



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:16 AM UTC

PDB ID : 1TF0 / pdb_00001tf0
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

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

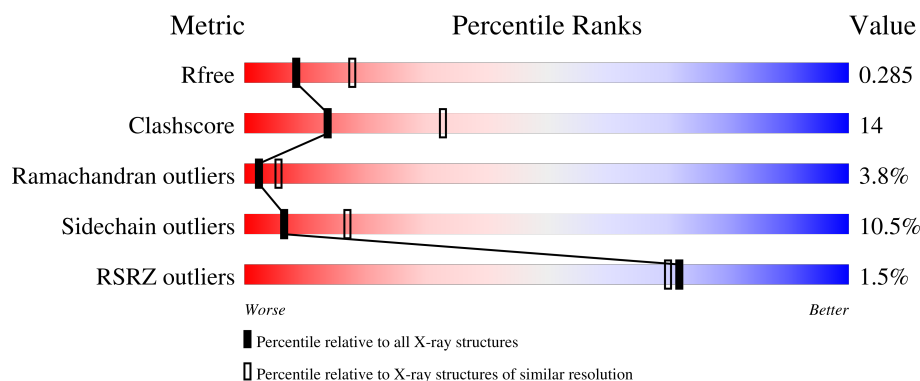
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	572	% 67% 24% 5% • •
2	B	53	2% 66% 21% 9% •

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	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.

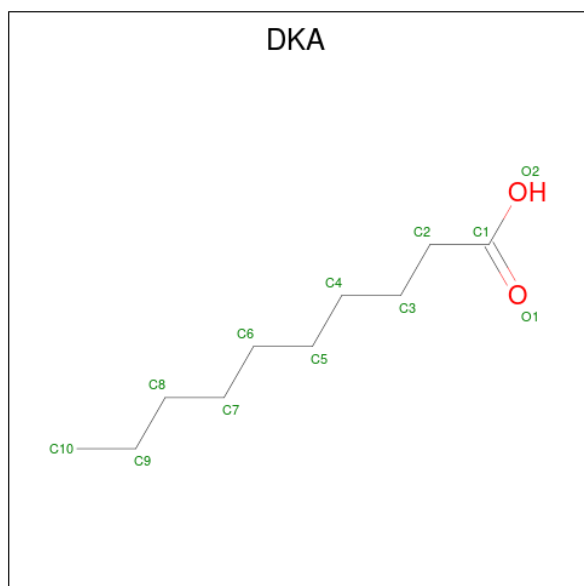
- Molecule 1 is a protein called Serum albumin.

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 (CCD ID: DKA) (formula: $C_{10}H_{20}O_2$).



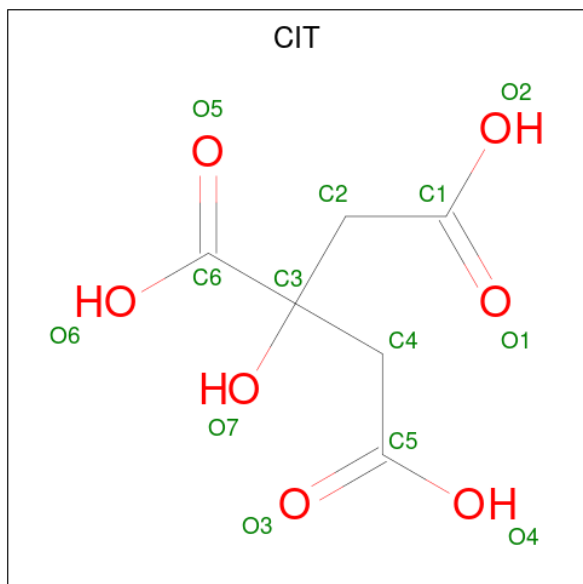
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	10	2		
3	A	1	Total	C	O	0	0
			12	10	2		

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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 (CCD ID: CIT) (formula: $C_6H_8O_7$).

