



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:12 AM UTC

PDB ID : 7Q40 / pdb_00007q40
Title : Crystal structure of RCC1-Like domain 2 of ubiquitin ligase HERC2
Authors : Demenge, A.; Howard, E.; Cousido-Siah, A.; Mitschler, A.; Podjarny, A.;
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Deposited on : 2021-10-29
Resolution : 2.35 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) : 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

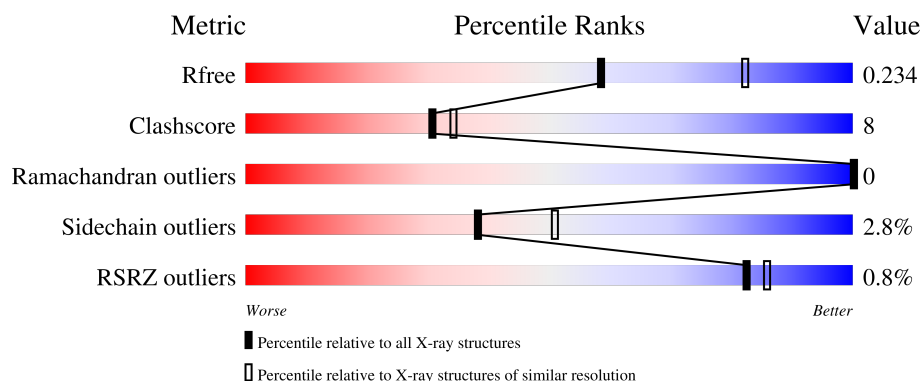
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	405	% 72% 18% • 9%
1	C	405	% 78% 13% 9%
1	E	405	79% 12% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8668 atoms, of which 45 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.

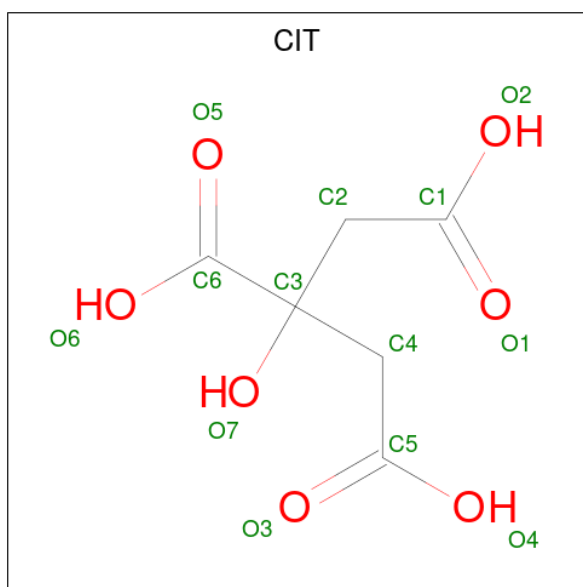
- Molecule 1 is a protein called E3 ubiquitin-protein ligase HERC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2747	1714	507	515	11			
1	C	370	Total	C	N	O	S	0	1	0
			2766	1726	512	517	11			
1	E	369	Total	C	N	O	S	0	1	0
			2756	1719	509	517	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2939	ALA	ASN	conflict	UNP O95714
A	2940	MET	SER	conflict	UNP O95714
C	2939	ALA	ASN	conflict	UNP O95714
C	2940	MET	SER	conflict	UNP O95714
E	2939	ALA	ASN	conflict	UNP O95714
E	2940	MET	SER	conflict	UNP O95714

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			18	6	5	7		
2	A	1	Total	C	H	O	0	0
			18	6	5	7		
2	C	1	Total	C	H	O	0	0
			18	6	5	7		
2	C	1	Total	C	H	O	0	0
			18	6	5	7		
2	C	1	Total	C	H	O	0	0
			18	6	5	7		
2	E	1	Total	C	H	O	0	0
			18	6	5	7		
2	E	1	Total	C	H	O	0	0
			18	6	5	7		
2	E	1	Total	C	H	O	0	0
			18	6	5	7		

