



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:11 AM UTC

PDB ID : 2B5U / pdb_00002b5u
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 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

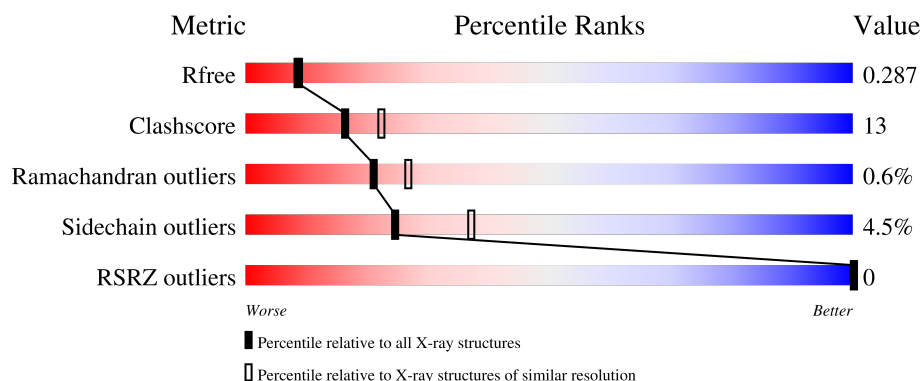
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

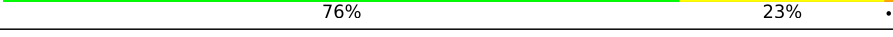
The reported resolution of this entry is 2.30 Å.

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	551	 64% 19% 15%
1	C	551	 62% 21% 15%
2	B	84	 71% 26%
2	D	84	 76% 23%

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 mutation	UNP P00646
C	206	CYS	VAL	engineered mutation	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 (CCD ID: 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		

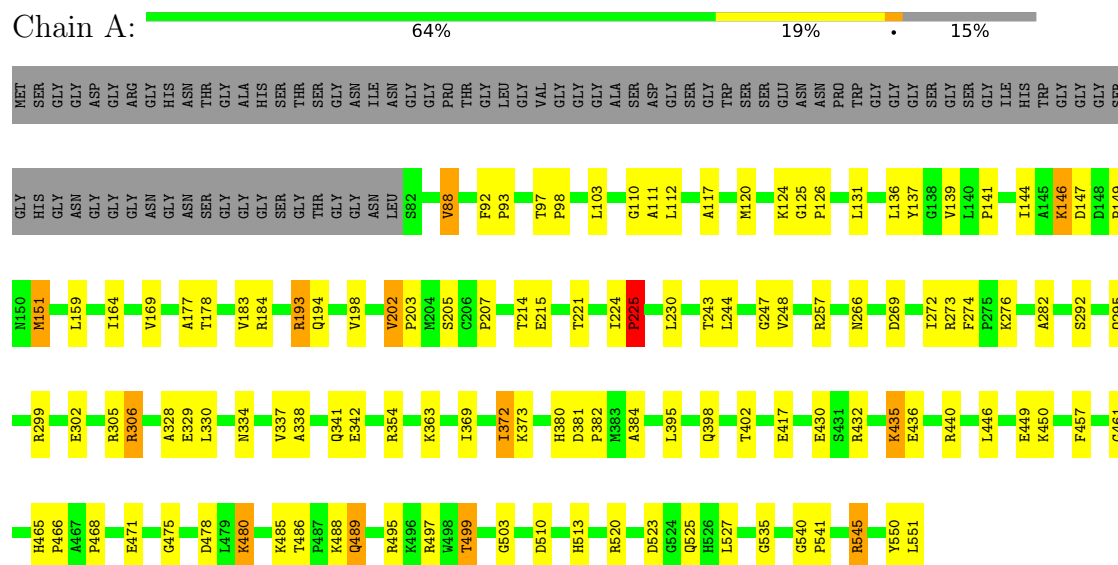
- Molecule 4 is water.

