



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2022 – 04:06 pm GMT

PDB ID : 7Q44
Title : Crystal structure of RCC1-Like domain 2 of ubiquitin ligase HERC2 in complex with DXDKDED motif of deubiquitinase USP35
Authors : Demenge, A.; Howard, E.; Cousido-Siah, A.; Mitschler, A.; Podjarny, A.; McEwen, A.G.; Trave, G.
Deposited on : 2021-10-29
Resolution : 2.20 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.31.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

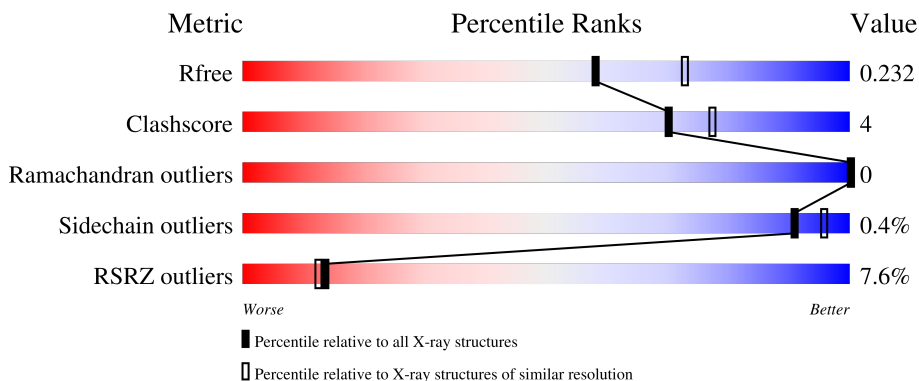
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div>
1	C	405	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div>
1	E	405	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div>
2	B	15	<div style="display: flex; align-items: center;"> <div style="width: 13%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: grey;"></div> </div>
2	D	15	<div style="display: flex; align-items: center;"> <div style="width: 27%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
2	F	15	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment (33%), a green segment (33%), a yellow segment (13%), and a grey segment (13%). The percentages are labeled above and below the segments.</p>

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9139 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
			Total	C	N	O	S			
1	A	369	Total 2747	C 1714	N 507	O 515	S 11	0	0	0
1	C	369	Total 2758	C 1720	N 511	O 516	S 11	0	1	0
1	E	369	Total 2750	C 1716	N 506	O 517	S 11	0	1	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2938	GLY	-	expression tag	UNP O95714
A	2939	ALA	-	expression tag	UNP O95714
A	2940	MET	-	expression tag	UNP O95714
C	2938	GLY	-	expression tag	UNP O95714
C	2939	ALA	-	expression tag	UNP O95714
C	2940	MET	-	expression tag	UNP O95714
E	2938	GLY	-	expression tag	UNP O95714
E	2939	ALA	-	expression tag	UNP O95714
E	2940	MET	-	expression tag	UNP O95714

- Molecule 2 is a protein called Deubiquitinase USP35 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	9	Total 69	C 38	N 10	O 21	0	0	0
2	B	10	Total 77	C 42	N 11	O 24	0	0	0
2	F	7	Total 55	C 30	N 8	O 17	0	0	0

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



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

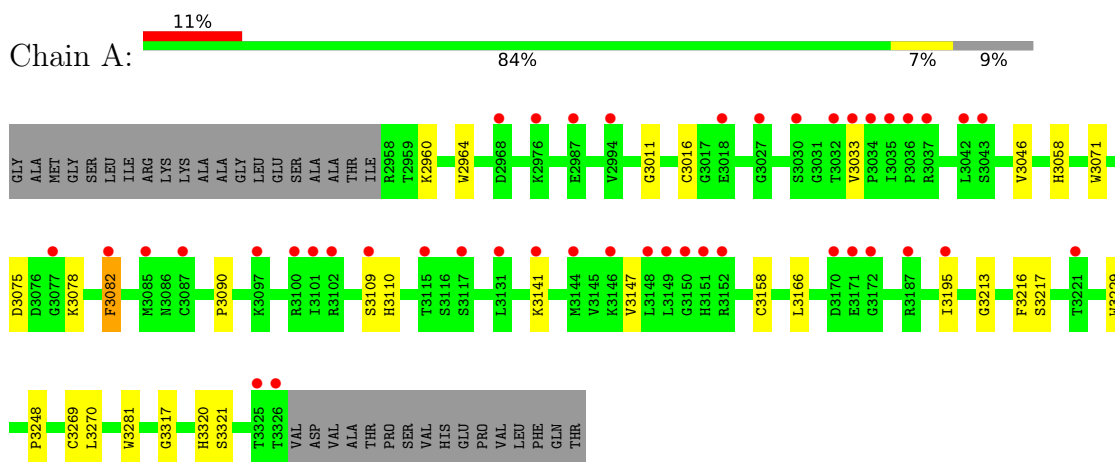
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	193	Total O 193 193	0	0
4	C	221	Total O 221 221	0	0
4	E	212	Total O 212 212	0	0
4	D	4	Total O 4 4	0	0
4	B	9	Total O 9 9	0	0
4	F	5	Total O 5 5	0	0

