



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 01:51 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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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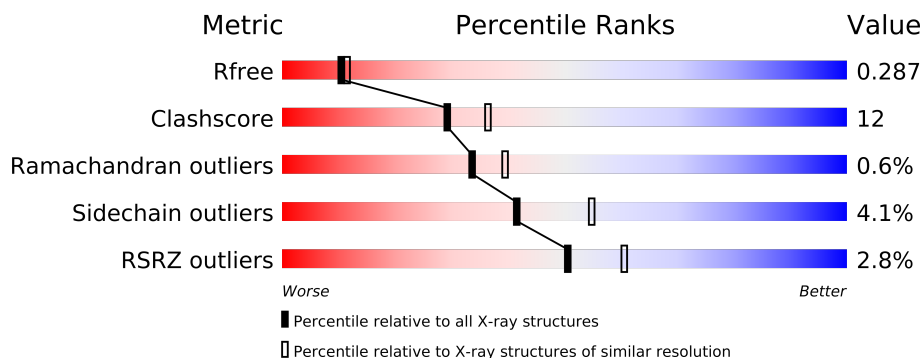
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance




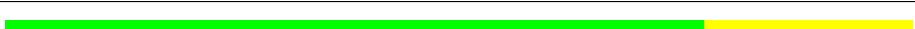
The reported resolution of this entry is 2.30 Å.

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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	551	
1	C	551	
2	B	84	
2	D	84	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CIT	A	602	-	X
3	CIT	C	601	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8791 atoms, of which 0 are hydrogen and 0 are deuterium.

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: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



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

- Molecule 4 is water.

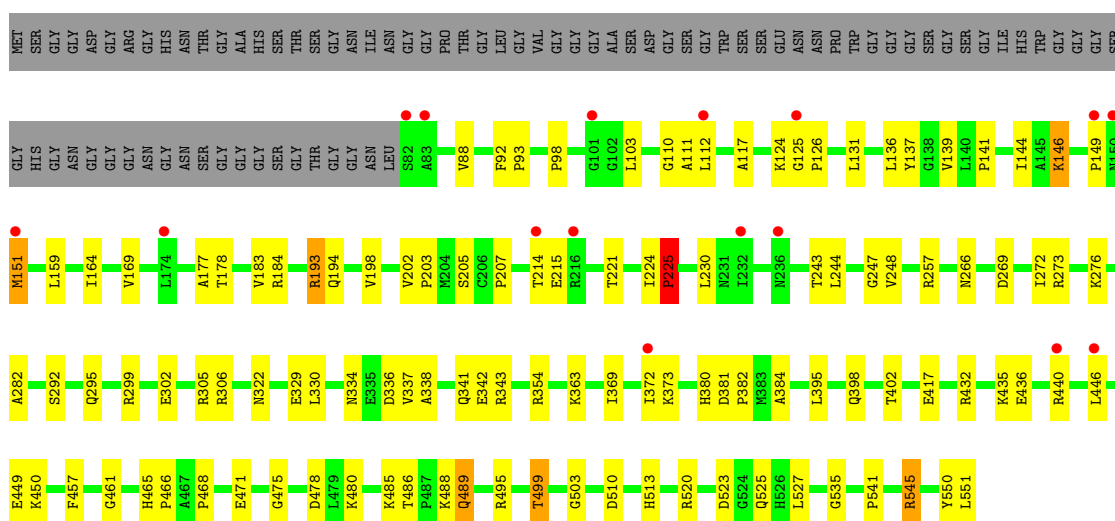
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	112	Total	O	0	0
			112	112		
4	B	23	Total	O	0	0
			23	23		
4	C	70	Total	O	0	0
			70	70		
4	D	14	Total	O	0	0
			14	14		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

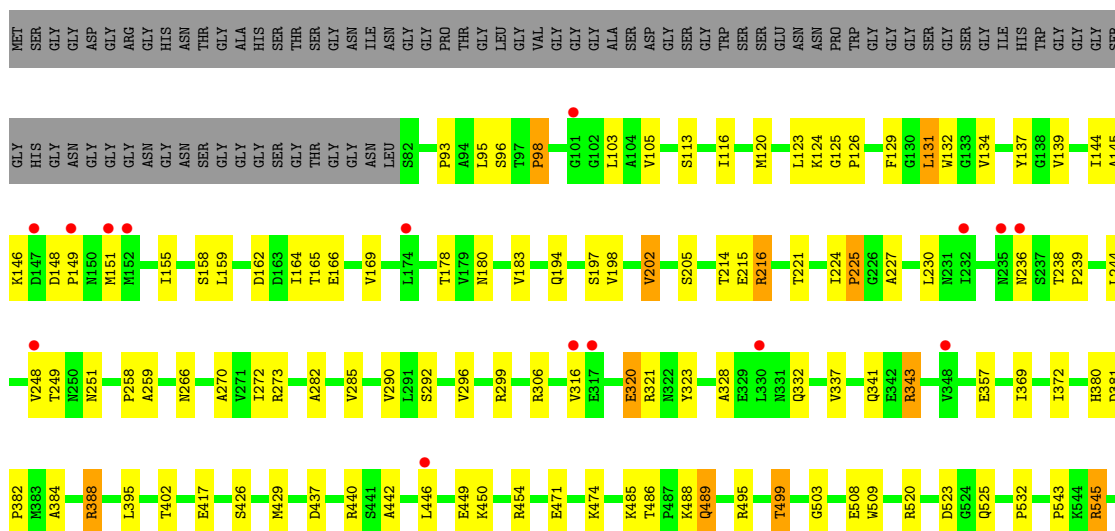
#### • Molecule 1: Colicin E3

Chain A: 