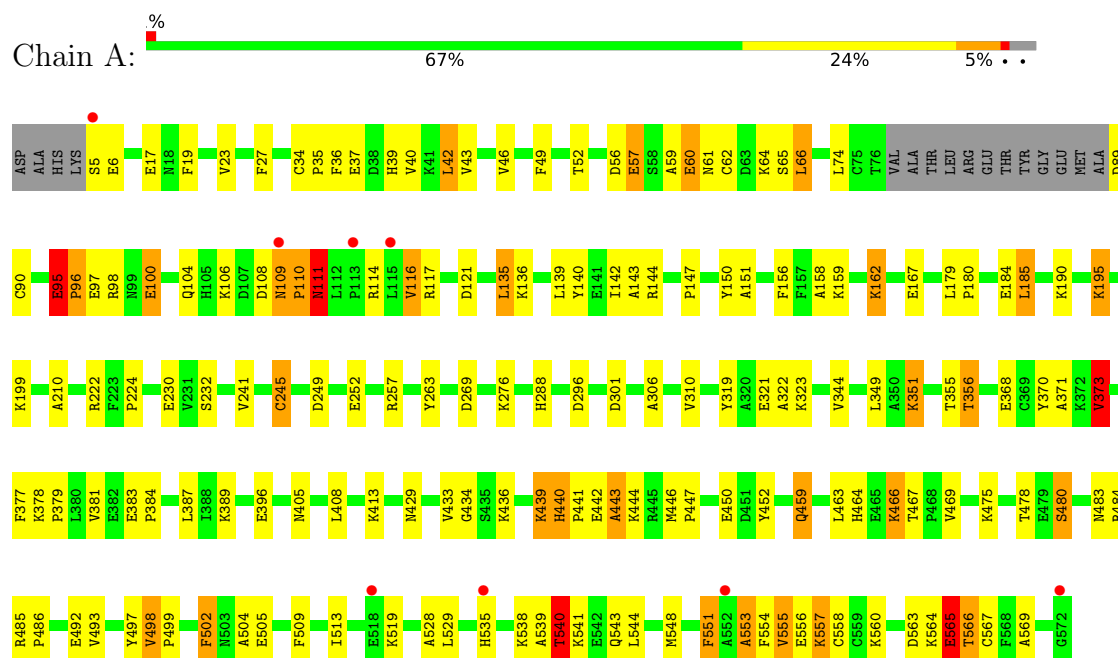


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		

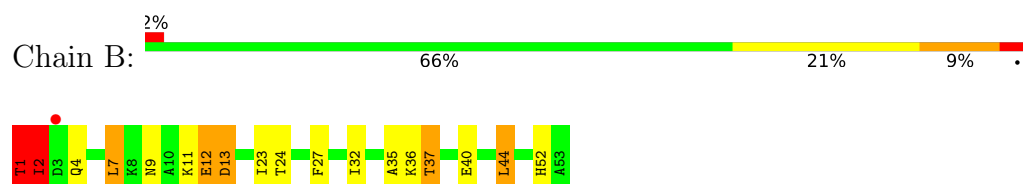
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: 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, α , β , γ	96.30Å 134.80Å 122.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.00 – 2.70 65.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.00-2.70) 99.9 (65.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.53 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0001	Depositor
R, R_{free}	0.249 , 0.295 0.235 , 0.285	Depositor DCC
R_{free} test set	1408 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4902	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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, DKA

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	0.98	1/4526 (0.0%)	1.10	9/6104 (0.1%)
2	B	1.05	0/419	1.20	2/564 (0.4%)
All	All	0.99	1/4945 (0.0%)	1.11	11/6668 (0.2%)

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	306	ALA	CA-CB	-5.27	1.45	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	12	GLU	N-CA-C	-8.22	98.16	110.24
1	A	373	VAL	N-CA-CB	6.86	118.13	110.51
1	A	373	VAL	CB-CA-C	-6.44	103.63	111.88
1	A	540	THR	N-CA-C	6.43	118.08	107.73
1	A	110	PRO	N-CA-C	6.24	122.21	113.53
1	A	551	PHE	N-CA-C	-5.76	104.69	110.97
1	A	497	TYR	CA-C-N	-5.67	118.51	122.59
1	A	497	TYR	C-N-CA	-5.67	118.51	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	528	ALA	N-CA-C	-5.58	105.20	112.23
2	B	27	PHE	N-CA-C	-5.17	105.64	111.28
1	A	66	LEU	N-CA-C	5.05	121.56	110.80

