



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2017 – 09:30 PM EDT

PDB ID : 3SPB  
Title : Unliganded E. Cloacae MurA  
Authors : Zhu, J.-Y.; Yang, Y.; Schonbrunn, E.  
Deposited on : unknown  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

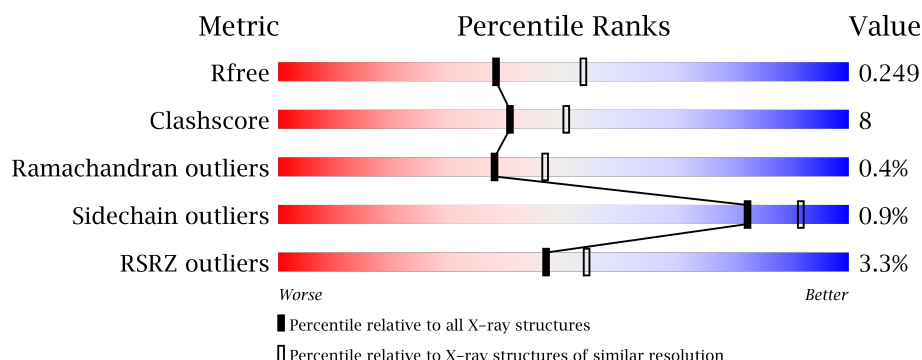
# 1 Overall quality at a glance

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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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. 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	419	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>17%</div> </div> </div>
1	B	419	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>21%</div> </div> </div>
1	C	419	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
1	D	419	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13229 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 UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	1	0	0
			3142	1976	554	598	14			
1	B	419	Total	C	N	O	S	1	0	0
			3142	1976	554	598	14			
1	C	419	Total	C	N	O	S	1	0	0
			3142	1976	554	598	14			
1	D	419	Total	C	N	O	S	1	0	0
			3142	1976	554	598	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	IAS	ASN	SEE REMARK 999	UNP P33038
B	67	IAS	ASN	SEE REMARK 999	UNP P33038
C	67	IAS	ASN	SEE REMARK 999	UNP P33038
D	67	IAS	ASN	SEE REMARK 999	UNP P33038

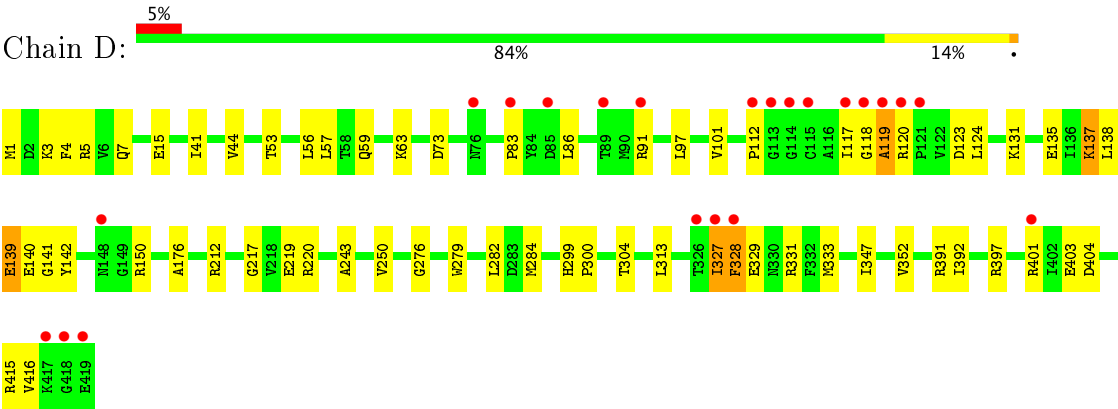
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	192	Total	O	0	0
			192	192		
2	B	163	Total	O	0	0
			163	163		
2	C	150	Total	O	0	0
			150	150		
2	D	156	Total	O	0	0
			156	156		



- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.14Å 101.22Å 213.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.30 19.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.92-2.30) 99.5 (19.92-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.37 (at 2.30Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.200 , 0.250 0.200 , 0.249	Depositor DCC
$R_{free}$ test set	1178 reflections (1.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13229	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: IAS

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	0.49	0/3178	0.88	0/4305
1	B	0.49	0/3178	0.89	1/4305 (0.0%)
1	C	0.47	0/3178	0.89	0/4305
1	D	0.47	0/3178	0.89	0/4305
All	All	0.48	0/12712	0.88	1/17220 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	GLU	N-CA-C	5.16	124.93	111.00

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	3142	0	3216	47	0
1	B	3142	0	3216	72	0
1	C	3142	0	3216	37	0
1	D	3142	0	3216	62	0
2	A	192	0	0	3	0
2	B	163	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	150	0	0	0	0
2	D	156	0	0	4	0
All	All	13229	0	12864	209	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 8.

All (209) 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:C:120:ARG:HB2	1:C:121:PRO:HD2	1.48	0.95
1:D:3:LYS:HG3	1:D:416:VAL:HG23	1.48	0.92
1:D:138:LEU:O	1:D:139:GLU:HG3	1.75	0.86
1:A:15:GLU:HG2	1:A:250:VAL:HB	1.61	0.82
1:D:7:GLN:NE2	2:D:571:HOH:O	2.13	0.81
1:B:139:GLU:HB3	1:B:142:TYR:CE2	2.18	0.79
1:D:3:LYS:HG3	1:D:416:VAL:CG2	2.13	0.78
1:A:403:GLU:HG3	2:A:426:HOH:O	1.86	0.74
1:B:317:ALA:O	1:B:356:GLY:HA3	1.88	0.73
2:B:569:HOH:O	1:D:131:LYS:HD2	1.87	0.73
1:D:304:THR:HB	1:D:327:ILE:HG13	1.71	0.71
1:C:333:MET:O	1:C:336:PRO:HD2	1.91	0.71
1:B:335:VAL:HB	1:B:336:PRO:HD3	1.74	0.67
1:B:287:LYS:HD2	2:B:490:HOH:O	1.93	0.66
1:B:335:VAL:HG11	1:B:347:ILE:HD11	1.76	0.66
1:D:135:GLU:HB2	2:D:482:HOH:O	1.95	0.65
1:D:91:ARG:HH11	1:D:91:ARG:HG3	1.62	0.65
1:C:353:ILE:N	1:C:353:ILE:HD12	2.10	0.64
1:A:333:MET:HE2	2:D:609:HOH:O	1.97	0.64
1:D:397:ARG:HG3	1:D:397:ARG:HH21	1.63	0.63
1:A:285:HIS:HB2	1:A:287:LYS:HE2	1.79	0.63