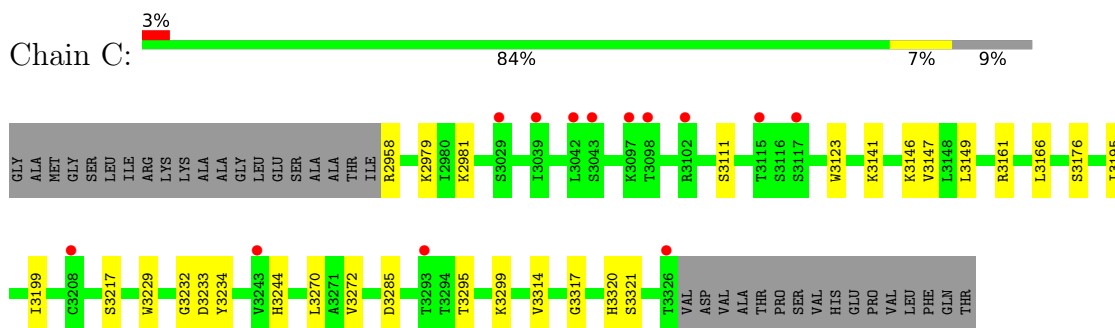
3 Residue-property plots [i](#)

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.

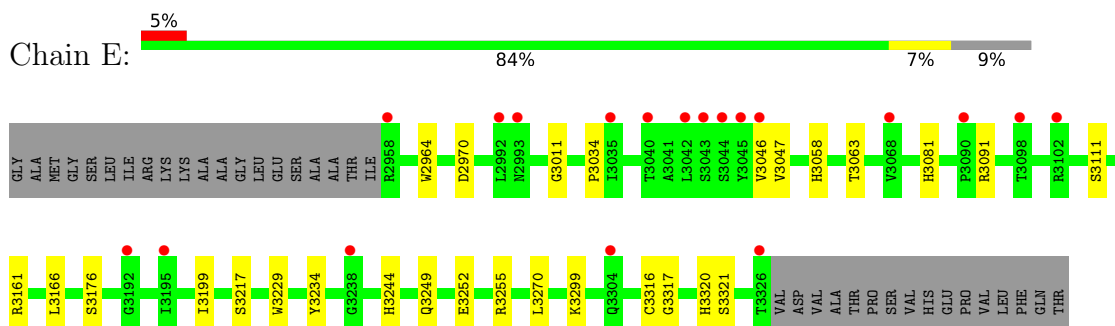
- Molecule 1: E3 ubiquitin-protein ligase HERC2



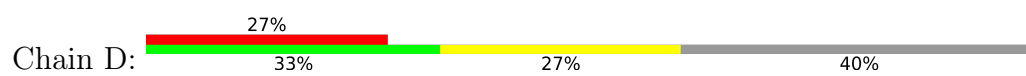
- Molecule 1: E3 ubiquitin-protein ligase HERC2



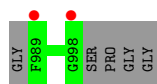
- Molecule 1: E3 ubiquitin-protein ligase HERC2



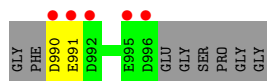
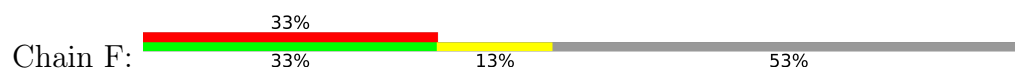
- Molecule 2: Deubiquitinase USP35 peptide



