



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:06 PM UTC

PDB ID : 7Q45 / pdb_00007q45
Title : Crystal structure of RCC1-Like domain 2 of ubiquitin ligase HERC2 in complex with DXDKDED motif of Myelin transcription factor 1
Authors : Demenge, A.; Howard, E.; Cousido-Siah, A.; Mitschler, A.; Podjarny, A.; McEwen, A.G.; Trave, G.
Deposited on : 2021-10-29
Resolution : 2.10 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

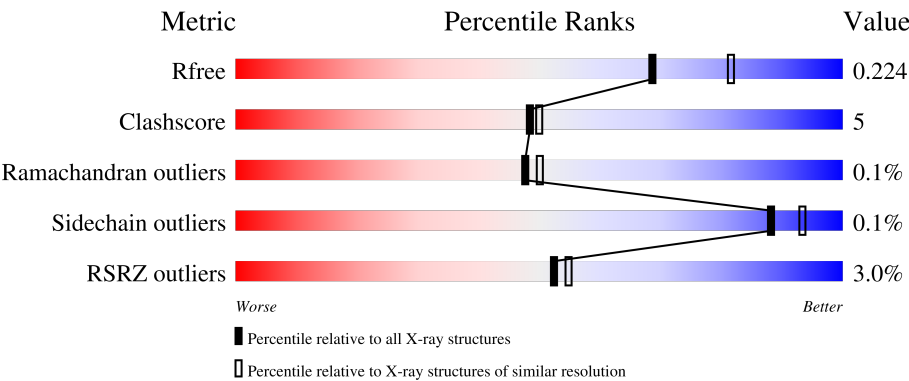
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	% 80%12%9%
1	C	405	2% 80%11%9%
1	E	405	% 80%10%9%
2	B	14	21% 36%29%36%
2	D	14	43% 64%7%29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	14	36%36%14%50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9322 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 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	368	Total	C	N	O	S	0	1	0
			2747	1714	507	515	11			
1	E	368	Total	C	N	O	S	0	1	0
			2745	1713	505	516	11			

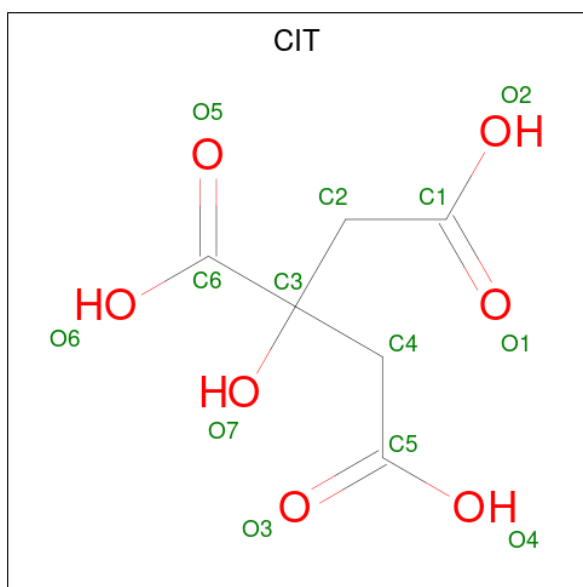
There are 6 discrepancies between the modelled and reference sequences:

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 a protein called Myelin transcription factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			70	38	10	22			
2	D	10	Total	C	N	O	0	0	0
			76	41	11	24			
2	F	7	Total	C	N	O	0	0	0
			58	31	8	19			

