



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:03 PM UTC

PDB ID : 2HAV / pdb_00002hav
Title : Apo-Human Serum Transferrin (Glycosylated)
Authors : Wally, J.; Everse, S.J.
Deposited on : 2006-06-13
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

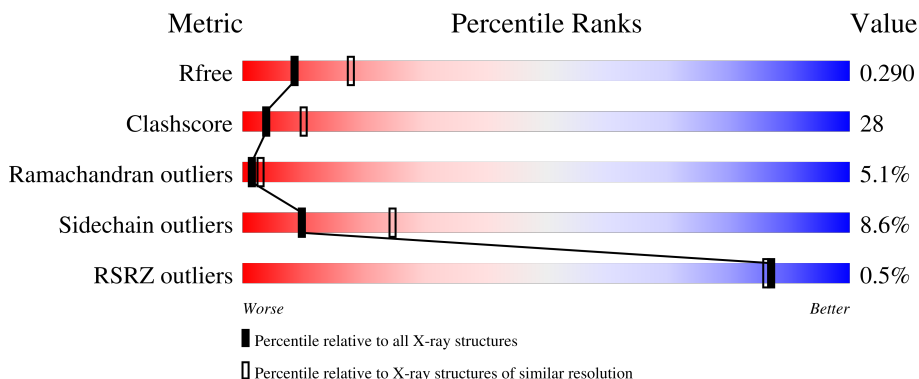
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

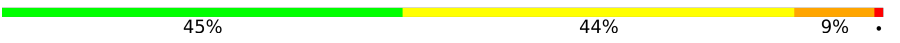
The reported resolution of this entry is 2.70 Å.

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	676	
1	B	676	

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
2	CIT	A	9202	-	-	X	-
2	CIT	A	9207	-	X	-	-
2	CIT	B	9201	-	X	-	-
2	CIT	B	9206	-	-	X	-
3	GOL	A	9103	-	-	X	-

2 Entry composition [i](#)

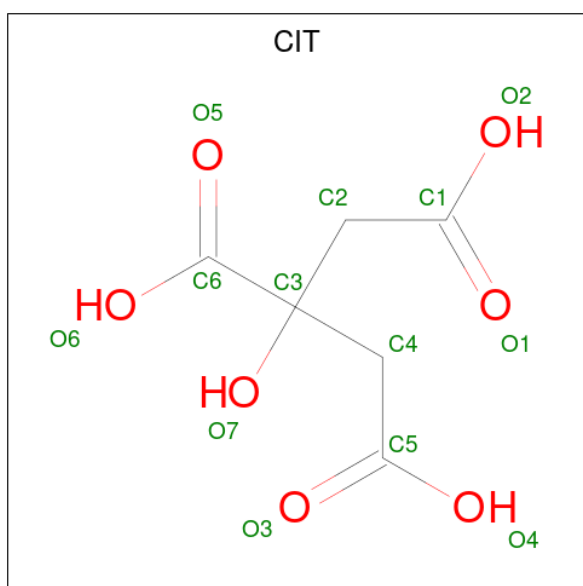
There are 3 unique types of molecules in this entry. The entry contains 10601 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	676	Total	C	N	O	S	0	0	0
			5243	3291	909	996	47			
1	B	676	Total	C	N	O	S	0	0	0
			5243	3291	909	996	47			