- Molecule 2: Deubiquitinase USP35 peptide



- Molecule 2: Deubiquitinase USP35 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.46Å 108.46Å 242.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 2.20 49.52 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.52-2.20) 99.9 (49.52-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.12_2829, PHENIX 1.12_2829	Depositor
R, R_{free}	0.182 , 0.231 0.183 , 0.232	Depositor DCC
R_{free} test set	3709 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtrriage
Anisotropy	0.143	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9139	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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	0.27	0/2797	0.49	0/3777
1	C	0.27	0/2808	0.50	0/3791
1	E	0.28	0/2800	0.50	0/3782
2	B	0.22	0/76	0.44	0/100
2	D	0.23	0/68	0.42	0/90
2	F	0.21	0/54	0.40	0/71
All	All	0.27	0/8603	0.49	0/11611

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 [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	20	0
1	C	2758	0	2767	18	0
1	E	2750	0	2751	23	0
2	B	77	0	51	0	0
2	D	69	0	44	5	0
2	F	55	0	36	5	0
3	C	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	26	0	10	1	0
4	A	193	0	0	1	0
4	B	9	0	0	0	0
4	C	221	0	0	1	0
4	D	4	0	0	0	0
4	E	212	0	0	2	0
4	F	5	0	0	0	0
All	All	9139	0	8419	60	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 4.