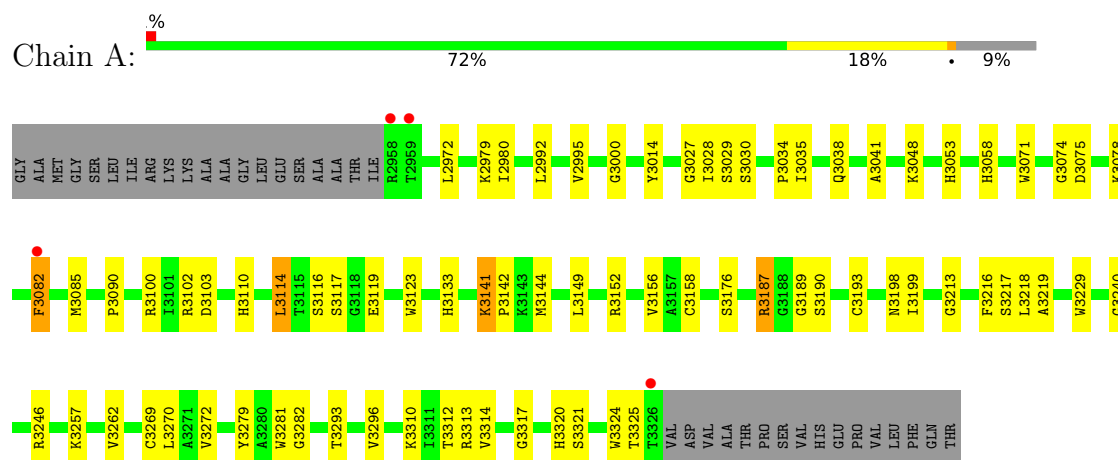
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	C	92	Total	O	0	0
			92	92		
3	E	77	Total	O	0	0
			77	77		

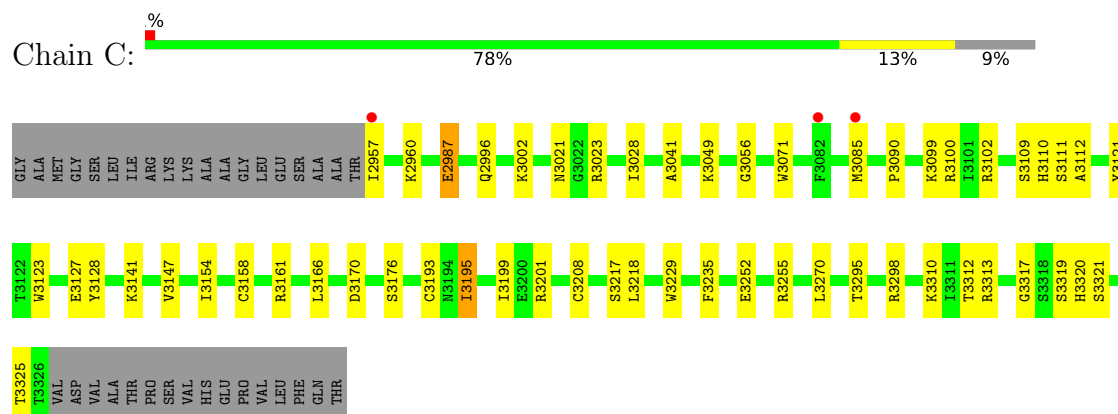
3 Residue-property plots

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 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.

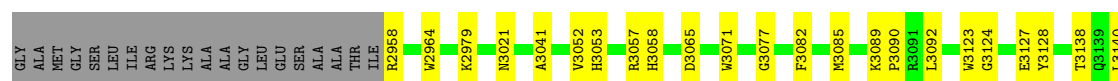
- Molecule 1: E3 ubiquitin-protein ligase HERC2