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

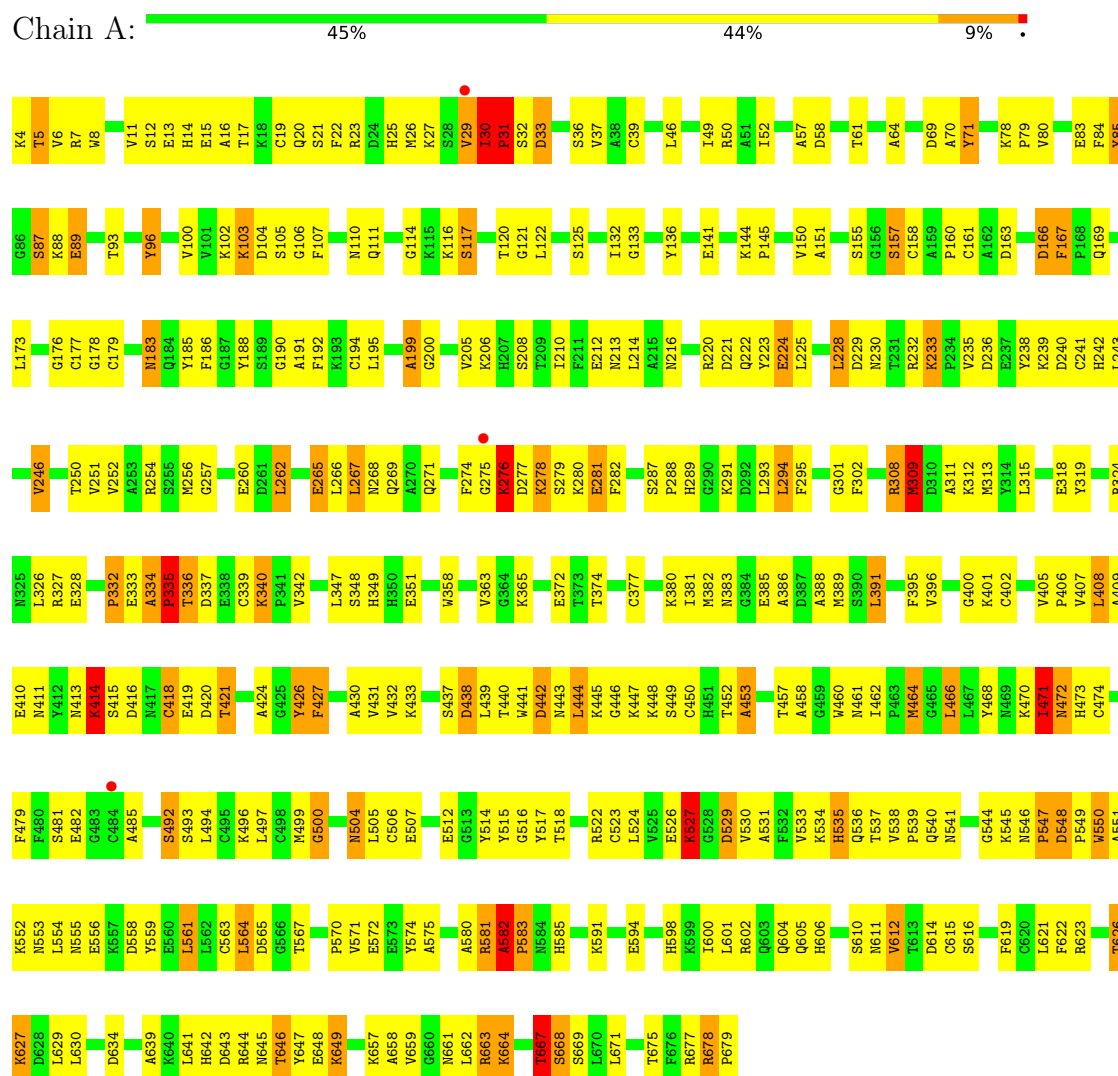


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Serotransferrin



• Molecule 1: Serotransferrin



S669	T589	E512	M443	R351	G257	T181	F107	K4
L670	G513	G513	L444	R352	G258	L182	Q108	A10
L671	Y514	Y514	K445	R353	K259	M183	M109	N110
T675	Y515	Y515	W358	W358		Q184	N110	N111
R678	G516	G516	K447	V363	L267	Y188	Q111	S12
P679	Y517	Y517	K448	V366	M268	S189	R113	E13
	F521	F521	S449	E367	Q269	G190	G114	H14
	L524	L524	V454	E367	A270	A191		E15
	V525	V525	T457	S370	Q271	K193	S117	C19
I600	E526	E526	A371	E372	F274	C194	T120	F22
L601	K527	K527	M461	A371	G275	L195	R124	H25
R602	G528	G528	L462	E372	K276	K196	S125	M26
Q603	D529	D529	P463	T378	K280	D197	A126	K27
Q604	H535	H535	M464	I381		G198	G127	S28
Q605			G465	I381	Q283	D201	W128	V29
G609	V538	V538	L466	K389	L284		M129	I30
V612	P539	P539	L467	D392	F285	F204	I130	P31
T613	Q540	Q540	Y468	D392	S286	V205	P131	S32
D614	N541	N541	M469	G393	S287	K206	I132	P35
C615	T542	T542	K470	G394	P288	H207	L135	
	G543	G543	I471	F395	H289	S208	Y136	I49
	G544	G544	N472	V396	G290	T209		
	R545	R545	H473	Y397	K291	I210		
N618	N546	N546	C474	L404	D292	F211	L139	I52
L621	P549	P549	R475	V407	L293	E212	P140	N55
R623	N550	N550	E478	L408	L294	N213	E141	
	A551	A551	F479	L408	G301	L214	P142	V60
K552	K552	K552	F480		P306	N216	K144	T61
N553	L554	L554	S481	N411	P307	K217	P145	
L554	N555	N555	E482	N412	R308		K148	Y71
N555	N556	N556	A485	N413	M309	R220	A149	L77
E556	E556	E556	P486	K414	D310	D221	V150	K78
Y559	Y559	Y559	G487	S415	A311	Q222	A151	P79
E560	E560	E560	S488	D416	K312	Y223	M152	
L561	L561	L561	K489	N417	M313	E224	F154	F84
L562	L562	L562	K490	C418	Y314	L225		Y85
C563	C563	C563	D491	D420	L315	L228	G158	G86
L564	L564	L564	S492	T421	Y319	D229	A159	S87
			S493		V320	N230	P160	K88
R568	R568	R568	K496	A424	T321	N231	D163	E89
K569	K569	K569	L497	G425	A322	R232		D90
P570	P570	P570	C498	Y426	I323	K233	D166	Q92
V571	V571	V571	M499	F427	E328	P234	P167	T93
E572	E572	E572	G500	A428		V235	Q169	F94
E573	E573	E573	S501	V429	E333	E237		Y95
Y574	Y574	Y574	N504	V432	A334	Y238	L173	A99
A575	A575	A575	L505	K433	P335	V246		V100
N576	N576	N576	K434	K434	T336	S247	G176	V101
C577	C577	C577	E506	D438	K340	H249	C177	K102