#### • Molecule 1: Colicin E3

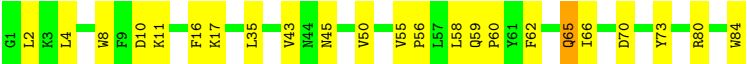
Chain C: 



Y550  
L551

- Molecule 2: Colicin E3 immunity protein

Chain B:



- Molecule 2: Colicin E3 immunity protein

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 27.8	EDS
Estimated twinning fraction	0.478 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 87291 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8791	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.38	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 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	70	0	0	2	0
4	D	14	0	0	0	0
All	All	8791	0	8320	207	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (207) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:C:306:ARG:NH1	1:C:306:ARG:HG2	2.10	0.66
2:B:59:GLN:HE22	2:B:66:ILE:H	1.42	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:488:LYS:HE2	1:C:489:GLN:HE22	1.62	0.65
1:C:169:VAL:HG11	1:C:282:ALA:HB3	1.79	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:D:35:LEU:HD11	2:D:58:LEU:HD21	1.83	0.60
1:C:525:GLN:HG3	4:C:633:HOH:O	2.02	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
2:B:59:GLN:HE22	2:B:66:ILE:N	2.03	0.56
1:A:146:LYS:HE2	1:A:146:LYS:O	2.06	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
1:C:486:THR:HG21	1:C:495:ARG:HE	1.71	0.55
2:B:8:TRP:HB3	2:B:73:TYR:CD2	2.41	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:C:205:SER:HB2	2:D:60:PRO:HG3	1.89	0.54
1:A:98:PRO:HG3	1:A:103:LEU:HD21	1.88	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:C:124:LYS:O	1:C:125:GLY:C	2.48	0.52
1:A:520:ARG:HE	1:A:523:ASP:HB3	1.75	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:489:GLN:HE21	1:C:495:ARG:NH1	2.07	0.52
1:A:330:LEU:HD21	1:A:436:GLU:HG3	1.90	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:545:ARG:CB	1:A:545:ARG:HH11	2.22	0.51
1:A:266:ASN:HD22	1:A:299:ARG:HH11	1.56	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:C:221:THR:HA	1:C:230:LEU:O	2.14	0.48
2:B:35:LEU:HD11	2:B:58:LEU:HD21	1.96	0.48
1:A:475:GLY:HA3	1:A:535:GLY:HA3	1.96	0.48
1:A:372:ILE:HG23	1:A:373:LYS:N	2.29	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:381:ASP:OD2	1:A:384:ALA:HB2	2.13	0.47
1:C:485:LYS:HZ1	1:C:551:LEU:HD21	1.79	0.47
1:A:440:ARG:HG3	1:A:440:ARG:HH11	1.80	0.47
1:A:257:ARG:NH2	4:A:702:HOH:O	2.47	0.47
1:C:369:ILE:O	1:C:372:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:545:ARG:HH11	1:C:545:ARG:HB3	1.79	0.47
1:C:216:ARG:HD3	1:C:216:ARG:H	1.80	0.47
1:A:292:SER:OG	1:A:295:GLN:HG3	2.14	0.47
1:C:485:LYS:HZ2	1:C:551:LEU:HD21	1.79	0.46
1:C:146:LYS:HB3	1:C:149:PRO:HG3	1.97	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:A:380:HIS:C	1:A:382:PRO:HD3	2.36	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:486:THR:CG2	1:C:495:ARG:HE	2.30	0.45
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: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
1:C:523:ASP:OD1	1:C:525:GLN:HB2	2.17	0.45
1:C:272:ILE:HD12	1:C:272:ILE:N	2.32	0.45
3:A:602:CIT:H22	4:A:699:HOH:O	2.16	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:124:LYS:O	1:A:125:GLY:C	2.54	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:446:LEU:HD13	1:A:446:LEU:C	2.37	0.44
1:A:302:GLU:HA	1:A:302:GLU:OE1	2.17	0.44
1:C:388:ARG:HH11	1:C:388:ARG:CB	2.26	0.44
1:C:146:LYS:HA	1:C:151:MET:CE	2.48	0.44
1:A:110:GLY:O	1:A:111:ALA:C	2.56	0.44
1:C:380:HIS:C	1:C:382:PRO:HD3	2.39	0.43
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:71:ASN:HB2	2:D:73:TYR:CE1	2.54	0.43
2:D:32:MET:HE1	2:D:43:VAL:HG22	2.00	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:485:LYS:NZ	1:C:551:LEU:CD2	2.79	0.43
1:C:113:SER:HB3	1:C:116:ILE:HD13	2.00	0.43
2:D:59:GLN:N	2:D:60:PRO:CD	2.82	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
1:C:144:ILE:HD11	1:C:290:VAL:HG11	2.00	0.42
2:B:11:LYS:HG3	2:B:70:ASP:O	2.19	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:178:THR:CG2	2:B:65:GLN:HE21	2.32	0.42
1:A:248:VAL:O	1:A:248:VAL:HG23	2.20	0.42
1:C:440:ARG:HH11	1:C:440:ARG:HG3	1.85	0.42
1:A:334:ASN:ND2	1:A:432:ARG:HH11	2.17	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:214:THR:CG2	1:C:215:GLU:H	2.20	0.42
1:A:178:THR:CG2	2:B:65:GLN:NE2	2.82	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:446:LEU:HD13	1:A:446:LEU:O	2.19	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:465:HIS:HA	1:A:466:PRO:HD3	1.93	0.41
1:C:520:ARG:HE	1:C:523:ASP:CB	2.34	0.41
1:A:457:PHE:CZ	2:B:2:LEU:HD22	2.55	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
1:C:105:VAL:HG13	4:C:664:HOH:O	2.21	0.41
1:A:177:ALA:HB3	2:B:65:GLN:HG2	2.03	0.41
1:A:146:LYS:H	1:A:146:LYS:HE2	1.85	0.41
1:A:334:ASN:HA	1:A:334:ASN:HD22	1.69	0.41
1:C:131:LEU:HD13	1:C:259:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:159:LEU:CD1	1:C:164:ILE:HD11	2.51	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:A:136:LEU:HD11	1:A:198:VAL:HG13	2.02	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