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		

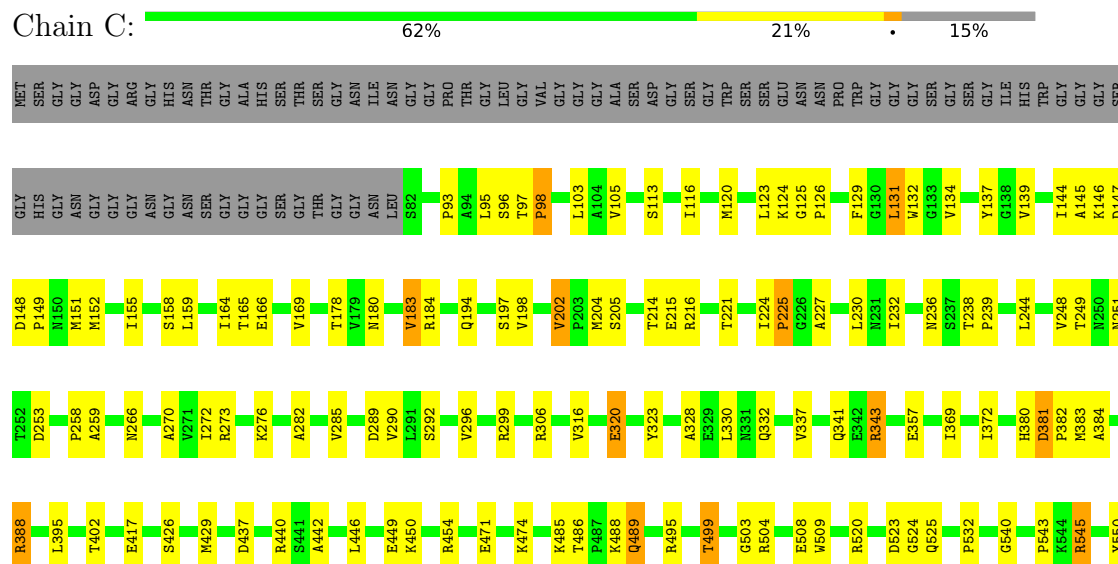
3 Residue-property plots

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: Colicin E3



• Molecule 1: Colicin E3

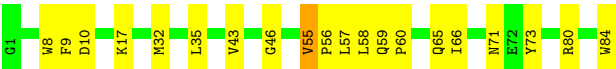


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● Molecule 2: Colicin E3 immunity protein



● 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 44.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.40-2.30) 99.3 (44.40-2.30)	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 , 28.2	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	0.96	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

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	0.47	0/3649	0.91	9/4935 (0.2%)
1	C	0.46	0/3649	0.91	9/4935 (0.2%)
2	B	0.53	1/714 (0.1%)	0.90	1/967 (0.1%)
2	D	0.49	0/714	0.94	2/967 (0.2%)
All	All	0.47	1/8726 (0.0%)	0.91	21/11804 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	55	VAL	CA-CB	5.44	1.56	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	540	GLY	CA-C-N	6.53	126.88	119.83
1	C	540	GLY	C-N-CA	6.53	126.88	119.83
2	D	55	VAL	CB-CA-C	-6.28	107.74	113.70
1	C	97	THR	CA-C-N	5.99	127.32	119.84
1	C	97	THR	C-N-CA	5.99	127.32	119.84
1	A	147	ASP	N-CA-C	-5.96	105.09	112.90
2	D	46	GLY	N-CA-C	5.67	119.14	111.72
1	A	540	GLY	CA-C-N	5.50	125.43	119.76
1	A	540	GLY	C-N-CA	5.50	125.43	119.76
1	C	524	GLY	N-CA-C	-5.42	108.16	115.21
1	A	497	ARG	N-CA-C	5.42	118.31	109.59
2	B	31	VAL	CB-CA-C	-5.35	104.91	112.14
1	A	372	ILE	N-CA-C	-5.33	105.34	110.72
1	A	274	PHE	CA-C-N	5.29	125.29	119.89
1	A	274	PHE	C-N-CA	5.29	125.29	119.89
1	C	381	ASP	CA-C-N	5.27	125.58	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	381	ASP	C-N-CA	5.27	125.58	119.47
1	C	147	ASP	N-CA-C	-5.22	106.86	113.18
1	A	97	THR	CA-C-N	5.17	126.30	119.84
1	A	97	THR	C-N-CA	5.17	126.30	119.84
1	C	253	ASP	N-CA-C	-5.06	101.86	109.15

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	96	0
1	C	3580	0	3538	100	0
2	B	693	0	617	21	0
2	D	693	0	617	15	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
4	D	14	0	0	0	0
All	All	8791	0	8320	219	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 13.