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		

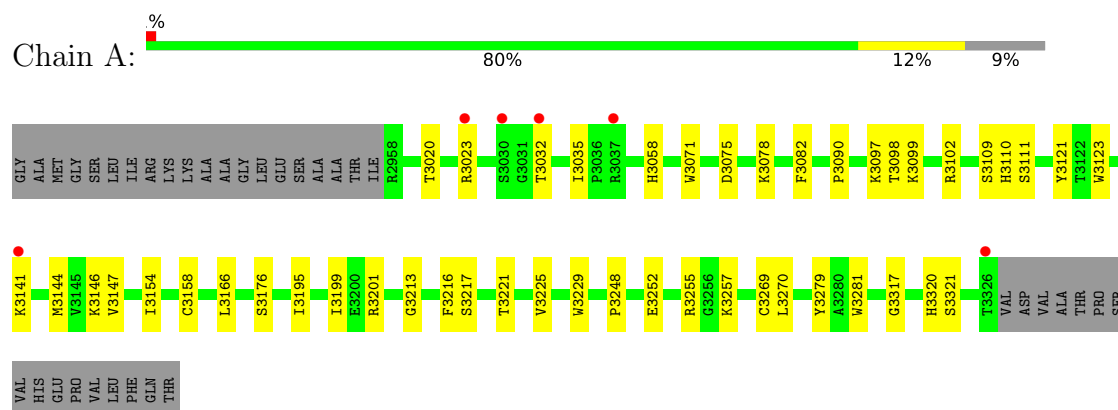
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	271	Total	O	0	0
			271	271		
4	C	279	Total	O	0	0
			279	279		
4	E	269	Total	O	0	0
			269	269		
4	B	8	Total	O	0	0
			8	8		
4	D	9	Total	O	0	0
			9	9		
4	F	4	Total	O	0	0
			4	4		

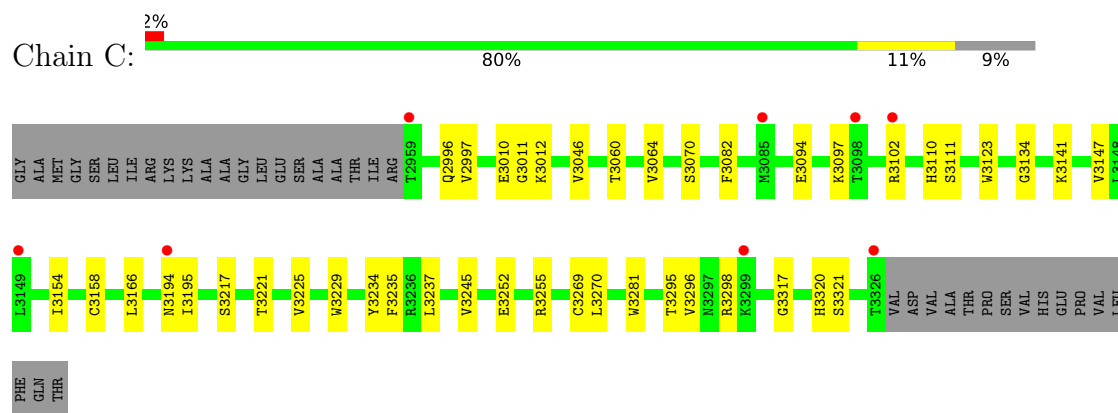
3 Residue-property plots [i](#)

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.

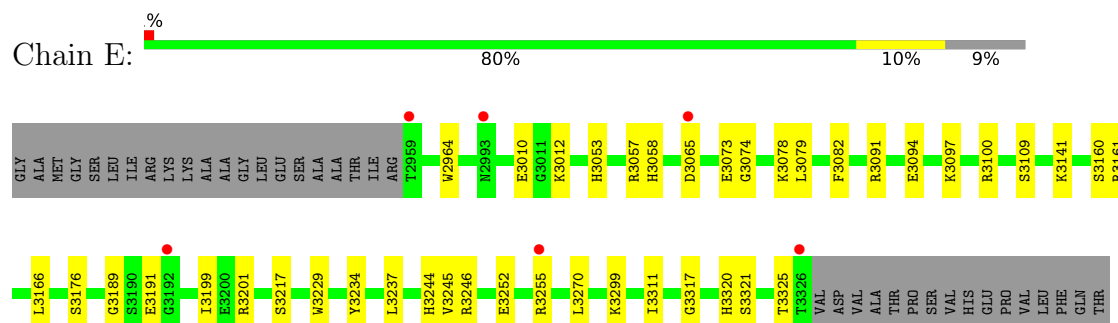
• Molecule 1: E3 ubiquitin-protein ligase HERC2