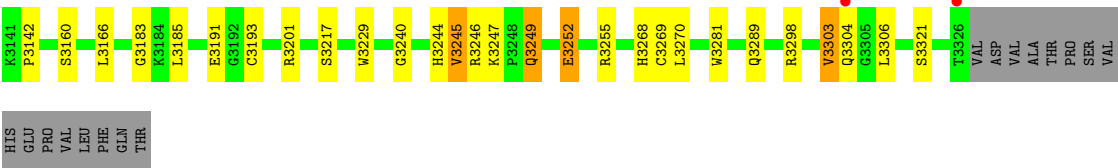


- Molecule 1: E3 ubiquitin-protein ligase HERC2



- Molecule 1: E3 ubiquitin-protein ligase HERC2





HIS
GLU
PRO
VAL
LEU
PHE
GLN
THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.54Å 108.54Å 243.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.27 – 2.35 54.27 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.8 (54.27-2.35) 98.9 (54.27-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.12_2829, PHENIX 1.12_2829	Depositor
R, R_{free}	0.179 , 0.230 0.183 , 0.234	Depositor DCC
R_{free} test set	3036 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.9	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	8668	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

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

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	0.31	0/2797	0.49	0/3777
1	C	0.32	0/2816	0.49	0/3802
1	E	0.31	0/2806	0.51	0/3789
All	All	0.31	0/8419	0.50	0/11368

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2747	0	2755	62	0
1	C	2766	0	2778	40	0
1	E	2756	0	2762	35	0
2	A	26	10	10	0	0
2	C	39	15	15	4	0
2	E	52	20	20	5	0
3	A	68	0	0	5	0
3	C	92	0	0	7	0
3	E	77	0	0	2	0
All	All	8623	45	8340	139	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 8.

