



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 09:35 pm GMT

PDB ID : 2B5U
Title : Crystal Structure Of Colicin E3 V206C Mutant In Complex With Its Immunity Protein
Authors : Nallini Vijayarangan, A.; Nithianantham, S.; Nan, W.; Jakes, K.; Shoham, M.
Deposited on : 2005-09-29
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

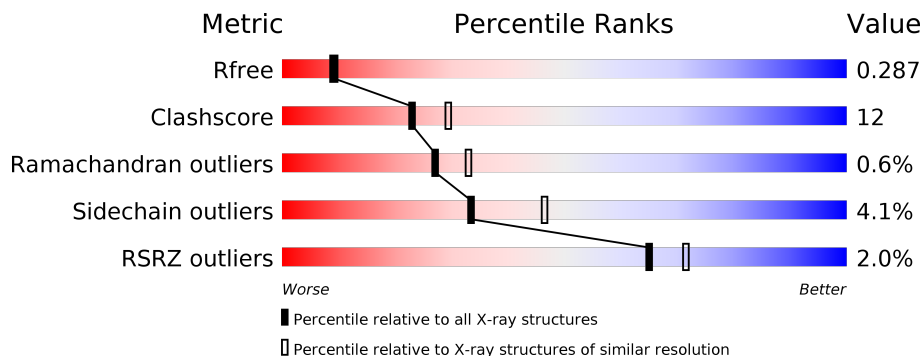
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	551	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>20%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	551	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>19%</div> <div>•</div> <div>15%</div> </div> </div>
2	B	84	<div> <div></div> <div> <div>73%</div> <div>26%</div> <div>•</div> </div> </div>
2	D	84	<div> <div></div> <div> <div>77%</div> <div>23%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8791 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 Colicin E3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3580	2210	661	700	9			
1	C	470	Total	C	N	O	S	0	0	0
			3580	2210	661	700	9			

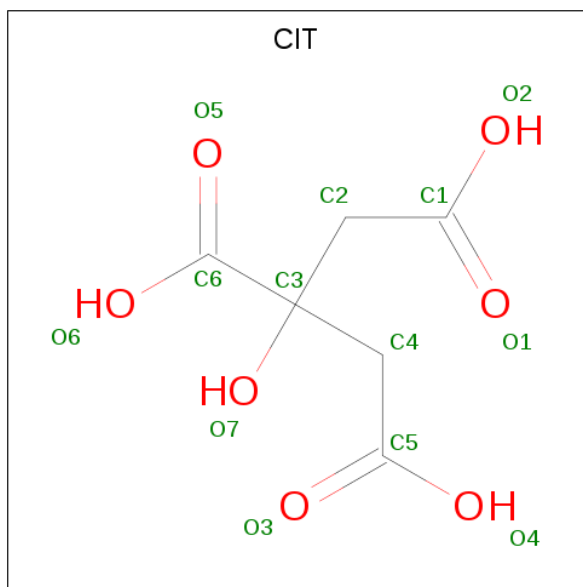
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	CYS	VAL	ENGINEERED	UNP P00646
C	206	CYS	VAL	ENGINEERED	UNP P00646

- Molecule 2 is a protein called Colicin E3 immunity protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	84	Total	C	N	O	S	0	0	0
			693	445	104	142	2			
2	D	84	Total	C	N	O	S	0	0	0
			693	445	104	142	2			

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

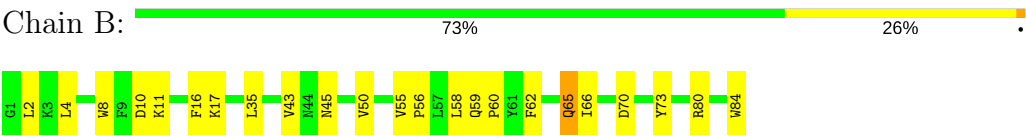


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		

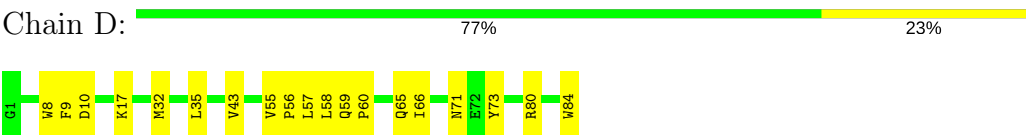
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	112	Total	O	0	0
			112	112		
4	B	23	Total	O	0	0
			23	23		
4	C	70	Total	O	0	0
			70	70		
4	D	14	Total	O	0	0
			14	14		