1:B:124:LEU:HD22	1:D:117:ILE:HD12	1.80	0.62
1:D:347:ILE:HD13	1:D:352:VAL:HG13	1.82	0.62
1:A:282:LEU:HD23	1:A:282:LEU:C	2.20	0.61
1:D:56:LEU:HD23	1:D:56:LEU:C	2.20	0.61
1:C:101:VAL:HG21	1:C:145:ALA:HB3	1.82	0.60
1:A:313:LEU:C	1:A:313:LEU:HD23	2.22	0.60
1:B:334:HIS:HB3	1:B:372:ALA:HB1	1.85	0.59
1:C:276:GLY:HA3	1:C:279:TRP:NE1	2.16	0.59
1:C:150:ARG:NH1	1:C:219:GLU:HA	2.16	0.59
1:D:97:LEU:O	1:D:101:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:VAL:HG21	1:B:110:SER:O	2.03	0.58
1:A:91:ARG:HE	1:A:112:PRO:HG3	1.68	0.58
1:C:3:LYS:NZ	1:C:418:GLY:HA3	2.18	0.58
1:D:347:ILE:CD1	1:D:352:VAL:HG22	2.34	0.58
1:A:334:HIS:HB3	1:A:372:ALA:HB1	1.86	0.57
1:C:9:PRO:HB3	1:C:359:LYS:HE3	1.86	0.57
1:A:336:PRO:O	1:A:340:ARG:HG3	2.04	0.57
1:B:117:ILE:CG2	1:D:131:LYS:HE3	2.35	0.57
1:C:276:GLY:HA3	1:C:279:TRP:CE2	2.39	0.57
1:B:150:ARG:NH1	1:B:219:GLU:HA	2.20	0.56
1:A:335:VAL:HB	1:A:336:PRO:HD3	1.85	0.56
1:A:324:THR:HG23	1:A:351:THR:HG22	1.86	0.56
1:A:97:LEU:O	1:A:101:VAL:HG23	2.06	0.56
1:C:126:ILE:HG12	1:C:143:VAL:HG21	1.88	0.56
1:D:91:ARG:NH1	1:D:91:ARG:HG3	2.20	0.56
1:D:15:GLU:HG2	1:D:250:VAL:HB	1.88	0.56
1:D:118:GLY:O	1:D:119:ALA:HB3	2.06	0.56
1:B:288:ARG:CG	1:B:289:PRO:HD2	2.36	0.55
1:B:370:LEU:HD11	1:B:399:TYR:CD1	2.42	0.55
1:A:288:ARG:HG3	1:A:289:PRO:HD2	1.87	0.55
1:B:51:ASP:O	1:B:55:LYS:HG3	2.07	0.55
1:A:3:LYS:HB2	1:A:416:VAL:CG2	2.36	0.55
1:D:131:LYS:HE2	2:D:517:HOH:O	2.07	0.55
1:B:324:THR:HG23	1:B:351:THR:HG22	1.89	0.55
1:B:140:GLU:CD	1:D:131:LYS:HZ3	2.10	0.55
1:A:91:ARG:HH11	1:A:91:ARG:HG3	1.72	0.55
1:D:313:LEU:HD23	1:D:313:LEU:C	2.28	0.54
1:B:313:LEU:HD23	1:B:313:LEU:C	2.27	0.54
1:D:176:ALA:O	1:D:217:GLY:HA3	2.06	0.54
1:B:64:VAL:HG22	1:B:72:ILE:CD1	2.38	0.54
1:D:138:LEU:C	1:D:139:GLU:HG3	2.27	0.54
1:B:124:LEU:HD22	1:D:117:ILE:CD1	2.38	0.54
1:D:83:PRO:HG2	1:D:86:LEU:HD12	1.88	0.54
1:B:363:ALA:O	1:B:387:THR:HG23	2.08	0.53
1:C:64:VAL:HG22	1:C:72:ILE:CD1	2.38	0.53
1:C:330:ASN:ND2	1:C:333:MET:SD	2.78	0.53
1:B:370:LEU:CD1	1:B:395:ILE:HA	2.39	0.53
1:B:366:MET:HG3	1:B:391:ARG:HD3	1.90	0.53
1:D:401:ARG:HG2	1:D:404:ASP:OD2	2.08	0.53