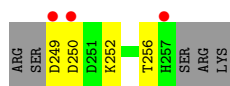
• Molecule 1: E3 ubiquitin-protein ligase HERC2



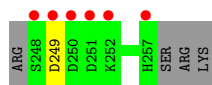
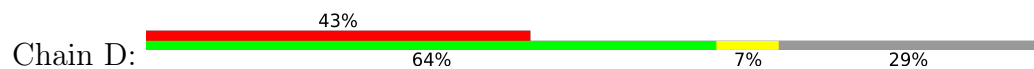
• Molecule 1: E3 ubiquitin-protein ligase HERC2



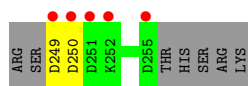
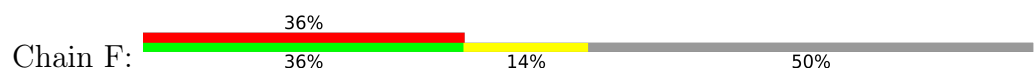
● Molecule 2: Myelin transcription factor 1



● Molecule 2: Myelin transcription factor 1



● Molecule 2: Myelin transcription factor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.39Å 108.39Å 242.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 2.10 48.47 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.47-2.10) 89.5 (48.47-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.12_2829, PHENIX 1.12_2829	Depositor
R, R_{free}	0.184 , 0.224 0.184 , 0.224	Depositor DCC
R_{free} test set	4242 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9322	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.24	1/2797 (0.0%)	0.45	0/3777
1	C	0.21	0/2797	0.44	0/3777
1	E	0.21	0/2795	0.45	0/3775
2	B	0.54	0/69	1.19	0/92
2	D	0.32	0/75	0.81	0/100
2	F	0.22	0/57	0.54	0/75
All	All	0.22	1/8590 (0.0%)	0.46	0/11596

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3035	ILE	CA-C	6.97	1.57	1.52

There are no bond angle outliers.

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	2747	0	2755	27	0
1	C	2747	0	2754	30	0
1	E	2745	0	2749	33	0
2	B	70	0	47	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	76	0	52	1	0
2	F	58	0	38	6	0
3	C	13	0	5	0	0
3	E	26	0	10	1	0
4	A	271	0	0	1	0
4	B	8	0	0	0	0
4	C	279	0	0	2	0
4	D	9	0	0	0	0
4	E	269	0	0	3	0
4	F	4	0	0	1	0
All	All	9322	0	8410	92	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 5.

