	5 (1%)	10	2
1	B	418/429 (97%)	402 (96%)	11 (3%)	5 (1%)	10	2
1	C	418/429 (97%)	400 (96%)	14 (3%)	4 (1%)	12	3
1	D	418/429 (97%)	398 (95%)	14 (3%)	6 (1%)	9	2
All	All	1672/1716 (97%)	1604 (96%)	48 (3%)	20 (1%)	10	2

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	210	THR
1	A	230	LEU
1	A	234	ASP
1	B	58	GLU
1	B	210	THR
1	B	230	LEU
1	B	234	ASP
1	C	58	GLU
1	C	211	THR
1	D	58	GLU
1	D	210	THR
1	D	234	ASP
1	D	230	LEU
1	C	234	ASP
1	D	413	GLU
1	D	212	ARG
1	A	212	ARG
1	B	212	ARG
1	C	230	LEU

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	348/360 (97%)	339 (97%)	9 (3%)	40	23
1	B	348/360 (97%)	337 (97%)	11 (3%)	34	17
1	C	348/360 (97%)	333 (96%)	15 (4%)	26	10
1	D	348/360 (97%)	334 (96%)	14 (4%)	28	12
All	All	1392/1440 (97%)	1343 (96%)	49 (4%)	32	15

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	34	THR
1	A	58	GLU
1	A	188	ARG
1	A	211	THR
1	A	213	LYS
1	A	285	LYS
1	A	341	GLU
1	A	404	PRO
1	B	1	MET
1	B	21	GLU
1	B	34	THR
1	B	66	VAL
1	B	84	GLU
1	B	125	SER
1	B	188	ARG
1	B	213	LYS
1	B	217	THR
1	B	341	GLU
1	B	351	LEU
1	C	21	GLU
1	C	56	GLN
1	C	58	GLU
1	C	66	VAL
1	C	188	ARG
1	C	192	LEU
1	C	213	LYS
1	C	234	ASP
1	C	246	GLU
1	C	248	LEU
1	C	290	VAL
1	C	341	GLU
1	C	364	THR
1	C	399	LEU
1	C	413	GLU
1	D	1	MET
1	D	13	ARG
1	D	21	GLU
1	D	26	SER
1	D	58	GLU
1	D	79	GLU
1	D	125	SER
1	D	188	ARG

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Mol	Chain	Res	Type
1	D	210	THR
1	D	213	LYS
1	D	246	GLU
1	D	270	ILE
1	D	341	GLU
1	D	364	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	56	GLN
1	A	129	ASN
1	A	201	ASN
1	A	268	ASN
1	A	348	ASN
1	A	386	ASN
1	B	12	HIS
1	B	25	GLN
1	B	56	GLN
1	B	129	ASN
1	B	235	HIS
1	B	268	ASN
1	B	269	ASN
1	B	286	GLN
1	B	348	ASN
1	B	386	ASN
1	C	12	HIS
1	C	15	GLN
1	C	25	GLN
1	C	56	GLN
1	C	150	GLN
1	C	167	ASN
1	C	184	GLN
1	C	268	ASN
1	C	362	GLN
1	C	420	ASN
1	D	12	HIS
1	D	15	GLN
1	D	25	GLN
1	D	167	ASN
1	D	201	ASN

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Mol	Chain	Res	Type
1	D	235	HIS
1	D	268	ASN
1	D	286	GLN
1	D	316	ASN
1	D	362	GLN
1	D	386	ASN
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 ⓘ

There are no chain breaks in this entry.

