



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:37 am BST

PDB ID : 1TF0  
Title : Crystal structure of the GA module complexed with human serum albumin  
Authors : Lejon, S.; Svensson, S.; Bjorck, L.; Frick, I.-M.; Wikstrom, M.  
Deposited on : 2004-05-26  
Resolution : 2.70 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

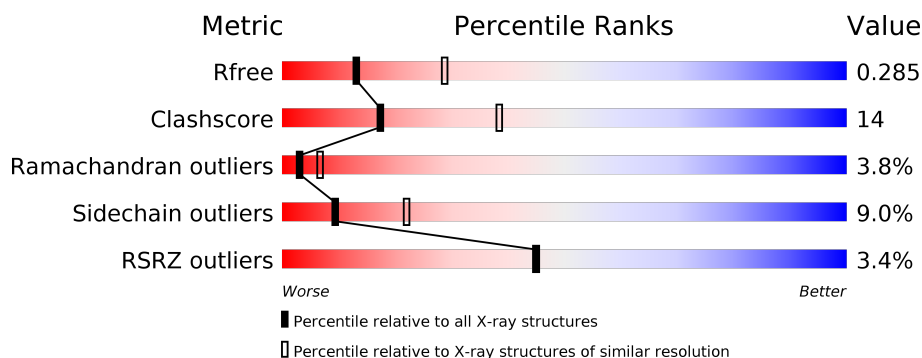
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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	572	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>24%</div> <div>5%</div> <div>••</div> </div> </div>
2	B	53	<div> <div>66%</div> <div>25%</div> <div>•</div> <div>6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DKA	A	1001	-	-	-	X
3	DKA	A	1002	-	-	X	-
3	DKA	A	1003	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4902 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.

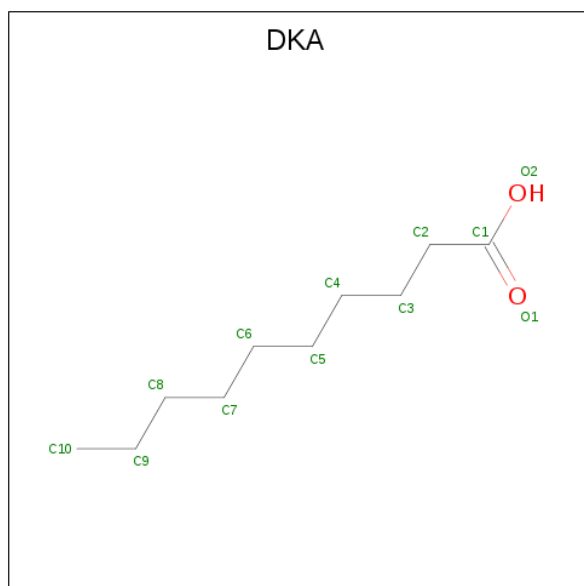
- Molecule 1 is a protein called Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	0	0
			4439	2803	748	848	40			

- Molecule 2 is a protein called Peptostreptococcal albumin-binding protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	53	Total	C	N	O	0	0	0
			414	266	70	78			

- Molecule 3 is DECANOIC ACID (three-letter code: DKA) (formula: C<sub>10</sub>H<sub>20</sub>O<sub>2</sub>).



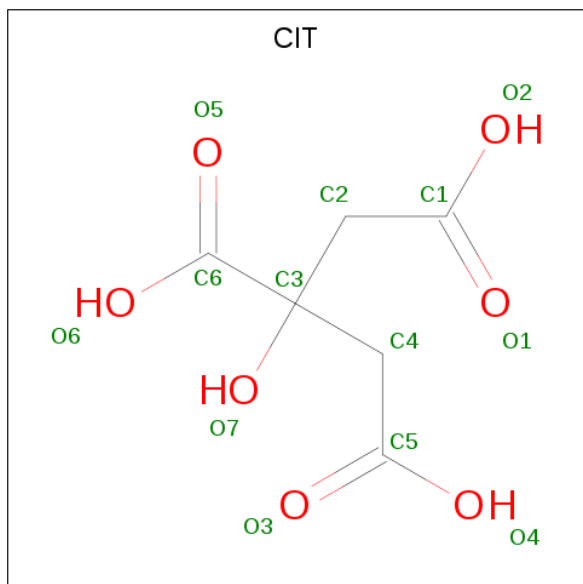
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	10	2		
3	A	1	Total	C	O	0	0
			12	10	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	10	2		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).