All (92) 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:A:3020:THR:O	1:A:3023:ARG:HD2	1.87	0.75
1:E:3270:LEU:HD11	1:E:3321:SER:HB3	1.68	0.75
1:E:3234:TYR:HE2	2:F:249:ASP:HB2	1.52	0.75
1:E:3234:TYR:CE2	2:F:249:ASP:HB2	2.24	0.72
1:C:3011:GLY:HA3	1:C:3046:VAL:HG23	1.72	0.72
1:E:3237:LEU:HD13	1:E:3245:VAL:HG22	1.76	0.68
1:C:3194:ASN:ND2	4:C:3502:HOH:O	2.25	0.68
1:C:3166:LEU:HD11	1:C:3217:SER:HB3	1.79	0.65
1:A:3082:PHE:CE2	1:A:3141:LYS:HD2	2.32	0.65
1:E:3229:TRP:HA	1:E:3245:VAL:HG23	1.78	0.65
1:E:3161:ARG:NH1	4:E:3501:HOH:O	2.30	0.64
1:C:3141:LYS:NZ	4:C:3504:HOH:O	2.30	0.62
1:C:3252:GLU:HG2	1:C:3255:ARG:NH2	2.15	0.62
1:E:3234:TYR:HH	2:F:249:ASP:N	1.99	0.60
1:C:3270:LEU:HD11	1:C:3321:SER:HB3	1.84	0.59
1:A:3078:LYS:HE2	1:A:3109:SER:HA	1.85	0.58
1:C:3147:VAL:HG21	1:C:3195:ILE:HD12	1.86	0.56
1:C:3317:GLY:HA3	1:C:3320:HIS:CE1	2.39	0.56
1:A:3201:ARG:HG2	1:A:3248:PRO:HG2	1.87	0.56
1:C:3082:PHE:CE1	1:C:3141:LYS:HD3	2.40	0.56
1:E:3166:LEU:HD11	1:E:3217:SER:HB3	1.88	0.55
1:C:3237:LEU:HD13	1:C:3245:VAL:HG22	1.88	0.54
1:A:3099:LYS:HE2	1:A:3121:TYR:OH	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3110:HIS:CE1	1:A:3158:CYS:HB3	2.42	0.54
1:E:3078:LYS:HE2	1:E:3109:SER:HA	1.90	0.54
1:C:3234:TYR:HE2	2:D:249:ASP:HB2	1.72	0.53
1:E:3161:ARG:HH22	2:F:250:ASP:HB3	1.72	0.53
1:C:3134:GLY:HA2	1:C:3194:ASN:HB3	1.90	0.53
1:E:3252:GLU:HG2	1:E:3255:ARG:NE	2.24	0.52
1:E:3074:GLY:HA2	1:E:3079:LEU:HG	1.91	0.52
1:A:3257:LYS:HE2	1:A:3279:TYR:OH	2.10	0.51
1:A:3166:LEU:HD11	1:A:3217:SER:HB3	1.91	0.51
1:E:3311:ILE:HD13	1:E:3325:THR:HG22	1.93	0.51
1:E:3229:TRP:HA	1:E:3245:VAL:CG2	2.41	0.51
1:C:3060:THR:HG22	1:C:3070:SER:HB3	1.93	0.50
1:C:3217:SER:HB2	1:C:3229:TRP:CE2	2.47	0.50
1:E:3317:GLY:HA3	1:E:3320:HIS:CE1	2.47	0.50
1:A:3102:ARG:HH12	1:A:3154:ILE:HG22	1.77	0.49
1:A:3071:TRP:HB3	1:A:3090:PRO:HA	1.94	0.49
1:C:3046:VAL:HG13	1:C:3064:VAL:HG22	1.94	0.49
1:A:3217:SER:HB2	1:A:3229:TRP:CE2	2.48	0.49
1:C:3229:TRP:HA	1:C:3245:VAL:CG2	2.43	0.49
1:A:3213:GLY:HA3	1:A:3216:PHE:CE1	2.48	0.48
1:C:3147:VAL:HG21	1:C:3195:ILE:HG23	1.96	0.48
1:A:3252:GLU:OE1	1:A:3255:ARG:NH2	2.45	0.47
1:A:3317:GLY:HA3	1:A:3320:HIS:CE1	2.49	0.47
1:C:3295:THR:HG21	1:E:3244:HIS:O	2.15	0.47
1:E:3217:SER:HB2	1:E:3229:TRP:CE2	2.50	0.47
1:A:3058:HIS:CE1	1:A:3078:LYS:HD3	2.50	0.47
1:A:3270:LEU:HD21	1:A:3321:SER:HB3	1.96	0.46
1:C:3235:PHE:CE1	1:C:3298:ARG:HG2	2.51	0.46
1:E:3058:HIS:CE1	1:E:3078:LYS:HD3	2.50	0.46
1:A:3147:VAL:HG21	1:A:3195:ILE:HD12	1.98	0.46
1:C:3094:GLU:O	1:C:3097:LYS:HG2	2.14	0.46
2:B:256:THR:O	2:B:256:THR:HG22	2.16	0.46
1:A:3075:ASP:O	1:A:3078:LYS:HE3	2.16	0.46
1:E:2964:TRP:CE2	1:E:3321:SER:HB2	2.51	0.46
1:A:3269:CYS:HB2	1:A:3281:TRP:CE2	2.51	0.45
1:A:3082:PHE:CZ	1:A:3141:LYS:HD2	2.50	0.45
1:A:3097:LYS:HG3	1:A:3098:THR:HG23	1.99	0.45
2:B:249:ASP:HB3	2:B:252:LYS:HG3	1.98	0.45
1:E:3201:ARG:HE	3:E:3402:CIT:H42	1.82	0.45
1:A:3176:SER:HB3	1:A:3199:ILE:HD11	1.98	0.45
1:E:3252:GLU:HG2	1:E:3255:ARG:CZ	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3057:ARG:HE	1:E:3073:GLU:CD	2.25	0.44
1:C:3269:CYS:HB2	1:C:3281:TRP:CE2	2.53	0.44
1:C:3010:GLU:OE1	1:C:3010:GLU:N	2.51	0.44
1:E:3176:SER:HB3	1:E:3199:ILE:HD11	1.99	0.44
1:E:3082:PHE:HD1	1:E:3141:LYS:HG3	1.83	0.43
1:A:3032:THR:HG21	4:A:3412:HOH:O	2.18	0.43
1:A:3111:SER:HB2	1:A:3123:TRP:CE2	2.54	0.43
1:C:2996:GLN:HG2	1:C:2997:VAL:N	2.34	0.43
1:C:3252:GLU:HG2	1:C:3255:ARG:HH22	1.84	0.43
1:C:3110:HIS:CE1	1:C:3158:CYS:HB3	2.54	0.42
1:E:3299:LYS:NZ	4:E:3502:HOH:O	2.31	0.42
1:E:3058:HIS:ND1	1:E:3078:LYS:HD3	2.35	0.42
1:C:3102:ARG:NH2	1:C:3154:ILE:O	2.52	0.42
1:A:3144:MET:O	1:A:3146:LYS:HD2	2.20	0.42
1:E:3010:GLU:HG2	1:E:3012:LYS:HG3	2.01	0.42
1:E:3161:ARG:NH2	2:F:250:ASP:HB3	2.34	0.42
1:E:3065:ASP:O	1:E:3100:ARG:NH1	2.53	0.41
1:A:3229:TRP:CE3	1:A:3248:PRO:HB3	2.54	0.41
1:E:3053:HIS:CE1	1:E:3160:SER:HB3	2.54	0.41
1:E:3094:GLU:OE1	1:E:3097:LYS:NZ	2.43	0.41
2:F:249:ASP:CG	4:F:301:HOH:O	2.62	0.41
1:C:3010:GLU:HG2	1:C:3012:LYS:HG3	2.03	0.41
1:E:3189:GLY:O	1:E:3246:ARG:HD3	2.20	0.41
1:C:3221:THR:OG1	1:C:3225:VAL:HG22	2.20	0.41
1:A:3221:THR:OG1	1:A:3225:VAL:HG22	2.21	0.41
1:C:3235:PHE:HD2	1:C:3296:VAL:HG21	1.86	0.40
1:E:3091:ARG:NH2	4:E:3507:HOH:O	2.46	0.40
1:C:3111:SER:HB2	1:C:3123:TRP:CE2	2.56	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	367/405 (91%)	354 (96%)	13 (4%)	0	100	100
1	C	367/405 (91%)	358 (98%)	9 (2%)	0	100	100
1	E	367/405 (91%)	357 (97%)	10 (3%)	0	100	100
2	B	7/14 (50%)	6 (86%)	0	1 (14%)	0	0
2	D	8/14 (57%)	8 (100%)	0	0	100	100
2	F	5/14 (36%)	5 (100%)	0	0	100	100
All	All	1121/1257 (89%)	1088 (97%)	32 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	250	ASP

