



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:44 AM UTC

PDB ID : 28MR / pdb\_000028mr  
Title : X-ray structure of the adduct between human serum transferrin with Fe<sup>3+</sup> bound at the C-lobe and diruthenium tetraacetate chloride  
Authors : Ferraro, G.; Merlino, A.  
Deposited on : 2026-02-08  
Resolution : 2.26 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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

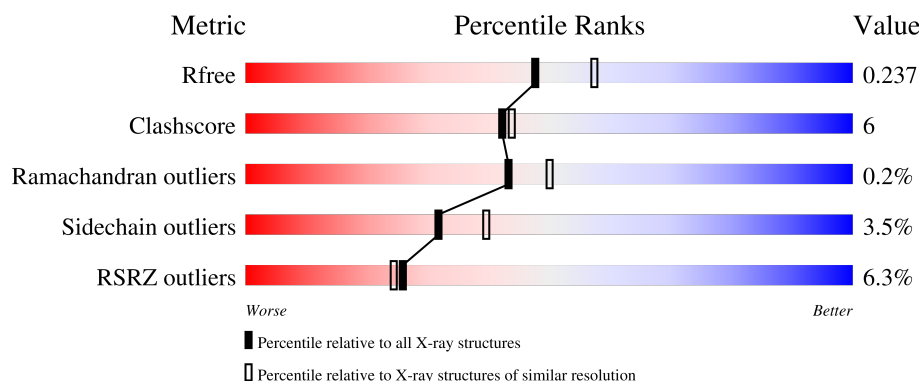
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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  $\geq 3$ , 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	679	<div> <div>6%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5656 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.

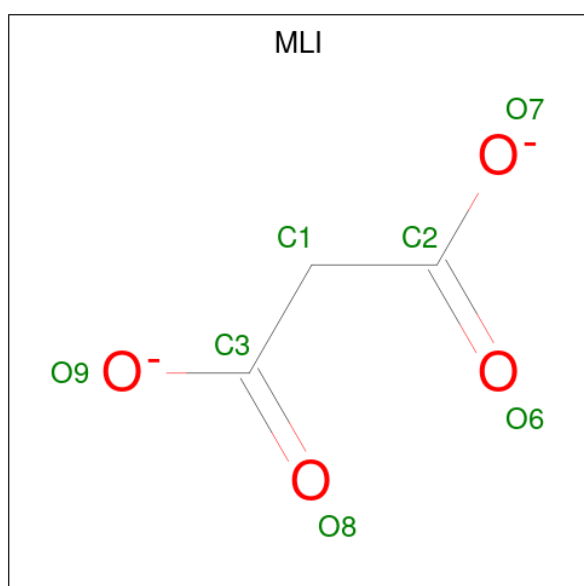
- Molecule 1 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	670	5252	3295	912	998	47	0	6	0

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0

- Molecule 3 is MALONATE ION (CCD ID: MLI) (formula: C<sub>3</sub>H<sub>2</sub>O<sub>4</sub>).



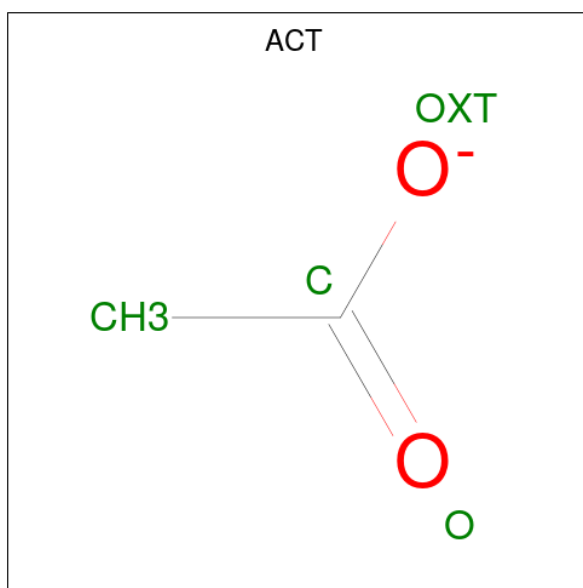
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 3 4	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is RUTHENIUM ION (CCD ID: RU) (formula: Ru) (labeled as "Ligand of

Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Ru 1	0	0

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Cl 1	0	0

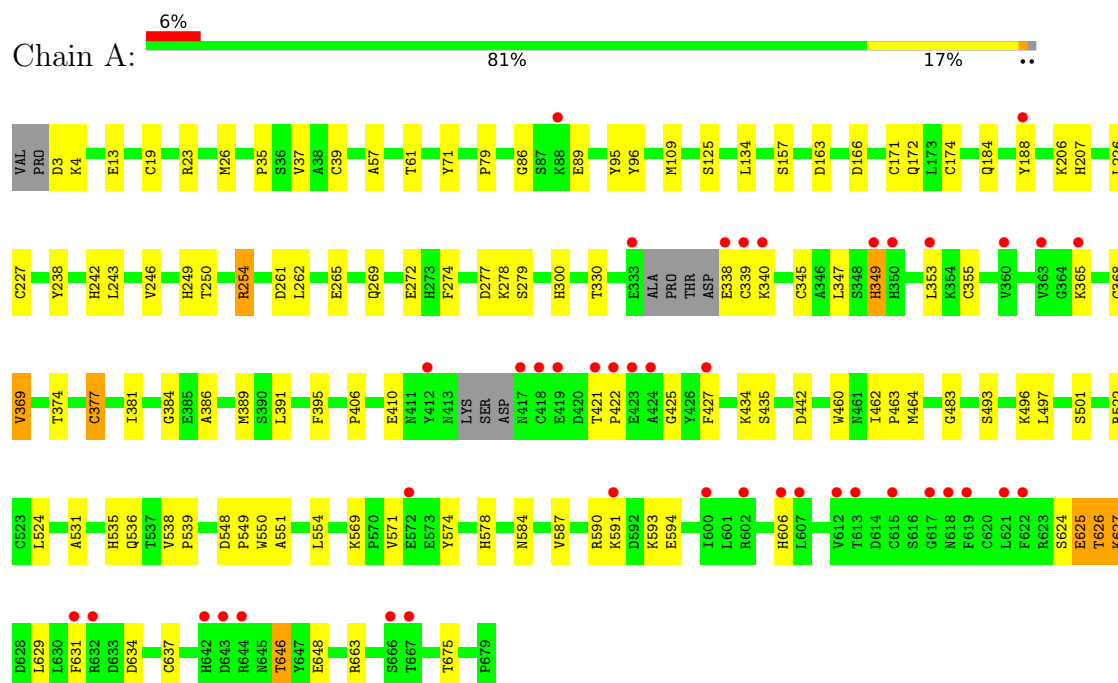
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	383	Total 384	O 384	0	1

### 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: Serotransferrin



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.94Å 156.71Å 107.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.12 – 2.26 103.12 – 2.26	Depositor EDS
% Data completeness (in resolution range)	56.8 (103.12-2.26) 56.8 (103.12-2.26)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.179 , 0.234 0.185 , 0.237	Depositor DCC
$R_{free}$ test set	1528 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, RU, MLI, ACT, FE

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	0.55	0/5368	1.08	9/7249 (0.1%)

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	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	646	THR	CA-CB-OG1	-6.06	100.51	109.60
1	A	3	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	548	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	634	ASP	CA-CB-CG	5.60	118.20	112.60
1	A	330	THR	CA-CB-OG1	-5.48	101.38	109.60
1	A	569	LYS	CB-CA-C	-5.30	102.77	110.03
1	A	442	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	13	GLU	CB-CG-CD	5.05	121.19	112.60
1	A	277	ASP	CA-CB-CG	5.05	117.65	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	SER	Peptide

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Mol	Chain	Res	Type	Group
1	A	254	ARG	Sidechain

## 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	5252	0	5067	65	0
2	A	1	0	0	0	0
3	A	7	0	2	0	0
4	A	6	0	8	2	0
5	A	4	0	3	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	384	0	0	3	0
All	All	5656	0	5080	65	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 6.