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	421/429 (98%)	0.56	27 (6%)	25 27	17, 39, 55, 72	6 (1%)
1	B	421/429 (98%)	0.74	36 (8%)	16 17	20, 42, 61, 79	8 (1%)
1	C	421/429 (98%)	0.81	46 (10%)	10 10	16, 43, 60, 78	6 (1%)
1	D	421/429 (98%)	1.40	105 (24%)	2 1	22, 47, 68, 83	6 (1%)
All	All	1684/1716 (98%)	0.88	214 (12%)	8 7	16, 42, 62, 83	26 (1%)

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	LEU	9.9
1	C	334	LEU	9.2
1	D	334	LEU	8.9
1	D	230	LEU	8.8
1	A	334	LEU	8.6
1	D	74	ALA	8.0
1	A	230	LEU	7.3
1	B	230	LEU	7.1
1	C	230	LEU	7.1
1	D	30	ALA	6.1
1	C	57	GLY	5.9
1	B	345	ASP	5.6
1	A	57	GLY	5.4
1	D	428	ALA	5.2
1	D	413	GLU	5.1
1	B	211	THR	5.1
1	D	57	GLY	5.0
1	A	305	CYS	4.9
1	D	272	TYR	4.8
1	D	233	ALA	4.7
1	D	270	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	211	THR	4.7
1	D	147	ALA	4.7
1	B	23	PHE	4.6
1	B	57	GLY	4.6
1	A	229	GLY	4.5
1	D	1	MET	4.3
1	D	18	ALA	4.3
1	A	244	PRO	4.3
1	D	309	ALA	4.2
1	A	234	ASP	4.2
1	B	290	VAL	4.1
1	D	269	ASN	4.0
1	C	233	ALA	4.0
1	B	301	GLY	3.9
1	C	23	PHE	3.9
1	D	424	SER	3.8
1	C	2	LYS	3.8
1	D	19	TRP	3.8
1	C	235	HIS	3.8
1	B	229	GLY	3.7
1	B	210	THR	3.7
1	B	244	PRO	3.7
1	D	28	TYR	3.7
1	C	234	ASP	3.7
1	A	235	HIS	3.6
1	D	410	VAL	3.6
1	B	234	ASP	3.6
1	C	22	ALA	3.6
1	D	36	VAL	3.6
1	A	210	THR	3.5
1	D	16	LEU	3.5
1	C	30	ALA	3.4
1	D	314	LEU	3.4
1	D	205	ASP	3.4
1	B	1	MET	3.4
1	B	233	ALA	3.3
1	C	56	GLN	3.3
1	B	235	HIS	3.3
1	D	408	VAL	3.3
1	D	235	HIS	3.3
1	D	159	ALA	3.3
1	C	214	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	345	ASP	3.2
1	D	427	THR	3.2
1	D	79	GLU	3.2
1	D	422	ILE	3.2
1	A	342	ALA	3.2
1	D	402	VAL	3.2
1	D	426	GLU	3.2
1	D	267	PRO	3.1
1	D	17	ASP	3.1
1	D	22	ALA	3.1
1	C	25	GLN	3.1
1	D	160	LEU	3.1
1	A	1	MET	3.0
1	C	1	MET	3.0
1	D	268	ASN	3.0
1	D	308	TYR	3.0
1	D	403	VAL	3.0
1	D	357	GLY	3.0
1	C	181	VAL	2.9
1	D	358	GLU	2.9
1	D	321	ASN	2.9
1	D	405	GLY	2.9
1	D	150	GLN	2.9
1	A	214	SER	2.9
1	C	24	GLN	2.9
1	D	207	ARG	2.9
1	B	350	THR	2.9
1	D	261	ASN	2.9
1	A	212	ARG	2.8
1	D	217	THR	2.8
1	B	358	GLU	2.8
1	C	79	GLU	2.8
1	D	2	LYS	2.8
1	D	81	ASP	2.8
1	D	275	TYR	2.8
1	C	248	LEU	2.8
1	B	48[A]	CYS	2.8
1	C	212	ARG	2.8
1	D	34	THR	2.8
1	B	212	ARG	2.7