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%)	290 (100%)	0	100	100
1	C	290/317 (92%)	290 (100%)	0	100	100
1	E	290/317 (92%)	289 (100%)	1 (0%)	86	91
2	B	8/14 (57%)	8 (100%)	0	100	100
2	D	9/14 (64%)	9 (100%)	0	100	100
2	F	7/14 (50%)	7 (100%)	0	100	100
All	All	894/993 (90%)	893 (100%)	1 (0%)	88	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3191	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3038	GLN
1	A	3136	ASN
1	C	3136	ASN
1	C	3194	ASN
1	C	3198	ASN
1	C	3203	ASN
1	C	3209	GLN
1	C	3304	GLN
1	E	3136	ASN
1	E	3198	ASN
1	E	3203	ASN
1	E	3209	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	$\# Z > 2$
3	CIT	C	3401	-	12,12,12	1.05	0	17,17,17	1.51	3 (17%)
3	CIT	E	3401	-	12,12,12	1.04	0	17,17,17	1.45	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CIT	E	3402	-	12,12,12	1.14	0	17,17,17	1.15	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CIT	C	3401	-	-	10/16/16/16	-
3	CIT	E	3401	-	-	9/16/16/16	-
3	CIT	E	3402	-	-	3/16/16/16	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3401	CIT	O6-C6-C3	3.94	120.69	113.14
3	C	3401	CIT	O6-C6-C3	3.88	120.59	113.14
3	E	3402	CIT	O5-C6-C3	-2.60	117.06	122.09
3	E	3402	CIT	O6-C6-C3	2.48	117.89	113.14
3	E	3401	CIT	O4-C5-C4	2.06	120.88	114.35
3	C	3401	CIT	C4-C3-C2	2.05	114.58	109.31
3	C	3401	CIT	O4-C5-C4	2.01	120.72	114.35