All (60) 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:E:3234:TYR:HH	2:F:990:ASP:N	1.67	0.91
1:C:3232:GLY:H	1:C:3244:HIS:HD2	1.27	0.80
3:E:3402:CIT:O4	3:E:3402:CIT:H21	1.88	0.72
1:C:3166:LEU:HD11	1:C:3217:SER:HB3	1.74	0.69
1:A:3270:LEU:HD11	1:A:3321:SER:HB3	1.73	0.69
1:C:3161:ARG:NH2	2:D:992:ASP:OD1	2.30	0.65
1:E:3299:LYS:NZ	4:E:3503:HOH:O	2.32	0.63
1:A:3147:VAL:HG21	1:A:3195:ILE:HD12	1.80	0.63
1:E:3234:TYR:CE2	2:F:990:ASP:HB2	2.36	0.60
1:C:3234:TYR:HE2	2:D:990:ASP:HB2	1.66	0.59
1:E:3166:LEU:HD11	1:E:3217:SER:HB3	1.84	0.59
1:E:3234:TYR:HE2	2:F:990:ASP:HB2	1.67	0.58
1:E:3270:LEU:HD11	1:E:3321:SER:HB3	1.83	0.58
1:A:3016:CYS:HA	1:A:3033:VAL:HG23	1.84	0.58
1:A:3078:LYS:HE2	1:A:3109:SER:HA	1.86	0.57
1:A:2960:LYS:NZ	4:A:3407:HOH:O	2.38	0.56
1:C:3270:LEU:HD11	1:C:3321:SER:HB3	1.87	0.56
1:C:3147:VAL:HG21	1:C:3195:ILE:HD12	1.87	0.56
1:A:3166:LEU:HD11	1:A:3217:SER:HB3	1.88	0.56
1:C:3146:LYS:HA	1:C:3149:LEU:HD23	1.88	0.55
1:A:3317:GLY:HA3	1:A:3320:HIS:CE1	2.43	0.53
1:E:3252:GLU:HG2	1:E:3255:ARG:NH2	2.24	0.53
1:A:3058:HIS:CE1	1:A:3078:LYS:HD3	2.46	0.51
1:C:2979:LYS:NZ	2:D:996:ASP:OD2	2.42	0.51
1:E:3317:GLY:HA3	1:E:3320:HIS:CE1	2.47	0.50
1:C:3285:ASP:OD2	2:D:993:LYS:HE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3176:SER:HB3	1:E:3199:ILE:HD11	1.93	0.49
1:A:3016:CYS:HA	1:A:3033:VAL:CG2	2.42	0.49
1:C:3234:TYR:CE2	2:D:990:ASP:HB2	2.45	0.49
1:C:3217:SER:HB2	1:C:3229:TRP:CE2	2.47	0.49
1:C:3317:GLY:HA3	1:C:3320:HIS:CE1	2.47	0.49
1:C:3299:LYS:NZ	4:C:3504:HOH:O	2.45	0.48
1:A:3217:SER:HB2	1:A:3229:TRP:CE2	2.49	0.48
1:A:3213:GLY:HA3	1:A:3216:PHE:CE1	2.49	0.47
1:A:3082:PHE:CE2	1:A:3141:LYS:HD2	2.50	0.47
1:E:3161:ARG:CZ	2:F:991:GLU:HG3	2.44	0.47
1:A:3075:ASP:O	1:A:3078:LYS:HG2	2.15	0.47
1:E:3047:VAL:HA	1:E:3063:THR:HA	1.97	0.47
1:C:2981:LYS:HE2	1:E:3249:GLN:HE22	1.80	0.46
1:E:3252:GLU:HG2	1:E:3255:ARG:HH22	1.80	0.46
1:A:3110:HIS:CE1	1:A:3158:CYS:HB3	2.50	0.46
1:E:3081:HIS:CE1	1:E:3091:ARG:HG2	2.50	0.46
1:A:2964:TRP:CE2	1:A:3321:SER:HB2	2.51	0.46
1:E:2964:TRP:CE2	1:E:3321:SER:HB2	2.52	0.46
1:E:3217:SER:HB2	1:E:3229:TRP:CE2	2.51	0.45
1:A:3011:GLY:HA3	1:A:3046:VAL:HG13	1.99	0.45
1:E:3058:HIS:HE1	1:E:3111:SER:OG	2.01	0.44
1:A:3141:LYS:HE3	1:A:3141:LYS:HB2	1.79	0.44
1:A:3071:TRP:HB3	1:A:3090:PRO:HA	2.00	0.43
1:A:3229:TRP:CE3	1:A:3248:PRO:HB3	2.54	0.42
1:E:3011:GLY:HA3	1:E:3046:VAL:HG13	2.02	0.41
1:C:3111:SER:HB2	1:C:3123:TRP:CE2	2.55	0.41
1:E:3058:HIS:HD2	4:E:3544:HOH:O	2.04	0.41
1:A:3269:CYS:HB2	1:A:3281:TRP:CE2	2.56	0.41
1:C:3176:SER:HB3	1:C:3199:ILE:HD11	2.02	0.41
1:E:3270:LEU:HG	1:E:3316:CYS:SG	2.61	0.41
1:C:3295:THR:HG21	1:E:3244:HIS:O	2.21	0.41
1:E:2970:ASP:HB3	1:E:3034:PRO:HA	2.03	0.40
1:C:3272:VAL:CG2	1:C:3314:VAL:HG13	2.51	0.40
1:E:3161:ARG:NH2	2:F:991:GLU:HG3	2.36	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	368/405 (91%)	360 (98%)	8 (2%)	0	100	100
1	E	368/405 (91%)	361 (98%)	7 (2%)	0	100	100
2	B	8/15 (53%)	8 (100%)	0	0	100	100
2	D	7/15 (47%)	7 (100%)	0	0	100	100
2	F	5/15 (33%)	5 (100%)	0	0	100	100
All	All	1123/1260 (89%)	1095 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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%)	289 (100%)	1 (0%)	92	97
1	C	291/317 (92%)	288 (99%)	3 (1%)	76	86
1	E	290/317 (92%)	290 (100%)	0	100	100
2	B	8/11 (73%)	8 (100%)	0	100	100
2	D	7/11 (64%)	7 (100%)	0	100	100
2	F	6/11 (54%)	6 (100%)	0	100	100
All	All	892/984 (91%)	888 (100%)	4 (0%)	91	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3082	PHE
1	C	2958	ARG
1	C	3141	LYS
1	C	3233	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3268	HIS
1	C	3133	HIS
1	C	3194	ASN
1	C	3244	HIS
1	E	3058	HIS
1	E	3215	GLN
1	E	3239	HIS
1	E	3249	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	E	3402	-	12,12,12	1.15	1 (8%)	17,17,17	1.44	2 (11%)
3	CIT	E	3401	-	12,12,12	1.05	0	17,17,17	1.39	1 (5%)
3	CIT	C	3401	-	12,12,12	1.04	0	17,17,17	1.39	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
3	CIT	E	3402	-	-	14/16/16/16	-
3	CIT	E	3401	-	-	0/16/16/16	-
3	CIT	C	3401	-	-	5/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3402	CIT	O2-C1	-2.06	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3401	CIT	O6-C6-C3	4.07	120.12	113.05
3	E	3401	CIT	O6-C6-C3	3.97	119.95	113.05
3	E	3402	CIT	O5-C6-C3	-3.74	116.96	122.25
3	E	3402	CIT	O6-C6-C3	2.78	117.88	113.05

There are no chirality outliers.