All (219) 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:HG2	1:C:306:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:485:LYS:HZ1	1:A:551:LEU:HD21	1.45	0.82
2:D:59:GLN:HE22	2:D:66:ILE:H	1.24	0.82
1:C:388:ARG:HH11	1:C:388:ARG:HB2	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:HH11	1:A:306:ARG:CG	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:A:489:GLN:H	1:A:489:GLN:CD	2.00	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:HH11	1:A:545:ARG:HB3	1.59	0.67
2:B:59:GLN:HE22	2:B:66:ILE:H	1.42	0.66
1:C:306:ARG:HG2	1:C:306:ARG:NH1	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: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
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:489:GLN:H	1:C:489:GLN:CD	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:124:LYS:O	1:C:125:GLY:C	2.48	0.57
1:C:152:MET:HE1	1:C:289:ASP:HB3	1.86	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:C:146:LYS:HA	1:C:151:MET:HE1	1.88	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:120:MET:HE3	1:A:183:VAL:HG11	1.88	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
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
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: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:HH11	1:A:545:ARG:CB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:LYS:HZ1	1:A:551:LEU:CD2	2.20	0.51
1:C:273:ARG:O	1:C:273:ARG:HG3	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:380:HIS:C	1:A:382:PRO:HD3	2.36	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:A:124:LYS:O	1:A:125:GLY:C	2.54	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:446:LEU:C	1:A:446:LEU:HD13	2.37	0.48
1:A:468:PRO:HG3	4:B:101:HOH:O	2.13	0.48
1:A:110:GLY:O	1:A:111:ALA:C	2.56	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:C:380:HIS:C	1:C:382:PRO:HD3	2.39	0.48
1:C:184:ARG:HE	1:C:204:MET:HE2	1.78	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:C:446:LEU:C	1:C:446:LEU:HD13	2.39	0.48
1:A:146:LYS:HB3	1:A:151:MET:SD	2.54	0.48
1:A:273:ARG:HG3	1:A:273:ARG:O	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
1:A:328:ALA:HB2	1:C:383:MET:HE3	1.96	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:SER:OG	1:A:295:GLN:HG3	2.14	0.47
1:A:302:GLU:CD	1:A:305:ARG:HH12	2.22	0.47
1:C:216:ARG:H	1:C:216:ARG:HD3	1.80	0.47
1:C:545:ARG:HH11	1:C:545:ARG:HB3	1.79	0.47
1:A:151:MET:O	1:A:151:MET:HE2	2.14	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: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: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
2:B:11:LYS:HG3	2:B:70:ASP:C	2.42	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: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:485:LYS:NZ	1:A:551:LEU:HD21	2.25	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
2:B:50:VAL:HB	2:B:73:TYR:HB2	2.00	0.44
1:C:383:MET:HE2	1:C:383:MET:HA	1.99	0.44
1:A:302:GLU:OE1	1:A:302:GLU:HA	2.17	0.44
1:C:388:ARG:HH11	1:C:388:ARG:CB	2.26	0.44
2:B:80:ARG:HB2	2:B:84:TRP:CD1	2.53	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:120:MET:HE3	1:C:183:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:ARG:HD2	1:C:508:GLU:OE1	2.19	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
2:D:32:MET:HE1	2:D:43:VAL:HG22	2.00	0.43
1:A:510:ASP:C	1:A:510:ASP:OD2	2.62	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:C:330:LEU:HD13	1:C:330:LEU:C	2.43	0.42
1:A:330:LEU:C	1:A:330:LEU:HD13	2.44	0.42
1:A:178:THR:CG2	2:B:65:GLN:HE21	2.32	0.42
1:A:184:ARG:HH11	1:A:269:ASP:CG	2.26	0.42
1:A:334:ASN:ND2	1:A:432:ARG:HH11	2.17	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:C:146:LYS:HA	1:C:151:MET:CE	2.48	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:193:ARG:HH11	1:A:193:ARG:CB	2.31	0.41
1:A:446:LEU:O	1:A:446:LEU:HD13	2.19	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:248:VAL:HG23	1:A:248:VAL:O	2.20	0.41
1:C:105:VAL:HG13	4:C:664:HOH:O	2.21	0.41
2:D:58:LEU:C	2:D:60:PRO:HD2	2.45	0.41
1:A:146:LYS:HE2	1:A:146:LYS:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ALA:HB3	2:B:65:GLN:HG2	2.03	0.41
1:A:334:ASN:HD22	1:A:334:ASN:HA	1.69	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: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:446:LEU:O	1:C:450:LYS:HB2	2.21	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%)	21	27
1	C	468/551 (85%)	447 (96%)	17 (4%)	4 (1%)	14	17
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%)	21	27