All (139) 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:3208:CYS:SG	3:C:3585:HOH:O	2.25	0.94
1:A:3144:MET:HE2	1:A:3149:LEU:HD21	1.49	0.91
1:A:3144:MET:CE	1:A:3149:LEU:HD21	1.99	0.91
1:C:3193:CYS:SG	3:C:3589:HOH:O	2.31	0.88
1:E:3193:CYS:SG	3:E:3576:HOH:O	2.33	0.85
1:E:3229:TRP:HA	1:E:3245:VAL:HG22	1.57	0.85
1:E:3270:LEU:HD11	1:E:3321:SER:HB3	1.63	0.81
1:E:3085:MET:HA	1:E:3085:MET:HE2	1.63	0.80
1:C:3085:MET:HE2	1:C:3085:MET:HA	1.62	0.80
1:A:3193:CYS:SG	3:A:3567:HOH:O	2.38	0.80
1:A:3103:ASP:HB3	1:A:3114:LEU:HD21	1.65	0.77
1:E:3077:GLY:HA3	1:E:3140:LEU:HD13	1.70	0.72
2:E:3401:CIT:O2	2:E:3401:CIT:O7	2.09	0.70
1:A:3119:GLU:HB3	1:A:3144:MET:HE3	1.71	0.69
1:E:3127:GLU:HG2	1:E:3128:TYR:CD2	2.27	0.69
1:C:3166:LEU:HD11	1:C:3217:SER:HB3	1.75	0.69
1:C:3099:LYS:HE3	1:C:3121:TYR:OH	1.93	0.69
1:E:3041:ALA:HB3	1:E:3090:PRO:HD2	1.78	0.66
1:C:3317:GLY:HA3	1:C:3320:HIS:CE1	2.30	0.66
1:E:3229:TRP:HA	1:E:3245:VAL:CG2	2.27	0.64
1:E:3021:ASN:ND2	1:E:3057:ARG:HD2	2.12	0.63
1:A:3218:LEU:C	1:A:3218:LEU:HD23	2.23	0.63
1:C:3127:GLU:HG2	1:C:3128:TYR:CD2	2.34	0.63
1:E:3041:ALA:CB	1:E:3090:PRO:HD2	2.29	0.63
2:E:3402:CIT:O3	2:E:3402:CIT:O7	2.12	0.63
1:C:3002:LYS:HE3	2:C:3403:CIT:O6	1.99	0.63
2:E:3403:CIT:O4	2:E:3403:CIT:O7	2.17	0.62
1:A:3312:THR:O	1:A:3313:ARG:HD3	1.99	0.61
1:E:3166:LEU:HD11	1:E:3217:SER:HB3	1.82	0.61
1:A:3027:GLY:C	1:A:3028:ILE:HD12	2.27	0.59
1:E:3201:ARG:HE	2:E:3403:CIT:H21	1.68	0.59
1:C:3176:SER:HB3	1:C:3199:ILE:HD11	1.84	0.59
1:E:3065:ASP:OD1	1:E:3065:ASP:N	2.34	0.58
1:A:3075:ASP:O	1:A:3078:LYS:HG2	2.04	0.58
2:C:3402:CIT:O3	2:C:3402:CIT:O7	2.21	0.57
1:C:3252:GLU:HG2	1:C:3255:ARG:NH1	2.20	0.56
1:C:3021:ASN:ND2	1:C:3023:ARG:HH21	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3123:TRP:HB3	1:A:3142:PRO:HA	1.87	0.55
1:A:3293:THR:HB	3:A:3540:HOH:O	2.07	0.55
1:A:3110:HIS:CE1	1:A:3158:CYS:HB3	2.42	0.55
1:A:3217:SER:HB2	1:A:3229:TRP:CE2	2.42	0.54
1:A:3189:GLY:O	1:A:3246:ARG:HD3	2.06	0.54
1:E:3082:PHE:HA	1:E:3140:LEU:HB3	1.90	0.54
1:A:3114:LEU:HD23	1:A:3114:LEU:H	1.74	0.53
1:A:3313:ARG:HB2	1:A:3324:TRP:CE2	2.44	0.53
1:A:3058:HIS:CE1	1:A:3078:LYS:HD2	2.44	0.53
1:A:3317:GLY:HA3	1:A:3320:HIS:CE1	2.44	0.52
1:C:3041:ALA:HB3	1:C:3090:PRO:HD2	1.91	0.52
1:A:3114:LEU:HD23	1:A:3114:LEU:N	2.24	0.52
1:A:3240:GLY:O	1:E:3304[B]:GLN:HG3	2.09	0.52
1:A:3144:MET:HE2	1:A:3149:LEU:CD2	2.32	0.51
1:C:3201:ARG:HB2	2:C:3401:CIT:O7	2.10	0.51
1:E:3071:TRP:HB3	1:E:3090:PRO:HA	1.92	0.51
1:A:3144:MET:HE2	1:A:3149:LEU:HD11	1.92	0.51
1:A:3213:GLY:HA3	1:A:3216:PHE:CE1	2.45	0.51
1:A:3272:VAL:CG2	1:A:3314:VAL:HG13	2.40	0.51
1:C:3252:GLU:HG2	1:C:3255:ARG:CZ	2.40	0.51
1:E:3269:CYS:HB2	1:E:3281:TRP:CE2	2.45	0.51
1:A:3100:ARG:HD2	1:A:3116:SER:OG	2.11	0.51
1:E:3077:GLY:CA	1:E:3140:LEU:HD13	2.40	0.51
1:A:3119:GLU:CB	1:A:3144:MET:HE3	2.41	0.50
1:A:3320:HIS:ND1	3:A:3502:HOH:O	2.20	0.50
1:A:3282:GLY:O	1:A:3296:VAL:HG23	2.12	0.50
1:A:3028:ILE:HD12	1:A:3028:ILE:N	2.27	0.50
1:A:3071:TRP:HB3	1:A:3090:PRO:HA	1.94	0.50
1:E:3240:GLY:O	1:E:3298:ARG:NH2	2.44	0.49
1:E:2964:TRP:CE2	1:E:3321:SER:HB2	2.47	0.49
1:C:3109:SER:HB2	3:C:3507:HOH:O	2.13	0.49
1:C:3217:SER:HB2	1:C:3229:TRP:CE2	2.48	0.49
1:C:3310:LYS:O	1:C:3325:THR:HG22	2.13	0.49
1:A:2972:LEU:HD12	1:A:2980:ILE:HG13	1.94	0.48
1:A:3190:SER:O	3:A:3501:HOH:O	2.20	0.48
1:C:3218:LEU:C	1:C:3218:LEU:HD23	2.39	0.48
1:A:3218:LEU:HD23	1:A:3219:ALA:N	2.29	0.48