1:B:370:LEU:HD11	1:B:399:TYR:HD1	1.74	0.53
1:D:219:GLU:O	1:D:220:ARG:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:GLY:HA3	1:D:279:TRP:CE2	2.45	0.52
1:D:282:LEU:HD23	1:D:282:LEU:C	2.29	0.52
1:A:59:GLN:OE1	1:A:86:LEU:HD12	2.10	0.52
1:D:112:PRO:HG2	1:D:120:ARG:HH22	1.75	0.52
1:B:120:ARG:HB3	1:B:123:ASP:OD2	2.11	0.51
1:C:120:ARG:HB2	1:C:121:PRO:CD	2.32	0.51
1:D:4:PHE:CD2	1:D:392:ILE:HG21	2.45	0.51
1:D:63:LYS:HB2	1:D:73:ASP:HB3	1.93	0.51
1:B:315:LEU:HD23	1:B:354:CYS:HB3	1.92	0.50
1:A:248:LYS:HD2	1:A:283:ASP:OD2	2.11	0.50
1:C:288:ARG:HH12	1:C:358:GLU:HG3	1.75	0.50
1:B:282:LEU:C	1:B:282:LEU:HD23	2.32	0.50
1:B:3:LYS:HE2	1:B:390:ASP:OD1	2.12	0.50
1:C:353:ILE:CD1	1:C:353:ILE:N	2.73	0.50
1:D:150:ARG:NH1	1:D:219:GLU:HA	2.27	0.50
1:C:138:LEU:CD2	1:C:143:VAL:HG23	2.42	0.50
1:B:243:ALA:HA	1:B:284:MET:CG	2.42	0.49
1:A:57:LEU:O	1:A:62:THR:HB	2.11	0.49
1:B:150:ARG:NH1	1:B:219:GLU:O	2.38	0.49
1:B:1:MET:CE	1:B:391:ARG:HG2	2.42	0.49
1:D:150:ARG:HG2	1:D:150:ARG:HH21	1.76	0.49
1:D:397:ARG:NH2	1:D:397:ARG:HG3	2.25	0.49
1:A:126:ILE:HG23	1:A:136:ILE:HG21	1.95	0.49
1:B:137:LYS:HG2	1:D:137:LYS:HG3	1.94	0.49
1:A:320:THR:HA	1:A:354:CYS:O	2.13	0.49
1:B:320:THR:HA	1:B:354:CYS:O	2.13	0.49
1:C:29:LEU:HD23	1:C:41:ILE:HD12	1.95	0.49
1:D:328:PHE:HB2	1:D:331:ARG:HG3	1.94	0.49
1:A:91:ARG:NH1	1:A:91:ARG:HG3	2.28	0.49
1:C:256:PRO:HG2	1:C:276:GLY:O	2.13	0.48
1:D:117:ILE:O	1:D:117:ILE:HD12	2.13	0.48
1:C:1:MET:HE3	1:C:391:ARG:HH12	1.79	0.48
1:A:51:ASP:O	1:A:55:LYS:HG3	2.14	0.48
1:A:370:LEU:HD13	1:A:394:HIS:O	2.13	0.48
1:B:243:ALA:HA	1:B:284:MET:HG3	1.95	0.48
1:B:117:ILE:HG22	1:D:131:LYS:HE3	1.95	0.48
1:A:243:ALA:HA	1:A:284:MET:CG	2.44	0.47
1:C:315:LEU:HD21	1:C:345:ALA:HB2	1.96	0.47
1:B:314:ASN:HB3	1:B:354:CYS:HB2	1.95	0.47
1:B:9:PRO:HD3	1:B:384:GLU:HA	1.95	0.47
1:B:25:ALA:O	1:B:29:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:GLU:OE2	1:B:137:LYS:HE3	2.15	0.47
1:B:84:TYR:O	1:B:88:LYS:HB3	2.13	0.47
1:B:347:ILE:HD12	1:B:352:VAL:HG22	1.96	0.47
1:D:327:ILE:HG22	1:D:328:PHE:N	2.30	0.47
1:C:4:PHE:CD2	1:C:392:ILE:HG21	2.50	0.46
1:C:64:VAL:HG22	1:C:72:ILE:HD12	1.97	0.46