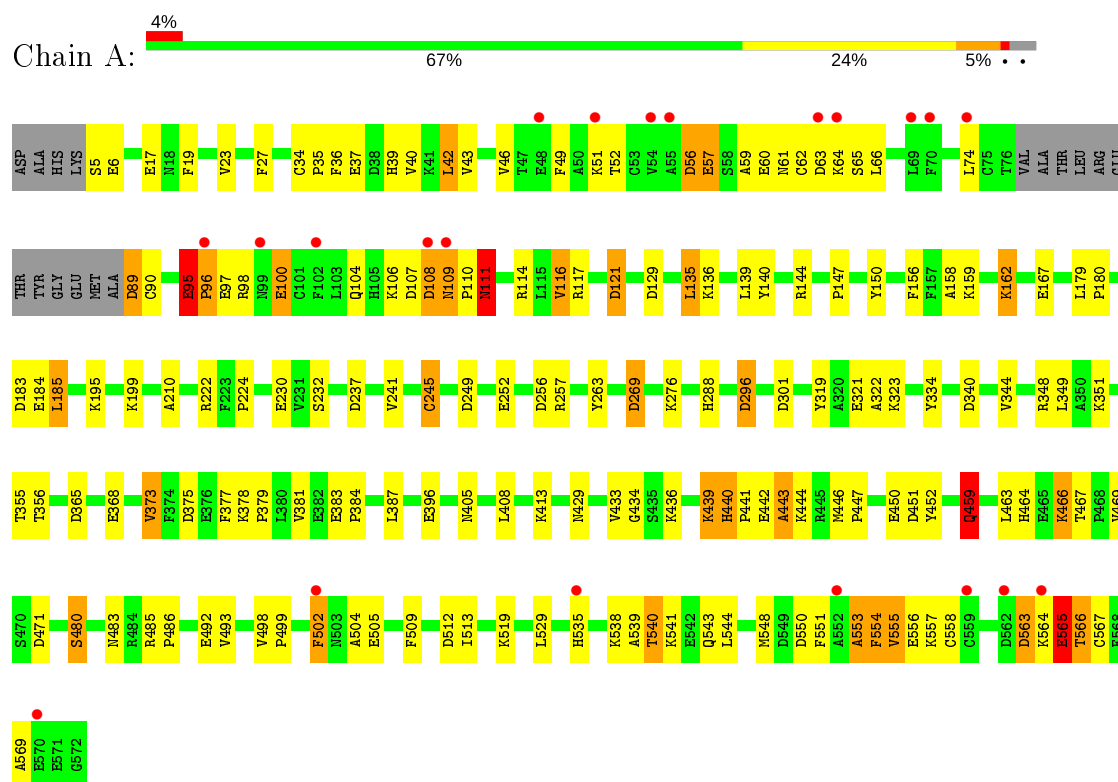


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		

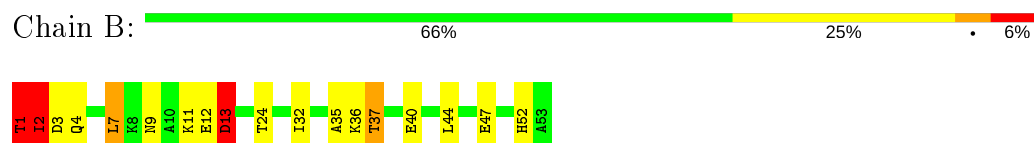
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Serum albumin



#### • Molecule 2: Peptostreptococcal albumin-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.30Å 134.80Å 122.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.00 – 2.70 66.00 – 2.49	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.00-2.70) 99.5 (66.00-2.49)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.53 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0001	Depositor
R, $R_{free}$	0.249 , 0.295 0.234 , 0.285	Depositor DCC
$R_{free}$ test set	1408 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.4	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4902	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: DKA, 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	0.79	1/4526 (0.0%)	0.91	21/6104 (0.3%)
2	B	0.82	0/419	0.98	2/564 (0.4%)
All	All	0.79	1/4945 (0.0%)	0.92	23/6668 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	459	GLN	CG-CD	5.17	1.62	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	ASP	CB-CG-OD2	7.77	125.29	118.30
1	A	269	ASP	CB-CG-OD2	7.10	124.69	118.30
2	B	13	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	56	ASP	CB-CG-OD2	6.48	124.14	118.30
1	A	256	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	451	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	129	ASP	CB-CG-OD2	6.25	123.92	118.30
1	A	512	ASP	CB-CG-OD2	6.17	123.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ASP	CB-CG-OD2	6.13	123.81	118.30
1	A	375	ASP	CB-CG-OD2	6.11	123.80	118.30
2	B	3	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	89	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	107	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	108	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	563	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	348	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	348	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	340	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	365	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	183	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	550	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	296	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	63	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ASN	Peptide
1	A	56	ASP	Peptide
1	A	95	GLU	Peptide
2	B	1	THR	Peptide