1:A:3176:SER:HB3	1:A:3199:ILE:HD11	1.96	0.48
1:A:3028:ILE:HG22	1:A:3030:SER:H	1.79	0.48
1:C:3201:ARG:HH21	2:C:3401:CIT:C2	2.27	0.48
1:A:3034:PRO:O	1:A:3035:ILE:HD13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3269:CYS:HB2	1:A:3281:TRP:CE2	2.49	0.48
1:A:3187:ARG:HD2	1:A:3198:ASN:O	2.13	0.47
1:C:3235:PHE:CE2	1:C:3298:ARG:HG2	2.49	0.47
1:E:3123:TRP:HB3	1:E:3142:PRO:HA	1.96	0.47
1:C:3028:ILE:O	3:C:3501:HOH:O	2.20	0.47
1:C:3111:SER:HB2	1:C:3123:TRP:CE2	2.49	0.47
1:A:3257:LYS:HE2	1:A:3279:TYR:OH	2.14	0.47
1:E:3183:GLY:HA3	1:E:3246:ARG:HA	1.97	0.46
1:C:3235:PHE:CD2	1:C:3298:ARG:HG2	2.50	0.46
1:A:3041:ALA:HB3	1:A:3090:PRO:HD2	1.97	0.46
1:E:3053:HIS:CE1	1:E:3160:SER:HB3	2.51	0.46
1:C:3110:HIS:HB2	1:C:3123:TRP:O	2.15	0.45
1:C:3147:VAL:HG21	1:C:3195:ILE:HD12	1.98	0.45
1:A:3000:GLY:HA2	1:A:3053:HIS:O	2.16	0.45
1:A:3149:LEU:HA	1:A:3149:LEU:HD23	1.59	0.45
1:E:3217:SER:HB2	1:E:3229:TRP:CE2	2.51	0.45
1:E:3247:LYS:HD3	2:E:3403:CIT:H42	1.99	0.45
1:A:3014:TYR:CE2	1:A:3038:GLN:HB2	2.52	0.45
1:C:3195:ILE:HA	1:C:3195:ILE:HD13	1.65	0.45
1:C:3154:ILE:HD13	1:C:3170:ASP:HA	1.98	0.45
1:A:3218:LEU:HD21	1:A:3262:VAL:HG21	1.99	0.44
1:A:3058:HIS:ND1	1:A:3078:LYS:HD2	2.31	0.44
1:E:3268:HIS:HB2	1:E:3289:GLN:HE22	1.80	0.44
1:C:3270:LEU:HD11	1:C:3321:SER:HB3	1.98	0.44
1:C:3099:LYS:HE3	1:C:3121:TYR:HH	1.81	0.44
1:C:3110:HIS:CE1	1:C:3158:CYS:HB3	2.53	0.44
1:A:3082:PHE:CE2	1:A:3141:LYS:HG2	2.53	0.44
1:A:3270:LEU:HD11	1:A:3321:SER:HB3	1.98	0.44
1:C:3085:MET:HA	1:C:3085:MET:CE	2.42	0.44
1:C:2960:LYS:HE3	1:C:3325:THR:OG1	2.18	0.43
1:A:3119:GLU:CG	1:A:3144:MET:HE3	2.48	0.43
1:A:2979:LYS:HE3	1:A:2979:LYS:HB2	1.59	0.43
1:A:3048:LYS:O	1:A:3048:LYS:HG2	2.17	0.43
1:A:3187:ARG:HH11	1:A:3187:ARG:HG2	1.83	0.42
1:E:3185:LEU:HB2	3:E:3514:HOH:O	2.19	0.42
1:E:3252:GLU:HG3	1:E:3255:ARG:NH1	2.34	0.42
1:E:3052:VAL:HG23	1:E:3058:HIS:O	2.20	0.42
1:C:2996:GLN:OE1	1:C:3049:LYS:HA	2.20	0.42
1:A:3119:GLU:HG2	1:A:3144:MET:HE3	2.02	0.42
1:A:3133:HIS:HB2	3:A:3508:HOH:O	2.20	0.42
1:C:3056:GLY:HA3	3:C:3517:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3295:THR:HG21	1:E:3244:HIS:O	2.19	0.42
1:A:3310:LYS:O	1:A:3325:THR:HG22	2.20	0.41
1:A:3028:ILE:HG22	1:A:3029:SER:N	2.34	0.41
1:A:3272:VAL:HG22	1:A:3314:VAL:HG13	2.02	0.41
1:C:3071:TRP:HB3	1:C:3090:PRO:HA	2.02	0.41
1:C:2987:GLU:N	3:C:3506:HOH:O	2.52	0.41
1:E:3124:GLY:O	1:E:3138:THR:HG23	2.20	0.41
1:A:3074:GLY:HA3	1:A:3085:MET:O	2.20	0.41
1:E:3249:GLN:HE21	1:E:3249:GLN:HB3	1.69	0.41
1:A:3103:ASP:HB3	1:A:3114:LEU:CD2	2.41	0.41
1:A:3313:ARG:HB3	1:A:3324:TRP:CZ2	2.56	0.41
1:C:3312:THR:O	1:C:3313:ARG:HD3	2.21	0.41
1:A:3028:ILE:CG2	1:A:3029:SER:N	2.84	0.41
1:E:3041:ALA:HB2	1:E:3089:LYS:HE2	2.02	0.41
1:E:3092:LEU:C	1:E:3092:LEU:HD23	2.46	0.41
1:E:3303:VAL:CG2	1:E:3306:LEU:HD12	2.51	0.41
1:C:3109:SER:N	3:C:3507:HOH:O	2.52	0.41
1:A:3103:ASP:O	1:A:3114:LEU:HD23	2.21	0.40
1:A:3114:LEU:HD22	1:A:3156:VAL:HG12	2.04	0.40
1:C:3112:ALA:HA	1:C:3121:TYR: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	367/405 (91%)	356 (97%)	11 (3%)	0	100	100
1	C	369/405 (91%)	360 (98%)	9 (2%)	0	100	100
1	E	368/405 (91%)	358 (97%)	10 (3%)	0	100	100
All	All	1104/1215 (91%)	1074 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	290/317 (92%)	281 (97%)	9 (3%)	35	47
1	C	292/317 (92%)	284 (97%)	8 (3%)	39	52
1	E	291/317 (92%)	284 (98%)	7 (2%)	43	57
All	All	873/951 (92%)	849 (97%)	24 (3%)	38	52