A580	A580	A580	E507	L439	P341	T250	G178	K103
R581	R581	R581	F508	T440			C179	D104
L662	L662	L662	N509	W441	H350		G179	S105
R663	R663	R663	N510	D442			S180	G106
N584	N584	N584	K511					
T667	T667	T667						
S668	S668	S668						

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.32Å 103.26Å 200.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.70) 96.1 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.232 , 0.293 0.237 , 0.290	Depositor DCC
R_{free} test set	2534 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	74.9	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10601	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: GOL, 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	0.51	0/5362	1.08	48/7247 (0.7%)
1	B	0.51	1/5362 (0.0%)	1.09	33/7247 (0.5%)
All	All	0.51	1/10724 (0.0%)	1.09	81/14494 (0.6%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	389	MET	SD-CE	-5.54	1.65	1.79

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	SER	N-CA-C	11.57	127.24	112.89
1	A	405	VAL	N-CA-C	9.35	116.86	109.19
1	B	439	LEU	N-CA-C	-9.34	95.86	109.59
1	B	415	SER	N-CA-C	9.19	125.42	109.80
1	A	85	TYR	N-CA-C	8.96	122.35	110.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	85	TYR	Sidechain

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	5243	0	5068	318	0
1	B	5243	0	5068	262	0
2	A	39	0	15	17	0
2	B	52	0	20	15	0
3	A	18	0	24	9	0
3	B	6	0	8	2	0
All	All	10601	0	10203	589	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 28.

The worst 5 of 589 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:B:108:GLN:HA	1:B:108:GLN:HE21	1.10	1.06
1:A:678:ARG:HB3	1:A:679:PRO:HD3	1.45	0.98
1:A:564:LEU:HD11	3:A:9103:GOL:H12	1.45	0.98
1:B:454:VAL:HG23	1:B:486:PRO:O	1.64	0.95
1:A:411:ASN:HD21	1:A:639:ALA:HB2	1.35	0.90

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	674/676 (100%)	552 (82%)	85 (13%)	37 (6%)	1	2
1	B	674/676 (100%)	554 (82%)	88 (13%)	32 (5%)	2	3
All	All	1348/1352 (100%)	1106 (82%)	173 (13%)	69 (5%)	1	3

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	LYS
1	A	335	PRO
1	A	336	THR
1	A	418	CYS
1	A	427	PHE

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	569/569 (100%)	512 (90%)	57 (10%)	7	19
1	B	569/569 (100%)	528 (93%)	41 (7%)	13	32
All	All	1138/1138 (100%)	1040 (91%)	98 (9%)	10	25