All (65) 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:A:188:TYR:CE1	1:A:206:LYS:HG3	2.15	0.82
1:A:261:ASP:HB2	8:A:964:HOH:O	1.88	0.73
1:A:538:VAL:HB	1:A:539:PRO:HD3	1.74	0.68
1:A:410:GLU:OE2	1:A:631:PHE:HB3	1.97	0.64
1:A:272:GLU:O	1:A:278:LYS:HE2	1.97	0.64
1:A:591[B]:LYS:HE2	8:A:981:HOH:O	1.99	0.63
1:A:425:GLY:HA2	1:A:584:ASN:OD1	1.99	0.62
1:A:23:ARG:HG3	1:A:37:VAL:O	2.00	0.62
1:A:493:SER:HA	1:A:496:LYS:HD3	1.85	0.59
1:A:57:ALA:O	1:A:254:ARG:NH2	2.36	0.58
1:A:26:MET:HE2	1:A:274:PHE:HE2	1.68	0.58
1:A:626:THR:OG1	1:A:627:LYS:N	2.37	0.57
1:A:26:MET:HE2	1:A:274:PHE:CE2	2.41	0.56
1:A:355:CYS:C	1:A:368:CYS:SG	2.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:CYS:HB3	4:A:703:GOL:H12	1.88	0.55
1:A:242:HIS:H	4:A:703:GOL:H32	1.73	0.54
1:A:349:HIS:H	1:A:349:HIS:HD1	1.53	0.54
1:A:462:ILE:HB	1:A:463:PRO:HD3	1.89	0.54
1:A:86:GLY:O	1:A:300:HIS:CD2	2.60	0.53
1:A:188:TYR:CE1	1:A:206:LYS:CG	2.91	0.53
1:A:26:MET:CE	1:A:274:PHE:CE2	2.92	0.52
1:A:391:LEU:HD13	1:A:395:PHE:HB3	1.91	0.52
1:A:26:MET:CE	1:A:274:PHE:CD2	2.93	0.52
1:A:381:ILE:HA	1:A:386:ALA:O	2.11	0.51
1:A:374:THR:HG21	1:A:395:PHE:CD2	2.46	0.50
1:A:79:PRO:HB3	1:A:250:THR:HG21	1.94	0.49
1:A:134:LEU:CD1	1:A:243:LEU:HB3	2.42	0.49
1:A:349:HIS:O	1:A:353:LEU:HG	2.14	0.48
1:A:109:MET:HE2	1:A:226:LEU:HB3	1.96	0.48
1:A:265:GLU:O	1:A:269:GLN:HG3	2.13	0.48
1:A:171:CYS:O	1:A:172:GLN:C	2.56	0.48
1:A:535:HIS:HB2	1:A:574:TYR:CD2	2.49	0.48
1:A:522:ARG:HA	1:A:550:TRP:CZ3	2.48	0.48
1:A:384:GLY:HA2	1:A:590:ARG:NH1	2.28	0.48
1:A:109:MET:HE2	1:A:226:LEU:CB	2.45	0.47
1:A:483:GLY:HA2	1:A:497:LEU:HD12	1.96	0.47
1:A:163:ASP:OD2	1:A:166:ASP:OD2	2.32	0.46
1:A:524:LEU:HB2	1:A:531:ALA:HB2	1.97	0.46
1:A:377:CYS:HB3	1:A:389:MET:SD	2.55	0.45
1:A:345:CYS:HA	1:A:369:VAL:O	2.16	0.45
1:A:184:GLN:HG2	8:A:1011:HOH:O	2.16	0.45
1:A:4:LYS:O	1:A:35:PRO:HA	2.16	0.45
1:A:551:ALA:HA	1:A:554:LEU:CD1	2.46	0.45
1:A:663:ARG:NH2	1:A:675[A]:THR:HG21	2.32	0.45
1:A:79:PRO:HB3	1:A:250:THR:CG2	2.47	0.44
1:A:134:LEU:HD11	1:A:243:LEU:HB3	2.00	0.44
1:A:207:HIS:HB2	1:A:238:TYR:CG	2.52	0.43
1:A:4:LYS:HA	1:A:262:LEU:HD21	2.00	0.43
1:A:535:HIS:CE1	1:A:536:GLN:OE1	2.72	0.43
1:A:19:CYS:C	1:A:39:CYS:SG	3.02	0.42
1:A:460:TRP:O	1:A:464:MET:HB2	2.19	0.42
1:A:26:MET:HE1	1:A:274:PHE:CD2	2.55	0.42
1:A:339:CYS:C	1:A:340:LYS:O	2.62	0.42
1:A:538:VAL:HB	1:A:539:PRO:CD	2.47	0.42
1:A:174:CYS:SG	1:A:174:CYS:O	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:PHE:CD1	1:A:578:HIS:ND1	2.88	0.41
1:A:624:SER:O	1:A:625:GLU:C	2.63	0.41
1:A:629:LEU:O	1:A:631:PHE:N	2.52	0.41
1:A:95:TYR:CZ	1:A:246:VAL:HG11	2.56	0.41
1:A:406:PRO:HA	1:A:587:VAL:O	2.20	0.41
1:A:646:THR:HG22	1:A:648:GLU:H	1.86	0.41
1:A:593:LYS:O	1:A:594:GLU:C	2.62	0.40
1:A:96:TYR:HB2	1:A:207:HIS:HB3	2.03	0.40
1:A:347:LEU:HD21	1:A:374:THR:HA	2.02	0.40
1:A:434:LYS:O	1:A:435:SER:C	2.64	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	670/679 (99%)	622 (93%)	47 (7%)	1 (0%)	48 56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	PRO