● Molecule 2: Colicin E3 immunity protein



● Molecule 2: Colicin E3 immunity protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.73Å 192.92Å 85.39Å 90.00° 112.98° 90.00°	Depositor
Resolution (Å)	44.40 – 2.30 44.42 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.40-2.30) 99.3 (44.42-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.259 , 0.295 0.252 , 0.287	Depositor DCC
R_{free} test set	8752 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8791	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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	0.38	0/3649	0.59	0/4935
1	C	0.38	0/3649	0.58	0/4935
2	B	0.47	0/714	0.61	0/967
2	D	0.46	0/714	0.62	0/967
All	All	0.39	0/8726	0.59	0/11804

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	3580	0	3538	91	0
1	C	3580	0	3538	94	0
2	B	693	0	617	20	0
2	D	693	0	617	14	0
3	A	13	0	5	1	0
3	C	13	0	5	0	0
4	A	112	0	0	3	0
4	B	23	0	0	1	0
4	C	70	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	14	0	0	0	0
All	All	8791	0	8320	207	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 12.

All (207) 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:306:ARG:HG2	1:A:306:ARG:HH11	1.23	1.02
1:C:249:THR:HG22	1:C:251:ASN:H	1.31	0.95
1:C:306:ARG:HH11	1:C:306:ARG:HG2	1.37	0.88
1:A:184:ARG:HD2	1:A:269:ASP:OD1	1.77	0.84
1:C:214:THR:HG22	1:C:215:GLU:H	1.40	0.84
1:A:369:ILE:O	1:A:372:ILE:HG22	1.76	0.83
1:A:139:VAL:HG12	1:A:194:GLN:O	1.79	0.83
2:D:59:GLN:HE22	2:D:66:ILE:H	1.24	0.82
1:C:388:ARG:HB2	1:C:388:ARG:HH11	1.49	0.78
1:A:164:ILE:HG13	1:A:183:VAL:HG13	1.64	0.78
1:C:164:ILE:HG13	1:C:183:VAL:HG13	1.68	0.76
1:C:550:TYR:O	1:C:551:LEU:HB2	1.87	0.74
1:C:98:PRO:HG3	1:C:103:LEU:CD2	2.20	0.72
1:C:238:THR:HB	1:C:239:PRO:HD2	1.71	0.72
1:A:306:ARG:CG	1:A:306:ARG:HH11	2.01	0.70
1:C:266:ASN:HD22	1:C:299:ARG:HH11	1.39	0.70
1:A:550:TYR:O	1:A:551:LEU:HB2	1.90	0.70
1:A:88:VAL:HG13	1:A:92:PHE:HB3	1.73	0.69
1:C:381:ASP:OD2	1:C:384:ALA:HB2	1.93	0.69
1:C:388:ARG:HB2	1:C:388:ARG:NH1	2.08	0.68
1:C:98:PRO:HG3	1:C:103:LEU:HD21	1.76	0.68
1:A:545:ARG:HB3	1:A:545:ARG:HH11	1.59	0.67