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	468/551 (85%)	450 (96%)	15 (3%)	3 (1%)	33	39
1	C	468/551 (85%)	447 (96%)	17 (4%)	4 (1%)	25	26
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%)	33	39

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
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%)	38	50
1	C	378/422 (90%)	360 (95%)	18 (5%)	35	46
2	B	76/76 (100%)	75 (99%)	1 (1%)	80	91
2	D	76/76 (100%)	75 (99%)	1 (1%)	80	91
All	All	908/996 (91%)	871 (96%)	37 (4%)	41	55

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 chains 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	-	12,12,12	1.89	2 (16%)	17,17,17	1.88	4 (23%)
3	CIT	C	601	-	12,12,12	1.84	2 (16%)	17,17,17	1.90	5 (29%)

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	-	-	0/16/16/16	0/0/0/0
3	CIT	C	601	-	-	0/16/16/16	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	C2-C3	4.66	1.59	1.53
3	A	602	CIT	C2-C3	4.61	1.59	1.53
3	A	602	CIT	C4-C3	3.65	1.58	1.53
3	C	601	CIT	C4-C3	3.29	1.58	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	CIT	O5-C6-C3	-4.10	116.55	122.20
3	A	602	CIT	O5-C6-C3	-3.98	116.70	122.20
3	C	601	CIT	O6-C6-O5	-3.72	112.06	123.76
3	A	602	CIT	O6-C6-O5	-3.66	112.24	123.76
3	C	601	CIT	O7-C3-C2	2.48	114.21	109.22
3	A	602	CIT	O7-C3-C2	2.46	114.19	109.22
3	C	601	CIT	C3-C2-C1	2.29	119.33	113.77
3	A	602	CIT	C3-C2-C1	2.29	119.31	113.77
3	C	601	CIT	C4-C3-C6	-2.02	105.43	110.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	470/551 (85%)	0.48	16 (3%) 43 53	27, 49, 81, 100	0
1	C	470/551 (85%)	0.47	15 (3%) 45 55	26, 49, 79, 101	0
2	B	84/84 (100%)	0.22	0 100 100	32, 44, 61, 64	0
2	D	84/84 (100%)	0.23	0 100 100	31, 43, 60, 70	0
All	All	1108/1270 (87%)	0.44	31 (2%) 50 60	26, 48, 80, 101	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	83	ALA	4.6
1	A	82	SER	4.1
1	A	149	PRO	3.7
1	A	101	GLY	3.6
1	A	446	LEU	3.4
1	A	112	LEU	3.3
1	C	149	PRO	3.2
1	A	150	ASN	3.1
1	A	174	LEU	3.1
1	C	101	GLY	3.0
1	C	151	MET	2.9
1	A	216	ARG	2.8
1	C	236	ASN	2.8
1	C	317	GLU	2.7
1	A	125	GLY	2.6
1	A	372	ILE	2.5
1	C	174	LEU	2.5
1	C	330	LEU	2.5
1	C	248	VAL	2.5
1	C	152	MET	2.4
1	C	446	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	348	VAL	2.2
1	C	316	VAL	2.2
1	A	440	ARG	2.1
1	A	151	MET	2.1
1	C	147	ASP	2.1
1	C	232	ILE	2.1
1	A	236	ASN	2.0
1	A	214	THR	2.0
1	A	232	ILE	2.0
1	C	235	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CIT	C	601	13/13	0.32	10.03	140,140,141,141	0
3	CIT	A	602	13/13	0.29	8.14	139,140,142,142	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.