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2992	LEU
1	A	2995	VAL
1	A	3082	PHE
1	A	3102	ARG
1	A	3114	LEU
1	A	3117	SER
1	A	3141	LYS
1	A	3152	ARG
1	A	3187	ARG
1	C	2957	ILE
1	C	2987	GLU
1	C	3100	ARG
1	C	3102	ARG
1	C	3141	LYS
1	C	3161	ARG
1	C	3195	ILE
1	C	3319	SER
1	E	2958	ARG
1	E	2979	LYS
1	E	3191	GLU
1	E	3245	VAL
1	E	3249	GLN
1	E	3252	GLU

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Mol	Chain	Res	Type
1	E	3303	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3038	GLN
1	A	3136	ASN
1	A	3198	ASN
1	A	3203	ASN
1	A	3205	GLN
1	A	3249	GLN
1	A	3304	GLN
1	C	3021	ASN
1	C	3058	HIS
1	C	3249	GLN
1	C	3304	GLN
1	E	3021	ASN
1	E	3136	ASN
1	E	3249	GLN
1	E	3268	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](#)

9 ligands are modelled in this entry.

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
2	CIT	A	3401	-	12,12,12	1.14	1 (8%)	17,17,17	1.13	2 (11%)
2	CIT	C	3403	-	12,12,12	1.04	0	17,17,17	1.59	3 (17%)
2	CIT	C	3401	-	12,12,12	0.98	0	17,17,17	1.63	4 (23%)
2	CIT	E	3403	-	12,12,12	1.10	0	17,17,17	1.54	1 (5%)
2	CIT	E	3401	-	12,12,12	1.00	0	17,17,17	1.58	3 (17%)
2	CIT	C	3402	-	12,12,12	1.17	1 (8%)	17,17,17	1.11	2 (11%)
2	CIT	E	3404	-	12,12,12	1.08	0	17,17,17	1.54	3 (17%)
2	CIT	A	3402	-	12,12,12	1.05	0	17,17,17	1.53	2 (11%)
2	CIT	E	3402	-	12,12,12	1.01	0	17,17,17	1.52	1 (5%)