1:D:347:ILE:HD12	1:D:352:VAL:HG22	1.97	0.46
1:A:140:GLU:O	1:A:142:TYR:HD1	1.99	0.46
1:D:53:THR:O	1:D:57:LEU:HG	2.16	0.46
1:A:289:PRO:HG2	1:A:317:ALA:HA	1.98	0.46
1:B:335:VAL:HG21	1:B:347:ILE:HD11	1.97	0.46
1:D:56:LEU:HD23	1:D:56:LEU:O	2.14	0.46
1:A:176:ALA:O	1:A:217:GLY:HA3	2.15	0.45
1:B:4:PHE:HB2	1:B:392:ILE:HG21	1.98	0.45
1:A:282:LEU:HD23	1:A:283:ASP:N	2.30	0.45
1:A:135:GLU:O	1:A:145:ALA:HA	2.17	0.45
1:A:77:VAL:HB	1:A:104:PHE:CZ	2.52	0.45
1:D:243:ALA:HA	1:D:284:MET:CG	2.46	0.45
1:D:1:MET:CE	1:D:391:ARG:NH2	2.80	0.45
2:A:509:HOH:O	1:D:329:GLU:HA	2.15	0.45
1:C:138:LEU:HD23	1:C:143:VAL:HG23	1.98	0.45
1:B:158:MET:SD	1:D:117:ILE:HD11	2.56	0.45
1:C:139:GLU:HB2	1:C:142:TYR:CE2	2.51	0.45
1:B:118:GLY:O	1:B:119:ALA:HB3	2.17	0.45
1:B:267:ARG:HD3	2:B:494:HOH:O	2.16	0.45
1:D:150:ARG:NH1	1:D:219:GLU:O	2.50	0.45
1:C:150:ARG:NH1	1:C:219:GLU:HG2	2.32	0.44
1:D:1:MET:HE3	1:D:391:ARG:NH2	2.33	0.44
1:A:3:LYS:HB2	1:A:416:VAL:HG22	1.98	0.44
1:C:321:GLY:HA2	1:D:212:ARG:NH1	2.33	0.44
1:A:4:PHE:CD2	1:A:392:ILE:HG21	2.53	0.44
1:C:335:VAL:HB	1:C:347:ILE:HD11	1.98	0.44
1:D:139:GLU:OE1	1:D:142:TYR:HB2	2.18	0.44
1:A:299:HIS:CG	1:A:300:PRO:HA	2.52	0.44
1:B:138:LEU:HD23	1:B:143:VAL:HG23	2.00	0.43
1:B:282:LEU:HD23	1:B:283:ASP:N	2.33	0.43
1:A:317:ALA:O	1:A:356:GLY:HA3	2.18	0.43
1:B:332:PHE:CZ	1:B:352:VAL:HG23	2.53	0.43
1:B:4:PHE:CD2	1:B:392:ILE:HG21	2.53	0.43
1:A:62:THR:HG22	1:A:64:VAL:CG2	2.48	0.43
1:B:2:ASP:HB3	1:B:392:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:GLU:O	1:C:140:GLU:C	2.57	0.43
1:A:204:LYS:HB2	1:A:216:GLU:HB3	2.01	0.43
1:C:3:LYS:HZ2	1:C:418:GLY:HA3	1.81	0.43
1:A:36:GLU:O	1:A:75:SER:HB3	2.19	0.43
1:A:87:VAL:HB	1:A:93:SER:OG	2.19	0.43
1:D:299:HIS:CG	1:D:300:PRO:HA	2.53	0.43
1:B:129:LEU:HA	1:B:129:LEU:HD23	1.92	0.43
1:A:370:LEU:CD1	1:A:395:ILE:HA	2.49	0.43
1:C:370:LEU:CD1	1:C:395:ILE:HA	2.49	0.42
1:C:150:ARG:HH11	1:C:219:GLU:HG2	1.85	0.42
1:D:276:GLY:HA3	1:D:279:TRP:NE1	2.34	0.42
1:B:288:ARG:HG3	1:B:289:PRO:HD2	2.01	0.42
1:B:289:PRO:HG2	1:B:317:ALA:HA	2.00	0.42
1:B:295:ARG:HD3	2:B:559:HOH:O	2.20	0.42