All (19) torsion outliers are listed below:

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

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

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 [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%)	0.93	43 (11%) 4 4	20, 37, 59, 74	0
1	C	369/405 (91%)	0.65	13 (3%) 44 42	21, 31, 47, 65	0
1	E	369/405 (91%)	0.78	19 (5%) 28 26	19, 32, 51, 70	0
2	B	10/15 (66%)	1.86	2 (20%) 1 1	49, 63, 81, 83	0
2	D	9/15 (60%)	2.23	4 (44%) 0 0	51, 63, 76, 77	0
2	F	7/15 (46%)	3.62	5 (71%) 0 0	74, 85, 91, 101	0
All	All	1133/1260 (89%)	0.82	86 (7%) 13 12	19, 34, 57, 101	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	989	PHE	6.0
2	F	995	GLU	5.8
2	F	992	ASP	5.3
2	D	989	PHE	4.5
1	E	2958	ARG	4.4
2	D	995	GLU	4.2
1	C	3029	SER	4.1
1	A	3115	THR	4.1
2	F	990	ASP	3.9
2	F	996	ASP	3.8
1	E	3326	THR	3.8
1	A	3097	LYS	3.8
2	B	998	GLY	3.7
1	A	3087	CYS	3.7
1	E	3040	THR	3.7
1	C	3102	ARG	3.6
1	E	3043	SER	3.5
1	A	3034	PRO	3.5
1	E	3304[A]	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	3326	THR	3.4
1	A	3032	THR	3.4
1	E	3035	ILE	3.4
1	A	3150	GLY	3.3
1	E	3102	ARG	3.3
1	E	2992	LEU	3.2
1	A	3195	ILE	3.2
2	F	991	GLU	3.2
1	A	3082	PHE	3.2
1	C	3115	THR	3.1
1	C	3043	SER	3.1
1	A	3036	PRO	3.1
2	D	992	ASP	3.0
1	A	3033	VAL	2.9
1	A	3152	ARG	2.9
1	C	3117	SER	2.9
1	C	3243	VAL	2.9
1	E	2993	ASN	2.8
1	A	3144	MET	2.8
1	A	3027	GLY	2.8
1	A	3151	HIS	2.7
1	E	3042	LEU	2.7
1	E	3045	TYR	2.6
1	A	3030	SER	2.6
1	C	3326	THR	2.6
1	E	3098	THR	2.6
1	A	3187	ARG	2.5
1	A	3035	ILE	2.5
1	A	3149	LEU	2.5
1	A	3100	ARG	2.5
1	C	3098	THR	2.5
1	A	3141	LYS	2.5
1	A	3042	LEU	2.5
1	A	3171	GLU	2.4
1	A	3043	SER	2.4
1	A	3172	GLY	2.4
1	E	3195	ILE	2.4
1	A	2987	GLU	2.4
1	A	3221	THR	2.4
1	C	3208	CYS	2.4
1	A	3117	SER	2.4
1	E	3068	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	3238	GLY	2.3
1	A	3146	LYS	2.3
1	A	2994	VAL	2.3
1	A	3102	ARG	2.3
1	C	3042	LEU	2.3
1	A	3101	ILE	2.3
1	A	3148	LEU	2.3
1	A	3085	MET	2.3
1	C	3097	LYS	2.3
1	A	3037	ARG	2.2
1	A	3077	GLY	2.2
1	E	3046	VAL	2.2
1	E	3090	PRO	2.2
1	E	3192	GLY	2.2
1	A	3325	THR	2.1
1	A	2976	LYS	2.1
1	C	3293	THR	2.1
2	D	996	ASP	2.1
1	A	3109	SER	2.1
1	E	3044	SER	2.1
1	A	3170	ASP	2.1
1	A	3018	GLU	2.0
1	A	3131	LEU	2.0
1	C	3039	ILE	2.0
1	A	2968	ASP	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 monosaccharides 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(\AA^2)	Q<0.9
3	CIT	C	3401	13/13	0.42	0.27	85,88,91,91	0
3	CIT	E	3401	13/13	0.66	0.33	72,78,80,80	0
3	CIT	E	3402	13/13	0.81	0.28	63,70,79,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.