## 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	4439	0	4348	106	0
2	B	414	0	428	21	0
3	A	36	0	57	22	0
4	A	13	0	5	2	0
All	All	4902	0	4838	134	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 14.

All (134) 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)
3:A:1003:DKA:O1	3:A:1003:DKA:H103	1.47	1.12
1:A:413:LYS:NZ	1:A:540:THR:HG21	1.71	1.05
1:A:413:LYS:HZ1	1:A:540:THR:HG21	1.28	0.96
1:A:351:LYS:HZ3	3:A:1002:DKA:H41	1.28	0.95
2:B:32:ILE:HD13	2:B:44:LEU:HD12	1.56	0.88
1:A:351:LYS:NZ	3:A:1002:DKA:H41	1.92	0.84
2:B:32:ILE:CD1	2:B:44:LEU:HD12	2.07	0.84
3:A:1003:DKA:O1	3:A:1003:DKA:C10	2.26	0.83
3:A:1001:DKA:C10	3:A:1002:DKA:H101	2.11	0.81
1:A:263:TYR:OH	2:B:37:THR:HG21	1.86	0.75
2:B:35:ALA:O	2:B:36:LYS:HB2	1.88	0.73
1:A:509:PHE:HB3	1:A:513:ILE:CD1	2.19	0.73
1:A:139:LEU:HD21	1:A:158:ALA:HB2	1.73	0.71
1:A:538:LYS:O	1:A:540:THR:OG1	2.09	0.70
1:A:42:LEU:O	1:A:46:VAL:HG23	1.94	0.68
1:A:210:ALA:HA	3:A:1002:DKA:H62	1.74	0.68
1:A:356:THR:HG21	1:A:373:VAL:HG13	1.76	0.67
3:A:1003:DKA:C1	3:A:1003:DKA:H103	2.25	0.67
2:B:12:GLU:O	2:B:13:ASP:CB	2.42	0.67
1:A:257:ARG:HE	3:A:1003:DKA:H42	1.60	0.67
1:A:539:ALA:HB1	1:A:543:GLN:HE22	1.61	0.66
1:A:540:THR:HG22	1:A:544:LEU:HD11	1.78	0.66
3:A:1001:DKA:H101	3:A:1002:DKA:H101	1.79	0.65
1:A:563:ASP:O	1:A:565:GLU:N	2.30	0.64
1:A:502:PHE:HA	1:A:535:HIS:CD2	2.32	0.64
1:A:540:THR:HG22	1:A:544:LEU:CD1	2.28	0.64
1:A:502:PHE:HA	1:A:535:HIS:NE2	2.12	0.63
1:A:539:ALA:O	1:A:540:THR:HG23	1.97	0.63
3:A:1001:DKA:H102	3:A:1002:DKA:H91	1.81	0.62
3:A:1003:DKA:H102	4:A:2001:CIT:O3	1.99	0.62
1:A:199:LYS:HE2	3:A:1003:DKA:O2	2.00	0.62
3:A:1001:DKA:C10	3:A:1002:DKA:C10	2.78	0.62
1:A:413:LYS:CE	1:A:540:THR:HG21	2.31	0.61
1:A:480:SER:HA	3:A:1002:DKA:O1	1.99	0.61
1:A:429:ASN:ND2	1:A:459:GLN:OE1	2.26	0.61
1:A:249:ASP:HB3	1:A:252:GLU:CD	2.21	0.61
1:A:95:GLU:HB3	1:A:96:PRO:CD	2.30	0.60
1:A:351:LYS:NZ	3:A:1002:DKA:C4	2.63	0.59
2:B:37:THR:HG22	2:B:40:GLU:H	1.68	0.58
1:A:464:HIS:CE1	1:A:469:VAL:H	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ILE:O	2:B:2:ILE:HG22	2.03	0.58