1:D:150:ARG:HG2	1:D:150:ARG:NH2	2.33	0.42
1:D:328:PHE:CD2	1:D:331:ARG:HD2	2.55	0.42
1:A:364:GLN:HG2	1:A:388:VAL:HB	2.00	0.42
1:B:152:LYS:N	1:B:152:LYS:HD2	2.34	0.42
1:B:288:ARG:HG2	1:B:289:PRO:HD2	2.00	0.42
1:A:91:ARG:HD3	2:A:590:HOH:O	2.19	0.42
1:B:64:VAL:HG22	1:B:72:ILE:HD12	2.01	0.42
1:D:403:GLU:OE2	1:D:415:ARG:NE	2.51	0.42
1:B:56:LEU:HD23	1:B:56:LEU:C	2.40	0.42
1:B:188:GLU:HA	1:B:189:PRO:HD3	1.94	0.42
1:B:347:ILE:HD13	1:B:352:VAL:HG13	2.02	0.42
1:B:372:ALA:O	1:B:376:LEU:HG	2.19	0.42
1:B:83:PRO:O	1:B:87:VAL:HG13	2.19	0.42
1:C:314:ASN:HB3	1:C:354:CYS:HB2	2.01	0.42
1:B:3:LYS:HG2	1:B:390:ASP:OD1	2.19	0.41
1:A:401:ARG:HB3	1:A:404:ASP:OD2	2.20	0.41
1:C:9:PRO:HD3	1:C:384:GLU:OE1	2.20	0.41
1:D:124:LEU:HD23	1:D:124:LEU:HA	1.92	0.41
1:B:315:LEU:HD21	1:B:345:ALA:HB2	2.02	0.41
1:D:5:ARG:NH1	1:D:416:VAL:HG11	2.35	0.41
1:A:157:VAL:HG22	1:A:183:GLU:HG3	2.02	0.41
1:A:244:ILE:HD12	1:A:382:ILE:HD13	2.03	0.41
1:B:176:ALA:O	1:B:217:GLY:HA3	2.21	0.41
1:C:256:PRO:HG3	1:C:280:ILE:HG12	2.02	0.41
1:C:348:GLU:O	1:C:349:SER:HB3	2.20	0.41
1:D:59:GLN:NE2	1:D:59:GLN:O	2.54	0.41
1:B:248:LYS:HA	1:B:282:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:MET:CE	1:B:391:ARG:NH1	2.84	0.41
1:B:9:PRO:HB3	1:B:382:ILE:O	2.19	0.41
1:C:243:ALA:HA	1:C:284:MET:CG	2.51	0.41
1:B:299:HIS:CG	1:B:300:PRO:HA	2.56	0.41
1:B:64:VAL:HG12	1:B:65:GLU:N	2.36	0.41
1:B:120:ARG:HG2	1:B:122:VAL:HG12	2.02	0.41
1:B:138:LEU:CD2	1:B:143:VAL:HG23	2.51	0.41
1:B:111:LEU:O	1:B:141:GLY:HA2	2.21	0.40
1:A:188:GLU:HA	1:A:189:PRO:HD3	1.91	0.40
1:D:41:ILE:HG22	1:D:44:VAL:CG2	2.51	0.40
1:A:416:VAL:HG23	1:A:416:VAL:O	2.22	0.40
1:A:116:ALA:HB1	1:C:159:ASP:OD1	2.21	0.40
1:D:120:ARG:HB2	1:D:123:ASP:OD2	2.21	0.40
1:D:141:GLY:O	1:D:142:TYR:CD1	2.74	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	415/419 (99%)	408 (98%)	7 (2%)	0	100	100
1	B	415/419 (99%)	397 (96%)	16 (4%)	2 (0%)	32	39
1	C	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	D	415/419 (99%)	399 (96%)	11 (3%)	5 (1%)	15	16
All	All	1660/1676 (99%)	1606 (97%)	47 (3%)	7 (0%)	38	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	327	ILE