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
2	CIT	A	3401	-	-	1/16/16/16	-
2	CIT	C	3403	-	-	4/16/16/16	-
2	CIT	C	3401	-	-	9/16/16/16	-
2	CIT	E	3403	-	-	10/16/16/16	-
2	CIT	E	3401	-	-	14/16/16/16	-
2	CIT	C	3402	-	-	3/16/16/16	-
2	CIT	E	3404	-	-	7/16/16/16	-
2	CIT	A	3402	-	-	7/16/16/16	-
2	CIT	E	3402	-	-	7/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3401	CIT	O4-C5	-2.12	1.23	1.30
2	C	3402	CIT	C3-C6	2.01	1.55	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3403	CIT	O6-C6-C3	4.46	121.69	113.14
2	E	3402	CIT	O6-C6-C3	4.19	121.18	113.14
2	A	3402	CIT	O6-C6-C3	3.96	120.73	113.14
2	C	3403	CIT	O6-C6-C3	3.88	120.58	113.14
2	E	3401	CIT	O6-C6-C3	3.80	120.44	113.14
2	E	3404	CIT	O6-C6-C3	3.73	120.29	113.14
2	C	3401	CIT	O6-C6-C3	3.48	119.81	113.14
2	C	3401	CIT	C4-C3-C2	2.86	116.66	109.31
2	E	3401	CIT	O4-C5-C4	2.85	123.38	114.35
2	C	3401	CIT	O7-C3-C6	-2.54	105.35	108.96
2	A	3401	CIT	O5-C6-C3	-2.42	117.41	122.09
2	C	3403	CIT	O4-C5-C4	2.41	121.99	114.35
2	C	3402	CIT	O5-C6-C3	-2.29	117.66	122.09
2	A	3401	CIT	O6-C6-C3	2.16	117.29	113.14
2	C	3402	CIT	O6-C6-C3	2.13	117.23	113.14
2	E	3401	CIT	O4-C5-O3	-2.13	117.86	123.33
2	E	3404	CIT	O2-C1-C2	2.12	121.05	114.35
2	E	3404	CIT	C3-C4-C5	-2.10	108.17	113.92
2	C	3403	CIT	O4-C5-O3	-2.07	118.00	123.33
2	A	3402	CIT	O2-C1-C2	2.07	120.90	114.35
2	C	3401	CIT	O4-C5-O3	-2.01	118.17	123.33

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3401	CIT	C1-C2-C3-O7
2	C	3401	CIT	C1-C2-C3-C4
2	C	3401	CIT	O7-C3-C6-O5
2	C	3401	CIT	O7-C3-C6-O6
2	C	3401	CIT	C4-C3-C6-O5
2	C	3401	CIT	C4-C3-C6-O6
2	C	3402	CIT	C2-C3-C4-C5
2	C	3402	CIT	C6-C3-C4-C5
2	E	3401	CIT	C1-C2-C3-C4
2	E	3401	CIT	C1-C2-C3-C6
2	E	3401	CIT	C2-C3-C6-O5
2	E	3401	CIT	C2-C3-C6-O6
2	E	3401	CIT	O7-C3-C6-O5
2	E	3401	CIT	O7-C3-C6-O6
2	E	3402	CIT	C2-C3-C4-C5
2	E	3402	CIT	C6-C3-C4-C5
2	E	3402	CIT	O7-C3-C6-O5