1:A:301:ASP:OD2	1:A:301:ASP:C	2.42	0.58
1:A:39:HIS:O	1:A:43:VAL:HG23	2.04	0.58
1:A:463:LEU:O	1:A:466:LYS:HD3	2.04	0.58
1:A:439:LYS:HD3	1:A:440:HIS:ND1	2.19	0.57
1:A:111:ASN:C	1:A:111:ASN:HD22	2.07	0.57
2:B:2:ILE:HD12	2:B:4:GLN:HE21	1.70	0.56
1:A:27:PHE:CD2	1:A:74:LEU:HD21	2.41	0.56
1:A:483:ASN:HD22	1:A:486:PRO:HG2	1.71	0.56
2:B:32:ILE:HD11	2:B:44:LEU:HD12	1.87	0.56
1:A:34:CYS:SG	1:A:35:PRO:HD2	2.47	0.55
1:A:539:ALA:C	1:A:540:THR:OG1	2.43	0.55
1:A:257:ARG:HE	3:A:1003:DKA:C4	2.21	0.54
1:A:249:ASP:HB3	1:A:252:GLU:CG	2.39	0.53
2:B:1:THR:O	2:B:2:ILE:HG12	2.08	0.53
1:A:464:HIS:HE1	1:A:469:VAL:H	1.56	0.52
1:A:554:PHE:HA	1:A:557:LYS:HB3	1.92	0.52
1:A:95:GLU:C	1:A:97:GLU:N	2.63	0.52
2:B:35:ALA:O	2:B:36:LYS:CB	2.55	0.52
1:A:19:PHE:O	1:A:23:VAL:HG23	2.10	0.51
1:A:548:MET:HE2	1:A:548:MET:HA	1.91	0.51
1:A:230:GLU:OE1	2:B:35:ALA:O	2.28	0.51
1:A:377:PHE:O	1:A:381:VAL:HG23	2.11	0.51
1:A:95:GLU:O	1:A:97:GLU:N	2.44	0.51
2:B:44:LEU:C	2:B:44:LEU:HD13	2.32	0.50
1:A:34:CYS:SG	1:A:35:PRO:CD	3.00	0.49
1:A:466:LYS:HZ2	1:A:467:THR:HG23	1.76	0.49
1:A:114:ARG:HB2	1:A:116:VAL:HG23	1.94	0.48
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.53	0.48
1:A:439:LYS:HD3	1:A:440:HIS:CE1	2.49	0.48
2:B:12:GLU:O	2:B:13:ASP:HB2	2.14	0.48
1:A:509:PHE:HB3	1:A:513:ILE:HD12	1.95	0.48
1:A:90:CYS:O	1:A:98:ARG:HG3	2.13	0.48
1:A:36:PHE:O	1:A:40:VAL:HG23	2.14	0.48
1:A:135:LEU:HD11	1:A:162:LYS:HB2	1.96	0.48
1:A:110:PRO:O	1:A:111:ASN:CB	2.62	0.47
1:A:405:ASN:HA	1:A:408:LEU:HD12	1.96	0.47
2:B:2:ILE:CD1	2:B:4:GLN:HE21	2.27	0.47
1:A:321:GLU:O	2:B:52:HIS:HD2	1.96	0.47
1:A:555:VAL:O	1:A:557:LYS:N	2.47	0.47
1:A:195:LYS:HE3	4:A:2001:CIT:H21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:MET:N	1:A:447:PRO:CD	2.78	0.47
1:A:104:GLN:O	1:A:106:LYS:N	2.47	0.47
1:A:156:PHE:CZ	1:A:288:HIS:CD2	3.03	0.47
1:A:551:PHE:O	1:A:553:ALA:N	2.39	0.46
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.97	0.46
3:A:1001:DKA:H102	3:A:1002:DKA:C9	2.44	0.46
1:A:111:ASN:ND2	1:A:111:ASN:O	2.48	0.46
2:B:9:ASN:O	2:B:12:GLU:O	2.34	0.46
1:A:140:TYR:O	1:A:144:ARG:HG2	2.16	0.46