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	29	VAL
1	B	276	LYS
1	B	89	GLU
1	B	201	ASP
1	B	310	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	553	ASN
1	B	585	HIS
1	B	604	GLN
1	A	661	ASN
1	A	611	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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
2	CIT	B	9206	-	12,12,12	2.02	6 (50%)	17,17,17	1.53	4 (23%)
3	GOL	A	9104	-	5,5,5	0.50	0	5,5,5	1.16	1 (20%)
3	GOL	A	9103	-	5,5,5	0.59	0	5,5,5	0.75	0
2	CIT	A	9203	-	12,12,12	1.92	2 (16%)	17,17,17	1.70	5 (29%)
2	CIT	A	9207	-	12,12,12	2.45	5 (41%)	17,17,17	1.59	4 (23%)
2	CIT	B	9205	-	12,12,12	2.10	2 (16%)	17,17,17	1.28	3 (17%)
3	GOL	A	9101	-	5,5,5	0.69	0	5,5,5	0.47	0
3	GOL	B	9102	-	5,5,5	0.55	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CIT	A	9202	-	12,12,12	2.02	2 (16%)	17,17,17	1.79	5 (29%)
2	CIT	B	9204	-	12,12,12	1.78	3 (25%)	17,17,17	1.68	4 (23%)
2	CIT	B	9201	-	12,12,12	2.78	5 (41%)	17,17,17	1.84	4 (23%)

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
2	CIT	B	9206	-	-	7/16/16/16	-
3	GOL	A	9104	-	-	2/4/4/4	-
3	GOL	A	9103	-	-	0/4/4/4	-
2	CIT	A	9203	-	-	5/16/16/16	-
2	CIT	A	9207	-	-	11/16/16/16	-
2	CIT	B	9205	-	-	3/16/16/16	-
3	GOL	A	9101	-	-	2/4/4/4	-
3	GOL	B	9102	-	-	2/4/4/4	-
2	CIT	A	9202	-	-	5/16/16/16	-
2	CIT	B	9204	-	-	6/16/16/16	-
2	CIT	B	9201	-	-	12/16/16/16	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9201	CIT	C3-C6	6.16	1.59	1.53
2	A	9202	CIT	C3-C6	5.30	1.59	1.53
2	A	9207	CIT	C3-C6	5.19	1.58	1.53
2	B	9205	CIT	C3-C6	4.37	1.58	1.53
2	B	9201	CIT	C2-C3	4.04	1.59	1.54

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9201	CIT	O6-C6-C3	4.39	121.55	113.14
2	B	9204	CIT	O6-C6-C3	3.82	120.48	113.14
2	A	9202	CIT	O6-C6-C3	3.57	119.99	113.14
2	B	9206	CIT	O6-C6-C3	3.55	119.95	113.14
2	A	9207	CIT	O6-C6-C3	3.39	119.64	113.14

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	9202	CIT	C1-C2-C3-O7
2	A	9202	CIT	C1-C2-C3-C4
2	A	9207	CIT	O7-C3-C6-O5
2	A	9207	CIT	O7-C3-C6-O6
2	A	9207	CIT	C4-C3-C6-O5

There are no ring outliers.

10 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	9206	CIT	6	0
3	A	9104	GOL	2	0
3	A	9103	GOL	7	0
2	A	9203	CIT	5	0
2	A	9207	CIT	5	0
2	B	9205	CIT	2	0
3	B	9102	GOL	2	0
2	A	9202	CIT	7	0
2	B	9204	CIT	4	0
2	B	9201	CIT	3	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	676/676 (100%)	-0.23	3 (0%) 88 87	38, 74, 105, 123	0
1	B	676/676 (100%)	-0.27	4 (0%) 85 85	38, 75, 107, 124	0
All	All	1352/1352 (100%)	-0.25	7 (0%) 87 86	38, 75, 106, 124	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	CYS	2.9
1	A	275	GLY	2.3
1	B	612	VAL	2.2
1	B	615	CYS	2.1
1	B	335	PRO	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
2	CIT	A	9202	13/13	0.38	0.13	76,81,87,90	0
2	CIT	B	9205	13/13	0.49	0.11	81,87,91,94	0
2	CIT	B	9206	13/13	0.51	0.14	76,78,81,81	0
2	CIT	A	9207	13/13	0.54	0.13	80,85,89,90	0
2	CIT	B	9201	13/13	0.61	0.13	68,71,82,84	0
3	GOL	A	9103	6/6	0.61	0.17	79,83,85,86	0
3	GOL	B	9102	6/6	0.61	0.13	78,82,86,88	0
2	CIT	B	9204	13/13	0.64	0.11	73,77,84,86	0
3	GOL	A	9101	6/6	0.65	0.13	82,86,87,88	0
2	CIT	A	9203	13/13	0.67	0.10	77,81,88,89	0
3	GOL	A	9104	6/6	0.82	0.11	73,75,78,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.