2:B:59:GLN:HE22	2:B:66:ILE:H	1.42	0.66
1:C:306:ARG:NH1	1:C:306:ARG:HG2	2.10	0.66
1:C:214:THR:HG22	1:C:215:GLU:N	2.09	0.65
1:A:523:ASP:OD1	1:A:525:GLN:HB2	1.97	0.65
1:A:446:LEU:O	1:A:450:LYS:HB2	1.97	0.65
1:A:489:GLN:CD	1:A:489:GLN:H	2.00	0.65
1:C:169:VAL:HG11	1:C:282:ALA:HB3	1.79	0.65
1:C:488:LYS:HE2	1:C:489:GLN:HE22	1.62	0.65
1:C:485:LYS:NZ	1:C:551:LEU:HD21	2.12	0.64
2:B:10:ASP:HB2	2:B:17:LYS:HD2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:LEU:HB3	1:C:248:VAL:HG23	1.80	0.63
1:A:205:SER:HB2	2:B:60:PRO:HG3	1.80	0.62
1:A:193:ARG:HH11	1:A:193:ARG:HB2	1.63	0.62
1:C:499:THR:HG23	1:C:503:GLY:HA2	1.82	0.62
1:A:169:VAL:HG11	1:A:282:ALA:HB3	1.83	0.61
1:A:306:ARG:HG2	1:A:306:ARG:NH1	2.02	0.61
1:C:120:MET:O	1:C:124:LYS:HG3	2.01	0.60
1:C:525:GLN:HG3	4:C:633:HOH:O	2.02	0.60
2:D:35:LEU:HD11	2:D:58:LEU:HD21	1.83	0.60
1:C:337:VAL:O	1:C:341:GLN:HG3	2.02	0.60
1:A:402:THR:HG22	1:C:417:GLU:OE1	2.02	0.59
1:C:224:ILE:HD12	1:C:270:ALA:HB3	1.85	0.59
1:A:329:GLU:HB3	1:A:435:LYS:HD2	1.85	0.58
1:A:178:THR:HG21	2:B:65:GLN:HE21	1.68	0.58
1:A:224:ILE:HG23	1:A:225:PRO:HD2	1.86	0.58
1:C:266:ASN:HD22	1:C:299:ARG:NH1	2.02	0.58
1:A:98:PRO:HG3	1:A:103:LEU:CD2	2.33	0.58
1:C:343:ARG:HD2	1:C:417:GLU:OE2	2.03	0.57
2:D:55:VAL:HB	2:D:56:PRO:HD3	1.85	0.57
1:C:328:ALA:O	1:C:332:GLN:HG3	2.04	0.57
1:A:244:LEU:HB3	1:A:248:VAL:HG23	1.88	0.56
1:A:146:LYS:HE2	1:A:146:LYS:O	2.06	0.56
2:B:59:GLN:HE22	2:B:66:ILE:N	2.03	0.56
1:A:139:VAL:CG1	1:A:194:GLN:HB3	2.36	0.56
2:B:55:VAL:HB	2:B:56:PRO:HD3	1.86	0.56
2:B:8:TRP:HB3	2:B:73:TYR:CD2	2.41	0.55
1:C:486:THR:HG21	1:C:495:ARG:HE	1.71	0.55
2:D:59:GLN:HE22	2:D:66:ILE:N	2.00	0.55
1:A:214:THR:HG22	1:A:215:GLU:N	2.21	0.55
1:C:485:LYS:HZ2	1:C:551:LEU:CD1	2.19	0.55
1:C:489:GLN:CD	1:C:489:GLN:H	2.09	0.54
2:D:10:ASP:HB2	2:D:17:LYS:HD2	1.89	0.54
1:C:485:LYS:HZ2	1:C:551:LEU:HD11	1.71	0.54
1:A:98:PRO:HG3	1:A:103:LEU:HD21	1.88	0.54
1:C:205:SER:HB2	2:D:60:PRO:HG3	1.89	0.54
1:A:141:PRO:O	1:A:144:ILE:HG12	2.08	0.54
1:C:95:LEU:HD13	1:C:155:ILE:HD11	1.90	0.54
1:C:230:LEU:HD21	1:C:285:VAL:HG11	1.91	0.53