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 ⓘ

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	113	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	141	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 (141) 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:H103	3:A:1003:DKA:O1	1.47	1.12
1:A:413:LYS:NZ	1:A:540:THR:HG21	1.71	1.05
1:A:351:LYS:HZ3	3:A:1002:DKA:H41	1.18	1.02
1:A:413:LYS:HZ1	1:A:540:THR:HG21	1.28	0.96
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:509:PHE:HB3	1:A:513:ILE:CD1	2.19	0.73
2:B:35:ALA:O	2:B:36:LYS:HB2	1.88	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:H103	3:A:1003:DKA:C1	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
1:A:249:ASP:HB3	1:A:252:GLU:CD	2.21	0.65
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
1:A:301:ASP:OD2	1:A:301:ASP:C	2.42	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:111:ASN:HD22	1:A:111:ASN:C	2.07	0.61
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:95:GLU:HB3	1:A:96:PRO:CD	2.30	0.60
1:A:539:ALA:C	1:A:540:THR:OG1	2.43	0.59
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
2:B:2:ILE:O	2:B:2:ILE:HG22	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:C	1:A:97:GLU:N	2.63	0.56
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:548:MET:HA	1:A:548:MET:HE2	1.88	0.55
2:B:44:LEU:C	2:B:44:LEU:HD13	2.32	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
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: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
1:A:95:GLU:C	1:A:97:GLU:H	2.20	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:554:PHE:C	1:A:554:PHE:CD2	2.91	0.48
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.53	0.48
1:A:114:ARG:HB2	1:A:116:VAL:HG23	1.94	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:90:CYS:O	1:A:98:ARG:HG3	2.13	0.48
1:A:509:PHE:HB3	1:A:513:ILE:HD12	1.95	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ASN:O	1:A:111:ASN:ND2	2.48	0.46
3:A:1001:DKA:H102	3:A:1002:DKA:C9	2.44	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: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:563:ASP:C	1:A:565:GLU:H	2.24	0.45
1:A:150:TYR:OH	3:A:1003:DKA:H21	2.17	0.45
1:A:230:GLU:OE2	2:B:37:THR:HB	2.17	0.45
1:A:387:LEU:HD22	1:A:485:ARG:NH1	2.32	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:95:GLU:HB3	1:A:96:PRO:HD3	1.99	0.44
1:A:466:LYS:NZ	1:A:467:THR:HG23	2.32	0.44
1:A:483:ASN:O	1:A:484:ARG:C	2.59	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: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:370:TYR:O	1:A:371:ALA:C	2.62	0.43
1:A:548:MET:HE1	1:A:551:PHE:CD2	2.52	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:529:LEU:HD13	1:A:548:MET:HE3	2.01	0.43
1:A:142:ILE:O	1:A:143:ALA:C	2.61	0.42
1:A:378:LYS:HB2	1:A:379:PRO:HD3	2.01	0.42
1:A:563:ASP:C	1:A:565:GLU:N	2.77	0.42
1:A:59:ALA:O	1:A:60:GLU:C	2.63	0.42
1:A:150:TYR:O	1:A:151:ALA:C	2.63	0.42
1:A:413:LYS:HZ3	1:A:540:THR:HG21	1.71	0.42
1:A:529:LEU:HB2	1:A:548:MET:HE3	2.02	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:383:GLU:N	1:A:384:PRO:HD2	2.34	0.41
1:A:349:LEU:HD22	1:A:377:PHE:CD1	2.56	0.41
3:A:1001:DKA:O1	3:A:1001:DKA:H41	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:VAL:HG13	1:A:434:GLY:N	2.36	0.41
1:A:6:GLU:OE1	1:A:6:GLU:HA	2.21	0.41
1:A:121:ASP:OD1	1:A:121:ASP:N	2.54	0.41
1:A:553:ALA:O	1:A:557:LYS:N	2.54	0.41
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:27:PHE:CE1	1:A:42:LEU:HD12	2.57	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: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%)	2	5
2	B	51/53 (96%)	44 (86%)	5 (10%)	2 (4%)	2	5
All	All	603/625 (96%)	537 (89%)	43 (7%)	23 (4%)	2	5

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%)	442 (90%)	49 (10%)	7	19
2	B	42/43 (98%)	35 (83%)	7 (17%)	2	6
All	All	533/546 (98%)	477 (90%)	56 (10%)	6	17

All (56) 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	57	GLU
1	A	65	SER

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Mol	Chain	Res	Type
1	A	89	ASP
1	A	100	GLU
1	A	111	ASN
1	A	117	ARG
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	190	LYS
1	A	195	LYS
1	A	232	SER
1	A	245	CYS
1	A	269	ASP
1	A	276	LYS
1	A	310	VAL
1	A	344	VAL
1	A	351	LYS
1	A	355	THR
1	A	356	THR
1	A	368	GLU
1	A	373	VAL
1	A	389	LYS
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	475	LYS
1	A	478	THR
1	A	480	SER
1	A	492	GLU
1	A	493	VAL
1	A	498	VAL
1	A	502	PHE
1	A	519	LYS
1	A	540	THR
1	A	557	LYS
1	A	560	LYS
1	A	565	GLU