There are no chirality outliers.

All (22) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	3401	CIT	C1-C2-C3-C4
3	E	3401	CIT	C2-C3-C6-O5
3	E	3401	CIT	C4-C3-C6-O5
3	E	3401	CIT	C4-C3-C6-O6
3	E	3401	CIT	C1-C2-C3-O7
3	E	3401	CIT	O7-C3-C6-O5
3	C	3401	CIT	C3-C4-C5-O4
3	C	3401	CIT	C3-C4-C5-O3
3	E	3401	CIT	C6-C3-C4-C5
3	C	3401	CIT	C2-C3-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	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

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	369/405 (91%)	-0.00	6 (1%) 70 73	20, 34, 55, 66	0
1	C	368/405 (90%)	-0.12	8 (2%) 62 65	19, 30, 47, 59	1 (0%)
1	E	368/405 (90%)	-0.11	6 (1%) 70 73	16, 32, 50, 67	1 (0%)
2	B	9/14 (64%)	1.98	3 (33%) 1 1	49, 60, 74, 80	0
2	D	10/14 (71%)	1.88	6 (60%) 0 0	56, 68, 85, 94	0
2	F	7/14 (50%)	2.85	5 (71%) 0 0	74, 88, 108, 117	0
All	All	1131/1257 (89%)	-0.03	34 (3%) 52 55	16, 32, 54, 117	2 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	257	HIS	5.0
1	C	2959	THR	4.2
1	A	3326	THR	4.2
2	F	249	ASP	4.1
1	E	3326	THR	3.9
1	C	3299	LYS	3.8
2	F	251	ASP	3.6
1	C	3149	LEU	3.5
2	B	249	ASP	3.3
1	A	3030	SER	3.2
2	D	249	ASP	3.0
2	F	250	ASP	3.0
2	F	252	LYS	3.0
2	F	255	ASP	2.9
1	E	3255	ARG	2.8
2	D	257	HIS	2.8
1	E	2959	THR	2.7
1	E	2993	ASN	2.7
1	A	3141	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	3192	GLY	2.5
1	C	3102	ARG	2.4
2	D	252	LYS	2.4
1	E	3065	ASP	2.4
2	D	250	ASP	2.4
1	C	3098	THR	2.2
1	C	3194	ASN	2.2
1	A	3023	ARG	2.2
1	A	3037	ARG	2.2
1	A	3032	THR	2.2
2	B	250	ASP	2.1
2	D	251	ASP	2.0
1	C	3326	THR	2.0
1	C	3085	MET	2.0
2	D	248	SER	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
3	CIT	E	3402	13/13	0.62	0.17	71,72,87,87	0
3	CIT	C	3401	13/13	0.70	0.18	87,89,91,91	0
3	CIT	E	3401	13/13	0.73	0.19	63,75,84,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.