1:A:510:ASP:OD1	1:A:513:HIS:HD2	1.92	0.53
1:A:144:ILE:HD13	1:A:247:GLY:HA3	1.91	0.53
1:A:480:LYS:HD3	2:B:16:PHE:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LYS:O	1:C:125:GLY:C	2.48	0.52
1:A:330:LEU:HD21	1:A:436:GLU:HG3	1.90	0.52
1:A:520:ARG:HE	1:A:523:ASP:HB3	1.75	0.52
1:C:489:GLN:HE21	1:C:495:ARG:NH1	2.07	0.52
1:A:485:LYS:NZ	1:A:551:LEU:HD21	2.25	0.52
1:C:489:GLN:HE21	1:C:495:ARG:HH12	1.58	0.52
1:A:266:ASN:HD22	1:A:299:ARG:HH11	1.56	0.51
1:A:545:ARG:CB	1:A:545:ARG:HH11	2.22	0.51
1:C:169:VAL:HG11	1:C:282:ALA:CB	2.41	0.51
1:A:306:ARG:CG	1:A:306:ARG:NH1	2.66	0.51
1:C:437:ASP:O	1:C:440:ARG:HB2	2.10	0.51
1:C:273:ARG:HG3	1:C:273:ARG:O	2.11	0.51
1:A:146:LYS:HD3	1:A:149:PRO:HG3	1.91	0.51
1:A:266:ASN:HD22	1:A:299:ARG:NH1	2.09	0.51
1:C:144:ILE:O	1:C:146:LYS:HG3	2.10	0.51
1:A:338:ALA:O	1:A:342:GLU:HG3	2.11	0.51
1:A:224:ILE:CG2	1:A:225:PRO:HD2	2.39	0.51
1:A:146:LYS:HE2	1:A:146:LYS:N	2.27	0.50
1:A:417:GLU:OE1	1:C:402:THR:HG22	2.11	0.50
1:C:158:SER:O	1:C:159:LEU:HD23	2.11	0.50
1:A:354:ARG:HD3	4:A:610:HOH:O	2.12	0.50
1:C:166:GLU:HG2	1:C:180:ASN:HB2	1.93	0.49
1:C:129:PHE:CZ	1:C:202:VAL:HG22	2.48	0.49
1:A:499:THR:HG23	1:A:503:GLY:HA2	1.94	0.49
1:A:520:ARG:HE	1:A:523:ASP:CB	2.26	0.49
1:C:93:PRO:HD3	1:C:137:TYR:CZ	2.47	0.49
1:A:485:LYS:HZ1	1:A:551:LEU:HD21	1.77	0.48
1:A:468:PRO:HG3	4:B:101:HOH:O	2.13	0.48
1:C:249:THR:HG22	1:C:251:ASN:N	2.13	0.48
1:A:488:LYS:HE3	2:B:45:ASN:OD1	2.13	0.48
1:A:272:ILE:N	1:A:272:ILE:HD12	2.27	0.48
1:A:527:LEU:O	1:A:541:PRO:HG3	2.13	0.48
1:C:139:VAL:CG2	1:C:194:GLN:HB3	2.43	0.48
1:A:475:GLY:HA3	1:A:535:GLY:HA3	1.96	0.48
2:B:35:LEU:HD11	2:B:58:LEU:HD21	1.96	0.48
1:C:221:THR:HA	1:C:230:LEU:O	2.14	0.48
1:A:146:LYS:HB3	1:A:151:MET:SD	2.54	0.48
1:A:273:ARG:O	1:A:273:ARG:HG3	2.14	0.48
1:A:372:ILE:HG23	1:A:373:LYS:N	2.29	0.48
1:A:381:ASP:OD2	1:A:384:ALA:HB2	2.13	0.47
1:A:257:ARG:NH2	4:A:702:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ARG:HG3	1:A:440:ARG:HH11	1.80	0.47
1:C:485:LYS:HZ1	1:C:551:LEU:HD21	1.79	0.47
1:C:369:ILE:O	1:C:372:ILE:HG12	2.15	0.47