1:A:95:GLU:C	1:A:97:GLU:H	2.20	0.46
1:A:554:PHE:O	1:A:558:CYS:HB2	2.16	0.45
1:A:222:ARG:HH12	3:A:1003:DKA:H102	1.82	0.45
1:A:433:VAL:CG1	1:A:434:GLY:N	2.80	0.45
1:A:109:ASN:HA	1:A:110:PRO:HD3	1.78	0.45
1:A:179:LEU:HB2	1:A:180:PRO:CD	2.46	0.45
1:A:150:TYR:OH	3:A:1003:DKA:H21	2.17	0.45
1:A:387:LEU:HD22	1:A:485:ARG:NH1	2.32	0.45
1:A:230:GLU:OE2	2:B:37:THR:HB	2.17	0.45
1:A:61:ASN:OD1	1:A:64:LYS:HE2	2.17	0.45
1:A:97:GLU:O	1:A:100:GLU:N	2.48	0.45
1:A:466:LYS:NZ	1:A:467:THR:HG23	2.32	0.44
1:A:95:GLU:HB3	1:A:96:PRO:HD3	1.99	0.44
2:B:12:GLU:O	2:B:13:ASP:HB3	2.17	0.44
1:A:49:PHE:O	1:A:52:THR:OG1	2.29	0.44
1:A:554:PHE:CD2	1:A:554:PHE:C	2.91	0.44
1:A:529:LEU:HB2	1:A:548:MET:CE	2.48	0.44
1:A:436:LYS:HE2	1:A:452:TYR:CD1	2.53	0.43
1:A:548:MET:HE2	1:A:551:PHE:CD2	2.54	0.43
1:A:257:ARG:NE	3:A:1003:DKA:H42	2.31	0.43
2:B:2:ILE:HD12	2:B:4:GLN:NE2	2.32	0.43
1:A:378:LYS:HB2	1:A:379:PRO:HD3	2.01	0.42
1:A:413:LYS:HZ3	1:A:540:THR:HG21	1.71	0.42
3:A:1003:DKA:O1	3:A:1003:DKA:C9	2.68	0.42
1:A:444:LYS:O	1:A:447:PRO:HD2	2.20	0.41
1:A:529:LEU:HD13	1:A:548:MET:HE3	2.02	0.41
1:A:383:GLU:N	1:A:384:PRO:HD2	2.34	0.41
3:A:1001:DKA:O1	3:A:1001:DKA:H41	2.20	0.41
1:A:349:LEU:HD22	1:A:377:PHE:CD1	2.56	0.41
2:B:7:LEU:HD21	2:B:11:LYS:HE3	2.01	0.41
1:A:319:TYR:CZ	1:A:323:LYS:HD3	2.55	0.41
1:A:433:VAL:HG13	1:A:434:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASP:N	1:A:121:ASP:OD1	2.54	0.41
1:A:6:GLU:OE1	1:A:6:GLU:HA	2.21	0.41
1:A:553:ALA:O	1:A:557:LYS:N	2.54	0.41
1:A:563:ASP:C	1:A:565:GLU:H	2.24	0.40
1:A:441:PRO:O	1:A:443:ALA:N	2.54	0.40
1:A:224:PRO:HD2	1:A:296:ASP:HB3	2.02	0.40
1:A:106:LYS:HG3	1:A:147:PRO:HB2	2.03	0.40
1:A:185:LEU:HD22	1:A:185:LEU:HA	1.84	0.40
1:A:241:VAL:O	1:A:245:CYS:HB2	2.22	0.40
1:A:27:PHE:CE1	1:A:42:LEU:HD12	2.57	0.40
1:A:498:VAL:HA	1:A:499:PRO:HD3	1.94	0.40
1:A:566:THR:O	1:A:569:ALA:N	2.54	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	552/572 (96%)	493 (89%)	38 (7%)	21 (4%)	3	7
2	B	51/53 (96%)	44 (86%)	5 (10%)	2 (4%)	3	6
All	All	603/625 (96%)	537 (89%)	43 (7%)	23 (4%)	3	7