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Mol	Chain	Res	Type
1	A	566	THR
2	B	1	THR
2	B	2	ILE
2	B	7	LEU
2	B	23	ILE
2	B	24	THR
2	B	37	THR
2	B	44	LEU

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

Mol	Chain	Res	Type
1	A	9	HIS
1	A	33	GLN
1	A	67	HIS
1	A	111	ASN
1	A	146	HIS
1	A	247	HIS
1	A	267	ASN
1	A	464	HIS
1	A	483	ASN
1	A	543	GLN
2	B	4	GLN
2	B	42	ASN
2	B	52	HIS

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

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
4	CIT	A	2001	-	12,12,12	1.08	0	17,17,17	2.20	5 (29%)
3	DKA	A	1001	-	11,11,11	0.53	0	11,11,11	1.42	2 (18%)
3	DKA	A	1002	-	11,11,11	0.77	1 (9%)	11,11,11	1.21	1 (9%)
3	DKA	A	1003	-	11,11,11	0.43	0	11,11,11	2.49	3 (27%)

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
4	CIT	A	2001	-	-	8/16/16/16	-
3	DKA	A	1001	-	-	6/9/9/9	-
3	DKA	A	1002	-	-	4/9/9/9	-
3	DKA	A	1003	-	-	6/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	DKA	O2-C1	-2.27	1.23	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	DKA	C3-C2-C1	-5.75	99.49	114.51
4	A	2001	CIT	O6-C6-C3	4.88	122.50	113.14
4	A	2001	CIT	C2-C3-C6	4.38	119.71	110.03
3	A	1003	DKA	O2-C1-C2	4.31	127.63	114.00
3	A	1001	DKA	C3-C2-C1	-3.34	105.79	114.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	DKA	O1-C1-C2	-3.33	112.53	123.09
4	A	2001	CIT	O7-C3-C2	-3.33	101.79	109.38
3	A	1002	DKA	O2-C1-C2	2.71	122.57	114.00
4	A	2001	CIT	O4-C5-C4	2.33	121.74	114.35
4	A	2001	CIT	O6-C6-O5	-2.25	116.65	123.86
3	A	1001	DKA	O1-C1-C2	-2.14	116.31	123.09

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2001	CIT	O7-C3-C6-O5
4	A	2001	CIT	O7-C3-C6-O6
3	A	1001	DKA	C5-C6-C7-C8
4	A	2001	CIT	C2-C3-C6-O6
3	A	1003	DKA	C3-C4-C5-C6
4	A	2001	CIT	C6-C3-C4-C5
3	A	1002	DKA	C5-C6-C7-C8
3	A	1003	DKA	C5-C6-C7-C8
3	A	1001	DKA	C3-C4-C5-C6
3	A	1003	DKA	C1-C2-C3-C4
3	A	1003	DKA	C4-C5-C6-C7
4	A	2001	CIT	C2-C3-C6-O5
3	A	1002	DKA	C6-C7-C8-C9
4	A	2001	CIT	O7-C3-C4-C5
3	A	1003	DKA	C7-C8-C9-C10
3	A	1003	DKA	C6-C7-C8-C9
3	A	1001	DKA	C7-C8-C9-C10
4	A	2001	CIT	C4-C3-C6-O5
4	A	2001	CIT	C4-C3-C6-O6
3	A	1001	DKA	O2-C1-C2-C3
3	A	1002	DKA	O1-C1-C2-C3
3	A	1001	DKA	O1-C1-C2-C3
3	A	1002	DKA	O2-C1-C2-C3
3	A	1001	DKA	C2-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	CIT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	DKA	6	0
3	A	1002	DKA	10	0
3	A	1003	DKA	11	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	556/572 (97%)	0.11	8 (1%) 73 72	17, 31, 44, 73	0
2	B	53/53 (100%)	0.07	1 (1%) 66 63	27, 31, 36, 38	0
All	All	609/625 (97%)	0.10	9 (1%) 72 70	17, 31, 43, 73	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	ASN	3.0
1	A	552	ALA	2.9
1	A	535	HIS	2.6
1	A	5	SER	2.3
2	B	3	ASP	2.3
1	A	113	PRO	2.3
1	A	572	GLY	2.2
1	A	115	LEU	2.1
1	A	518	GLU	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 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($\text{\AA}^2$)	Q<0.9
4	CIT	A	2001	13/13	0.66	0.18	84,88,94,94	0
3	DKA	A	1003	12/12	0.70	0.22	51,52,57,60	0
3	DKA	A	1001	12/12	0.81	0.24	50,62,75,77	0
3	DKA	A	1002	12/12	0.87	0.17	50,58,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.