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Mol	Chain	Res	Type
1	D	119	ALA
1	B	315	LEU
1	D	140	GLU
1	D	328	PHE
1	D	333	MET
1	B	392	ILE

### 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	329/329 (100%)	328 (100%)	1 (0%)	94	97
1	B	329/329 (100%)	324 (98%)	5 (2%)	70	83
1	C	329/329 (100%)	325 (99%)	4 (1%)	75	87
1	D	329/329 (100%)	327 (99%)	2 (1%)	89	95
All	All	1316/1316 (100%)	1304 (99%)	12 (1%)	82	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	417	LYS
1	B	85	ASP
1	B	216	GLU
1	B	220	ARG
1	B	229	LEU
1	B	307	GLN
1	C	42	GLN
1	C	220	ARG
1	C	229	LEU
1	C	307	GLN
1	D	137	LYS
1	D	139	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	IAS	A	67	1	3,7,8	0.76	0	2,8,10	1.08	0
1	IAS	B	67	1	3,7,8	0.87	0	2,8,10	1.14	0
1	IAS	C	67	1	3,7,8	0.88	0	2,8,10	1.03	0
1	IAS	D	67	1	3,7,8	0.77	0	2,8,10	0.96	0

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
1	IAS	A	67	1	-	0/3/7/8	0/0/0/0
1	IAS	B	67	1	-	0/3/7/8	0/0/0/0
1	IAS	C	67	1	-	0/3/7/8	0/0/0/0
1	IAS	D	67	1	-	0/3/7/8	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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, 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	418/419 (99%)	-0.27	8 (1%) 67 73	14, 26, 45, 77	1 (0%)
1	B	418/419 (99%)	-0.11	11 (2%) 56 63	12, 28, 51, 84	1 (0%)
1	C	418/419 (99%)	-0.11	14 (3%) 47 54	17, 29, 49, 82	1 (0%)
1	D	418/419 (99%)	-0.03	22 (5%) 27 34	16, 29, 55, 84	1 (0%)
All	All	1672/1676 (99%)	-0.13	55 (3%) 47 54	12, 28, 51, 84	4 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	119	ALA	9.6
1	D	418	GLY	8.9
1	C	119	ALA	7.9
1	A	113	GLY	7.6
1	C	115	CYS	7.4
1	B	419	GLU	6.6
1	D	118	GLY	6.1
1	C	116	ALA	5.6
1	D	419	GLU	5.4
1	A	419	GLU	5.3
1	A	418	GLY	5.0
1	C	114	GLY	4.9
1	C	113	GLY	4.9
1	D	328	PHE	4.5
1	C	419	GLU	4.3
1	C	118	GLY	3.9
1	D	112	PRO	3.9
1	B	417	LYS	3.8
1	D	113	GLY	3.7
1	D	120	ARG	3.6
1	D	327	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	120	ARG	3.6
1	D	115	CYS	3.6
1	B	418	GLY	3.6
1	C	327	ILE	3.3
1	A	417	LYS	3.2
1	D	89	THR	3.2
1	D	117	ILE	3.1
1	B	328	PHE	3.1
1	B	119	ALA	3.0
1	C	117	ILE	3.0
1	A	119	ALA	2.9
1	C	85	ASP	2.9
1	A	114	GLY	2.9
1	B	1	MET	2.8
1	D	114	GLY	2.8
1	D	401	ARG	2.8
1	D	91	ARG	2.7
1	D	83	PRO	2.6
1	B	91	ARG	2.6
1	C	121	PRO	2.5
1	B	139	GLU	2.4
1	D	148	ASN	2.4
1	D	417	LYS	2.4
1	D	121	PRO	2.4
1	C	76	ASN	2.4
1	D	326	THR	2.4
1	B	401	ARG	2.3
1	A	121	PRO	2.2
1	B	113	GLY	2.1
1	A	120	ARG	2.1
1	D	76	ASN	2.1
1	B	140	GLU	2.0
1	C	328	PHE	2.0
1	D	85	ASP	2.0

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

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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	IAS	B	67	8/9	0.94	0.12	-	18,25,28,30	0
1	IAS	A	67	8/9	0.93	0.22	-	33,35,38,38	0
1	IAS	D	67	8/9	0.88	0.18	-	40,42,43,44	0
1	IAS	C	67	8/9	0.91	0.18	-	36,40,42,42	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.