1	D	10	LEU	2.7
1	B	346	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	166	LEU	2.7
1	D	80	GLU	2.7
1	C	29	LYS	2.7
1	C	19	TRP	2.7
1	D	164	ALA	2.7
1	C	358	GLU	2.6
1	A	24	GLN	2.6
1	D	24	GLN	2.6
1	D	75	THR	2.6
1	D	234	ASP	2.6
1	D	125	SER	2.6
1	B	343	ILE	2.6
1	A	23	PHE	2.6
1	D	174	LEU	2.6
1	C	272	TYR	2.6
1	D	144	TRP	2.6
1	D	210	THR	2.5
1	D	124	LEU	2.5
1	D	229	GLY	2.5
1	D	211	THR	2.5
1	B	344	PRO	2.5
1	D	9	ALA	2.5
1	D	324	VAL	2.5
1	D	86	ILE	2.5
1	D	332	PRO	2.5
1	D	26	SER	2.5
1	B	205	ASP	2.5
1	B	428	ALA	2.5
1	C	103	TYR	2.5
1	D	122	VAL	2.5
1	B	217	THR	2.5
1	A	295	ALA	2.4
1	B	299	VAL	2.4
1	B	56	GLN	2.4
1	D	27	PRO	2.4
1	C	423	VAL	2.4
1	D	419	VAL	2.4
1	A	349	LEU	2.4
1	D	154	ALA	2.4
1	A	209	VAL	2.4
1	C	209	VAL	2.4
1	C	138	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	32	PRO	2.3
1	D	245	GLU	2.3
1	A	233	ALA	2.3
1	D	123	ALA	2.3
1	D	37	TRP	2.3
1	C	270	ILE	2.3
1	A	304	VAL	2.3
1	C	137	ASN	2.3
1	C	3	GLY	2.3
1	D	329	GLY	2.3
1	D	204	VAL	2.3
1	B	29	LYS	2.3
1	A	34	THR	2.3
1	C	18	ALA	2.3
1	B	351	LEU	2.3
1	D	157	LEU	2.3
1	D	359	LEU	2.3
1	A	300	ALA	2.2
1	B	214	SER	2.2
1	A	17	ASP	2.2
1	D	23	PHE	2.2
1	D	88	GLY	2.2
1	D	102	PHE	2.2
1	B	213	LYS	2.2
1	D	184	GLN	2.2
1	D	313	TYR	2.2
1	D	317	TYR	2.2
1	B	216	PRO	2.2
1	C	261	ASN	2.2
1	A	338	VAL	2.2
1	D	355	VAL	2.2
1	A	125	SER	2.2
1	D	83	ALA	2.2
1	D	153	ALA	2.2
1	C	317	TYR	2.2
1	D	131	THR	2.2
1	B	372	VAL	2.1
1	C	290	VAL	2.1
1	D	248	LEU	2.1
1	D	158	SER	2.1
1	C	244	PRO	2.1
1	D	404	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	3	GLY	2.1
1	C	34	THR	2.1
1	C	31	PRO	2.1
1	D	212	ARG	2.1
1	C	136	ILE	2.1
1	D	85	TYR	2.1
1	D	429	LYS	2.1
1	D	341	GLU	2.1
1	C	124	LEU	2.1
1	D	399	LEU	2.1
1	D	418	LEU	2.1
1	A	336	THR	2.1
1	C	429	LYS	2.1
1	B	272	TYR	2.1
1	D	195	GLY	2.0
1	B	342	ALA	2.0
1	C	321	ASN	2.0
1	C	428	ALA	2.0
1	C	130	LEU	2.0
1	D	353	THR	2.0
1	D	29	LYS	2.0
1	C	207	ARG	2.0
1	C	164	ALA	2.0
1	D	82	ALA	2.0
1	D	161	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	1004	1/1	0.93	0.09	46,46,46,46	0
2	CA	B	1002	1/1	0.99	0.02	40,40,40,40	0
2	CA	C	1003	1/1	0.99	0.03	42,42,42,42	0
2	CA	A	1001	1/1	0.99	0.02	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.