1:C:545:ARG:HH11	1:C:545:ARG:HB3	1.79	0.47
1:A:292:SER:OG	1:A:295:GLN:HG3	2.14	0.47
1:C:216:ARG:HD3	1:C:216:ARG:H	1.80	0.47
1:C:146:LYS:HB3	1:C:149:PRO:HG3	1.97	0.46
1:C:485:LYS:HZ2	1:C:551:LEU:HD21	1.79	0.46
1:A:93:PRO:HD3	1:A:137:TYR:CZ	2.51	0.46
1:C:316:VAL:HG21	1:C:454:ARG:HD3	1.96	0.46
1:A:221:THR:HA	1:A:230:LEU:O	2.15	0.46
1:A:380:HIS:C	1:A:382:PRO:HD3	2.36	0.46
1:C:123:LEU:HD22	1:C:198:VAL:HG23	1.98	0.46
1:C:485:LYS:HZ2	1:C:551:LEU:CD2	2.28	0.46
1:C:116:ILE:N	1:C:116:ILE:HD12	2.31	0.46
1:C:144:ILE:CD1	1:C:290:VAL:HG11	2.46	0.45
1:C:316:VAL:O	1:C:320:GLU:HB2	2.16	0.45
1:C:486:THR:CG2	1:C:495:ARG:HE	2.30	0.45
1:C:148:ASP:O	1:C:151:MET:HB3	2.16	0.45
1:A:159:LEU:HD13	1:A:164:ILE:HD11	1.98	0.45
1:C:96:SER:O	1:C:98:PRO:HD3	2.16	0.45
1:C:146:LYS:HA	1:C:151:MET:HE1	1.99	0.45
1:A:337:VAL:O	1:A:341:GLN:HG3	2.17	0.45
1:C:323:TYR:HA	1:C:442:ALA:HB1	1.98	0.45
2:D:80:ARG:HB2	2:D:84:TRP:CD1	2.51	0.45
3:A:602:CIT:H22	4:A:699:HOH:O	2.16	0.45
1:C:272:ILE:HD12	1:C:272:ILE:N	2.32	0.45
1:C:523:ASP:OD1	1:C:525:GLN:HB2	2.17	0.45
1:A:124:LYS:O	1:A:125:GLY:C	2.54	0.44
1:A:202:VAL:HG13	1:A:203:PRO:HD2	1.99	0.44
1:C:132:TRP:CZ3	1:C:258:PRO:HG3	2.51	0.44
1:A:461:GLY:HA2	2:B:43:VAL:HG11	1.99	0.44
1:A:164:ILE:HG13	1:A:183:VAL:CG1	2.41	0.44
1:C:306:ARG:NH1	1:C:306:ARG:CG	2.73	0.44
2:D:8:TRP:HB3	2:D:73:TYR:CD2	2.53	0.44
1:A:485:LYS:HZ2	1:A:551:LEU:CD1	2.31	0.44
2:B:50:VAL:HB	2:B:73:TYR:HB2	2.00	0.44
1:A:302:GLU:HA	1:A:302:GLU:OE1	2.17	0.44
1:A:446:LEU:HD13	1:A:446:LEU:C	2.37	0.44
1:C:388:ARG:HH11	1:C:388:ARG:CB	2.26	0.44
1:A:110:GLY:O	1:A:111:ALA:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:LYS:HA	1:C:151:MET:CE	2.48	0.44
2:B:80:ARG:HB2	2:B:84:TRP:CD1	2.53	0.43
1:C:380:HIS:C	1:C:382:PRO:HD3	2.39	0.43
2:B:59:GLN:N	2:B:60:PRO:CD	2.81	0.43
1:C:139:VAL:HG22	1:C:194:GLN:O	2.18	0.43
1:C:446:LEU:C	1:C:446:LEU:HD13	2.39	0.43
1:C:495:ARG:HD2	1:C:508:GLU:OE1	2.19	0.43
2:D:32:MET:HE1	2:D:43:VAL:HG22	2.00	0.43
2:D:71:ASN:HB2	2:D:73:TYR:CE1	2.54	0.43
1:C:134:VAL:O	1:C:197:SER:HB3	2.18	0.43
1:C:426:SER:O	1:C:429:MET:HB2	2.19	0.43