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	GLU
1	A	66	LEU
1	A	95	GLU
1	A	96	PRO
1	A	111	ASN
1	A	442	GLU

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Mol	Chain	Res	Type
1	A	443	ALA
1	A	541	LYS
1	A	564	LYS
1	A	567	CYS
2	B	2	ILE
2	B	13	ASP
1	A	167	GLU
1	A	504	ALA
1	A	60	GLU
1	A	505	GLU
1	A	553	ALA
1	A	108	ASP
1	A	322	ALA
1	A	555	VAL
1	A	556	GLU
1	A	565	GLU
1	A	116	VAL

### 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	491/503 (98%)	449 (91%)	42 (9%)	10	24
2	B	42/43 (98%)	36 (86%)	6 (14%)	3	8
All	All	533/546 (98%)	485 (91%)	48 (9%)	9	22

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	17	GLU
1	A	37	GLU
1	A	42	LEU
1	A	51	LYS
1	A	57	GLU

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Mol	Chain	Res	Type
1	A	65	SER
1	A	89	ASP
1	A	100	GLU
1	A	111	ASN
1	A	117	ARG
1	A	121	ASP
1	A	135	LEU
1	A	136	LYS
1	A	159	LYS
1	A	162	LYS
1	A	184	GLU
1	A	185	LEU
1	A	232	SER
1	A	245	CYS
1	A	269	ASP
1	A	276	LYS
1	A	334	TYR
1	A	344	VAL
1	A	355	THR
1	A	368	GLU
1	A	373	VAL
1	A	396	GLU
1	A	439	LYS
1	A	440	HIS
1	A	450	GLU
1	A	459	GLN
1	A	466	LYS
1	A	480	SER
1	A	492	GLU
1	A	493	VAL
1	A	502	PHE
1	A	519	LYS
1	A	540	THR
1	A	554	PHE
1	A	565	GLU
1	A	566	THR
2	B	1	THR
2	B	2	ILE
2	B	7	LEU
2	B	24	THR
2	B	37	THR
2	B	47	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	111	ASN
1	A	146	HIS
1	A	196	GLN
1	A	338	HIS
1	A	385	GLN
1	A	464	HIS
1	A	483	ASN
1	A	543	GLN
2	B	4	GLN
2	B	9	ASN
2	B	42	ASN
2	B	52	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	DKA	A	1003	-	8,11,11	0.40	0	7,11,11	0.57	0
4	CIT	A	2001	-	3,12,12	0.61	0	3,17,17	1.59	1 (33%)
3	DKA	A	1001	-	8,11,11	0.13	0	7,11,11	0.76	0
3	DKA	A	1002	-	8,11,11	0.38	0	7,11,11	0.59	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
3	DKA	A	1003	-	-	6/7/9/9	-
4	CIT	A	2001	-	-	2/6/16/16	-
3	DKA	A	1001	-	-	5/7/9/9	-
3	DKA	A	1002	-	-	2/7/9/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	CIT	C3-C4-C5	-2.13	111.57	114.98

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	DKA	C1-C2-C3-C4
4	A	2001	CIT	C6-C3-C4-C5
3	A	1003	DKA	C3-C4-C5-C6
3	A	1001	DKA	C5-C6-C7-C8
3	A	1003	DKA	C5-C6-C7-C8
3	A	1001	DKA	C3-C4-C5-C6
3	A	1002	DKA	C5-C6-C7-C8
3	A	1003	DKA	C4-C5-C6-C7
4	A	2001	CIT	O7-C3-C4-C5
3	A	1002	DKA	C6-C7-C8-C9
3	A	1003	DKA	C7-C8-C9-C10
3	A	1003	DKA	C6-C7-C8-C9
3	A	1001	DKA	C7-C8-C9-C10
3	A	1001	DKA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	1001	DKA	C1-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	DKA	11	0
4	A	2001	CIT	2	0
3	A	1001	DKA	6	0
3	A	1002	DKA	10	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, 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	556/572 (97%)	0.23	21 (3%) 40 39	17, 31, 44, 73	0
2	B	53/53 (100%)	-0.18	0 100 100	27, 31, 36, 38	0
All	All	609/625 (97%)	0.19	21 (3%) 45 45	17, 31, 43, 73	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	564	LYS	6.5
1	A	109	ASN	4.8
1	A	535	HIS	4.3
1	A	559	CYS	4.1
1	A	70	PHE	3.9
1	A	96	PRO	3.4
1	A	69	LEU	3.4
1	A	74	LEU	3.2
1	A	64	LYS	3.2
1	A	552	ALA	3.1
1	A	48	GLU	3.0
1	A	54	VAL	3.0
1	A	51	LYS	2.7
1	A	63	ASP	2.5
1	A	99	ASN	2.5
1	A	102	PHE	2.4
1	A	55	ALA	2.2
1	A	570	GLU	2.2
1	A	502	PHE	2.2
1	A	562	ASP	2.1
1	A	108	ASP	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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DKA	A	1003	12/12	0.70	0.29	51,52,57,60	0
3	DKA	A	1001	12/12	0.71	0.41	50,62,75,77	0
4	CIT	A	2001	13/13	0.77	0.30	84,88,94,94	0
3	DKA	A	1002	12/12	0.85	0.25	50,58,62,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.