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Mol	Chain	Res	Type	Atoms
2	E	3402	CIT	O7-C3-C6-O6
2	E	3402	CIT	C4-C3-C6-O5
2	E	3402	CIT	C4-C3-C6-O6
2	E	3403	CIT	C2-C3-C4-C5
2	E	3403	CIT	C6-C3-C4-C5
2	E	3404	CIT	C1-C2-C3-O7
2	E	3404	CIT	C1-C2-C3-C4
2	E	3404	CIT	O7-C3-C6-O5
2	E	3404	CIT	O7-C3-C6-O6
2	E	3404	CIT	C4-C3-C6-O5
2	E	3404	CIT	C4-C3-C6-O6
2	C	3402	CIT	O7-C3-C4-C5
2	E	3404	CIT	C1-C2-C3-C6
2	A	3402	CIT	C1-C2-C3-C4
2	C	3401	CIT	C1-C2-C3-C6
2	E	3401	CIT	C1-C2-C3-O7
2	E	3402	CIT	O7-C3-C4-C5
2	E	3403	CIT	O7-C3-C4-C5
2	E	3401	CIT	C6-C3-C4-C5
2	A	3402	CIT	C1-C2-C3-C6
2	C	3403	CIT	C1-C2-C3-C4
2	E	3401	CIT	C2-C3-C4-C5
2	E	3401	CIT	C3-C4-C5-O3
2	E	3401	CIT	C3-C4-C5-O4
2	C	3403	CIT	C1-C2-C3-C6
2	C	3401	CIT	C2-C3-C6-O5
2	C	3403	CIT	C3-C4-C5-O4
2	C	3403	CIT	C3-C4-C5-O3
2	A	3402	CIT	C2-C3-C6-O5
2	A	3402	CIT	C2-C3-C6-O6
2	A	3402	CIT	C4-C3-C6-O5
2	A	3402	CIT	C4-C3-C6-O6
2	C	3401	CIT	C2-C3-C6-O6
2	E	3403	CIT	C2-C3-C6-O6
2	E	3403	CIT	C4-C3-C6-O5
2	E	3403	CIT	C4-C3-C6-O6
2	A	3401	CIT	C2-C3-C4-C5
2	E	3403	CIT	C2-C3-C6-O5
2	E	3403	CIT	O7-C3-C6-O5
2	E	3401	CIT	O1-C1-C2-C3
2	E	3401	CIT	O2-C1-C2-C3
2	E	3403	CIT	C3-C4-C5-O4

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Mol	Chain	Res	Type	Atoms
2	E	3403	CIT	C3-C4-C5-O3
2	A	3402	CIT	C1-C2-C3-O7
2	E	3401	CIT	O7-C3-C4-C5

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3403	CIT	1	0
2	C	3401	CIT	2	0
2	E	3403	CIT	3	0
2	E	3401	CIT	1	0
2	C	3402	CIT	1	0
2	E	3402	CIT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	369/405 (91%)	0.08	4 (1%) 78 82	37, 57, 82, 107	0
1	C	370/405 (91%)	-0.10	3 (0%) 82 86	28, 50, 70, 94	1 (0%)
1	E	369/405 (91%)	-0.04	2 (0%) 87 90	25, 53, 76, 92	1 (0%)
All	All	1108/1215 (91%)	-0.02	9 (0%) 82 86	25, 53, 78, 107	2 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3326	THR	3.4
1	E	3326	THR	3.4
1	C	2957	ILE	3.3
1	A	2958	ARG	2.6
1	A	2959	THR	2.5
1	C	3082	PHE	2.5
1	C	3085	MET	2.3
1	A	3082	PHE	2.2
1	E	3304[A]	GLN	2.1

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	CIT	E	3403	13/13	0.64	0.13	98,103,125,125	0
2	CIT	E	3402	13/13	0.72	0.15	105,118,143,145	0
2	CIT	C	3401	13/13	0.74	0.13	107,113,135,138	0
2	CIT	A	3401	13/13	0.76	0.15	58,81,92,104	0
2	CIT	C	3403	13/13	0.76	0.14	83,106,132,141	0
2	CIT	A	3402	13/13	0.79	0.14	103,112,140,144	0
2	CIT	C	3402	13/13	0.81	0.14	65,95,109,114	0
2	CIT	E	3404	13/13	0.81	0.12	100,103,124,127	0
2	CIT	E	3401	13/13	0.86	0.11	76,111,129,132	0

6.5 Other polymers [i](#)

There are no such residues in this entry.