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
1	A	126	PRO
1	C	126	PRO

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Mol	Chain	Res	Type
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%)	358 (95%)	20 (5%)	20	30
1	C	378/422 (90%)	359 (95%)	19 (5%)	22	33
2	B	76/76 (100%)	75 (99%)	1 (1%)	61	77
2	D	76/76 (100%)	75 (99%)	1 (1%)	61	77
All	All	908/996 (91%)	867 (96%)	41 (4%)	24	37

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	VAL
1	A	131	LEU
1	A	146	LYS
1	A	151	MET
1	A	193	ARG
1	A	202	VAL
1	A	225	PRO
1	A	243	THR
1	A	306	ARG
1	A	363	LYS
1	A	395	LEU
1	A	430	GLU
1	A	435	LYS
1	A	449	GLU
1	A	471	GLU
1	A	478	ASP
1	A	480	LYS
1	A	489	GLN
1	A	499	THR
1	A	545	ARG

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Mol	Chain	Res	Type
2	B	65	GLN
1	C	131	LEU
1	C	183	VAL
1	C	202	VAL
1	C	225	PRO
1	C	232	ILE
1	C	236	ASN
1	C	276	LYS
1	C	320	GLU
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	504	ARG
1	C	545	ARG
2	D	57	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	180	ASN
1	A	182	ASN
1	A	242	GLN
1	A	266	ASN
1	A	280	HIS
1	A	298	GLN
1	A	304	ASN
1	A	307	GLN
1	A	308	GLN
1	A	314	HIS
1	A	322	ASN
1	A	331	ASN
1	A	334	ASN
1	A	362	ASN
1	A	391	GLN
1	A	401	GLN

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Mol	Chain	Res	Type
1	A	406	ASN
1	A	444	ASN
1	A	447	ASN
1	A	472	ASN
1	A	489	GLN
1	A	490	ASN
1	A	513	HIS
2	B	59	GLN
2	B	65	GLN
1	C	180	ASN
1	C	263	GLN
1	C	266	ASN
1	C	280	HIS
1	C	298	GLN
1	C	304	ASN
1	C	307	GLN
1	C	322	ASN
1	C	331	ASN
1	C	332	GLN
1	C	334	ASN
1	C	387	HIS
1	C	391	GLN
1	C	401	GLN
1	C	405	ASN
1	C	444	ASN
1	C	472	ASN
1	C	489	GLN
1	C	490	ASN
2	D	59	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

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	C	601	-	12,12,12	1.90	2 (16%)	17,17,17	1.73	4 (23%)
3	CIT	A	602	-	12,12,12	1.96	2 (16%)	17,17,17	1.71	3 (17%)

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	601	-	-	2/16/16/16	-
3	CIT	A	602	-	-	2/16/16/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	CIT	C2-C3	4.72	1.59	1.54
3	A	602	CIT	C2-C3	4.66	1.59	1.54
3	A	602	CIT	C4-C3	3.64	1.58	1.54
3	C	601	CIT	C4-C3	3.25	1.58	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	CIT	O6-C6-O5	-3.69	112.06	123.86
3	A	602	CIT	O6-C6-O5	-3.63	112.24	123.86
3	C	601	CIT	O5-C6-C3	-2.86	116.55	122.09
3	A	602	CIT	O5-C6-C3	-2.78	116.70	122.09
3	C	601	CIT	O7-C3-C2	2.12	114.21	109.38
3	A	602	CIT	O7-C3-C2	2.11	114.19	109.38
3	C	601	CIT	C4-C3-C6	-2.08	105.43	110.03

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	CIT	C2-C3-C6-O5
3	A	602	CIT	O7-C3-C6-O5
3	C	601	CIT	C2-C3-C6-O5
3	C	601	CIT	O7-C3-C6-O5

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 [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	470/551 (85%)	-0.99	0 100 100	27, 49, 81, 100	0
1	C	470/551 (85%)	-1.04	0 100 100	26, 49, 79, 101	0
2	B	84/84 (100%)	-1.13	0 100 100	32, 44, 61, 64	0
2	D	84/84 (100%)	-1.11	0 100 100	31, 43, 60, 70	0
All	All	1108/1270 (87%)	-1.03	0 100 100	26, 48, 80, 101	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
3	CIT	C	601	13/13	0.97	0.12	140,140,141,141	0
3	CIT	A	602	13/13	0.98	0.12	139,140,142,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.