1:C:113:SER:HB3	1:C:116:ILE:HD13	2.00	0.43
1:C:485:LYS:NZ	1:C:551:LEU:CD2	2.79	0.43
1:A:112:LEU:HG	1:A:117:ALA:HB2	2.01	0.43
1:C:509:TRP:HZ3	1:C:532:PRO:HG2	1.84	0.43
2:D:59:GLN:N	2:D:60:PRO:CD	2.82	0.43
2:B:11:LYS:HG3	2:B:70:ASP:O	2.19	0.42
1:C:144:ILE:HD11	1:C:290:VAL:HG11	2.00	0.42
1:A:398:GLN:OE1	1:A:402:THR:HG23	2.19	0.42
2:B:4:LEU:HB3	2:B:62:PHE:HZ	1.84	0.42
1:A:302:GLU:CD	1:A:305:ARG:HH12	2.22	0.42
1:A:248:VAL:O	1:A:248:VAL:HG23	2.20	0.42
1:A:334:ASN:ND2	1:A:432:ARG:HH11	2.17	0.42
1:A:178:THR:CG2	2:B:65:GLN:HE21	2.32	0.42
1:C:440:ARG:HH11	1:C:440:ARG:HG3	1.85	0.42
1:A:372:ILE:CG2	1:A:373:LYS:N	2.83	0.42
1:A:486:THR:CG2	1:A:495:ARG:HE	2.33	0.42
1:A:178:THR:CG2	2:B:65:GLN:NE2	2.82	0.42
1:C:214:THR:CG2	1:C:215:GLU:H	2.20	0.42
1:C:164:ILE:HG22	1:C:165:THR:N	2.35	0.42
1:C:525:GLN:NE2	1:C:543:PRO:O	2.53	0.42
1:C:224:ILE:HB	1:C:227:ALA:HB3	2.00	0.41
2:D:59:GLN:NE2	2:D:66:ILE:H	2.06	0.41
1:A:178:THR:HG22	1:A:207:PRO:HA	2.01	0.41
1:A:446:LEU:HD13	1:A:446:LEU:O	2.19	0.41
1:A:193:ARG:HH11	1:A:193:ARG:CB	2.31	0.41
1:A:465:HIS:HA	1:A:466:PRO:HD3	1.93	0.41
1:A:457:PHE:CZ	2:B:2:LEU:HD22	2.55	0.41
1:C:520:ARG:HE	1:C:523:ASP:CB	2.34	0.41
2:D:9:PHE:CD1	2:D:9:PHE:N	2.88	0.41
1:A:485:LYS:HZ2	1:A:551:LEU:HD11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:VAL:HG13	4:C:664:HOH:O	2.21	0.41
1:A:146:LYS:HE2	1:A:146:LYS:H	1.85	0.41
1:A:334:ASN:HA	1:A:334:ASN:HD22	1.69	0.41
1:A:177:ALA:HB3	2:B:65:GLN:HG2	2.03	0.41
1:C:131:LEU:HD13	1:C:259:ALA:CB	2.51	0.41
1:A:136:LEU:HD11	1:A:198:VAL:HG13	2.02	0.41
1:A:510:ASP:OD1	1:A:513:HIS:CD2	2.72	0.41
1:C:446:LEU:O	1:C:450:LYS:HB2	2.21	0.41
1:C:159:LEU:CD1	1:C:164:ILE:HD11	2.51	0.41
1:C:292:SER:O	1:C:296:VAL:HG23	2.20	0.41
1:C:178:THR:HG23	2:D:65:GLN:HG3	2.03	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	468/551 (85%)	450 (96%)	15 (3%)	3 (1%)	27	33
1	C	468/551 (85%)	447 (96%)	17 (4%)	4 (1%)	19	22
2	B	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
2	D	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
All	All	1100/1270 (87%)	1055 (96%)	38 (4%)	7 (1%)	27	33

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	PRO
1	C	98	PRO
1	C	145	ALA
1	A	276	LYS

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Mol	Chain	Res	Type
1	A	126	PRO
1	C	126	PRO
1	C	225	PRO

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	378/422 (90%)	361 (96%)	17 (4%)	30	42
1	C	378/422 (90%)	360 (95%)	18 (5%)	28	39
2	B	76/76 (100%)	75 (99%)	1 (1%)	71	84
2	D	76/76 (100%)	75 (99%)	1 (1%)	71	84
All	All	908/996 (91%)	871 (96%)	37 (4%)	33	46

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LEU
1	A	146	LYS
1	A	151	MET
1	A	193	ARG
1	A	225	PRO
1	A	243	THR
1	A	322	ASN
1	A	336	ASP
1	A	343	ARG
1	A	363	LYS
1	A	395	LEU
1	A	449	GLU
1	A	471	GLU
1	A	478	ASP
1	A	489	GLN
1	A	499	THR
1	A	545	ARG
2	B	65	GLN

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Mol	Chain	Res	Type
1	C	131	LEU
1	C	162	ASP
1	C	202	VAL
1	C	216	ARG
1	C	225	PRO
1	C	236	ASN
1	C	320	GLU
1	C	321	ARG
1	C	343	ARG
1	C	357	GLU
1	C	388	ARG
1	C	395	LEU
1	C	449	GLU
1	C	471	GLU
1	C	474	LYS
1	C	489	GLN
1	C	499	THR
1	C	545	ARG
2	D	57	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	180	ASN
1	A	266	ASN
1	A	298	GLN
1	A	304	ASN
1	A	308	GLN
1	A	314	HIS
1	A	322	ASN
1	A	331	ASN
1	A	334	ASN
1	A	387	HIS
1	A	391	GLN
1	A	401	GLN
1	A	444	ASN
1	A	447	ASN
1	A	451	ASN
1	A	472	ASN
1	A	489	GLN
1	A	513	HIS

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Mol	Chain	Res	Type
1	A	525	GLN
2	B	59	GLN
2	B	65	GLN
1	C	180	ASN
1	C	242	GLN
1	C	266	ASN
1	C	298	GLN
1	C	304	ASN
1	C	314	HIS
1	C	331	ASN
1	C	334	ASN
1	C	374	GLN
1	C	376	ASN
1	C	387	HIS
1	C	401	GLN
1	C	405	ASN
1	C	444	ASN
1	C	447	ASN
1	C	472	ASN
1	C	489	GLN
1	C	525	GLN
1	C	536	ASN
2	D	59	GLN
2	D	65	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	A	602	-	3,12,12	2.48	2 (66%)	3,17,17	2.55	2 (66%)
3	CIT	C	601	-	3,12,12	2.40	2 (66%)	3,17,17	2.72	2 (66%)

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	A	602	-	-	0/6/16/16	0/0/0/0
3	CIT	C	601	-	-	0/6/16/16	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	CIT	C4-C3	2.23	1.58	1.54
3	A	602	CIT	C4-C3	2.55	1.58	1.54
3	A	602	CIT	C2-C3	3.42	1.59	1.54
3	C	601	CIT	C2-C3	3.47	1.59	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	CIT	C3-C4-C5	-3.68	109.43	114.95
3	A	602	CIT	C3-C4-C5	-3.30	109.99	114.95
3	A	602	CIT	C3-C2-C1	2.91	119.31	114.95
3	C	601	CIT	C3-C2-C1	2.92	119.33	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	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	470/551 (85%)	0.33	12 (2%) 56 63	27, 49, 81, 100	0
1	C	470/551 (85%)	0.31	10 (2%) 63 70	26, 49, 79, 101	0
2	B	84/84 (100%)	0.04	0 100 100	32, 44, 61, 64	0
2	D	84/84 (100%)	0.06	0 100 100	31, 43, 60, 70	0
All	All	1108/1270 (87%)	0.28	22 (1%) 65 71	26, 48, 80, 101	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	83	ALA	4.2
1	A	149	PRO	4.0
1	A	82	SER	4.0
1	A	101	GLY	3.4
1	A	446	LEU	3.2
1	A	112	LEU	3.2
1	A	174	LEU	3.2
1	C	149	PRO	3.0
1	A	150	ASN	2.8
1	C	101	GLY	2.8
1	A	216	ARG	2.8
1	C	174	LEU	2.6
1	C	317	GLU	2.6
1	C	151	MET	2.6
1	C	236	ASN	2.4
1	A	372	ILE	2.3
1	C	330	LEU	2.3
1	C	152	MET	2.3
1	A	125	GLY	2.2
1	C	248	VAL	2.2
1	C	348	VAL	2.1
1	A	440	ARG	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 carbohydrates 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	A	602	13/13	0.60	0.28	139,140,142,142	0
3	CIT	C	601	13/13	0.69	0.32	140,140,141,141	0

6.5 Other polymers [i](#)

There are no such residues in this entry.