### 5.3.2 Protein sidechains [i](#)

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	570/572 (100%)	549 (96%)	21 (4%)	30	37

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	THR
1	A	71	TYR
1	A	89	GLU
1	A	125[A]	SER
1	A	125[B]	SER
1	A	249	HIS
1	A	279	SER
1	A	338	GLU
1	A	349	HIS
1	A	365	LYS
1	A	369	VAL
1	A	377	CYS
1	A	421	THR
1	A	501	SER
1	A	549	PRO
1	A	571	VAL
1	A	606	HIS
1	A	625	GLU
1	A	626	THR
1	A	627	LYS
1	A	637	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	213	ASN
1	A	222	GLN
1	A	230	ASN
1	A	283	GLN
1	A	300	HIS
1	A	555	ASN
1	A	611	ASN

### 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 ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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	GOL	A	703	-	5,5,5	0.10	0	5,5,5	0.29	0
5	ACT	A	704	-	3,3,3	1.17	0	3,3,3	0.82	0
3	MLI	A	702	2	6,6,6	1.12	0	7,7,7	1.61	1 (14%)

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	GOL	A	703	-	-	2/4/4/4	-
3	MLI	A	702	2	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	MLI	O6-C2-C1	-2.06	116.25	122.11

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	GOL	O1-C1-C2-C3
3	A	702	MLI	C2-C1-C3-O9
3	A	702	MLI	C2-C1-C3-O8
4	A	703	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	GOL	2	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	670/679 (98%)	0.21	42 (6%) 26 24	14, 39, 94, 143	6 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	424	ALA	6.5
1	A	412	TYR	4.9
1	A	613	THR	4.6
1	A	340	LYS	4.6
1	A	422	PRO	4.4
1	A	349	HIS	3.8
1	A	365	LYS	3.4
1	A	417	ASN	3.4
1	A	421	THR	3.3
1	A	606	HIS	3.3
1	A	88	LYS	3.3
1	A	339	CYS	3.3
1	A	642	HIS	3.1
1	A	423	GLU	3.0
1	A	350	HIS	3.0
1	A	353	LEU	2.9
1	A	607	LEU	2.9
1	A	333	GLU	2.8
1	A	338	GLU	2.8
1	A	363	VAL	2.8
1	A	419	GLU	2.8
1	A	591[A]	LYS	2.8
1	A	619	PHE	2.7
1	A	612	VAL	2.7
1	A	632	ARG	2.6
1	A	618	ASN	2.6
1	A	572[A]	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	643	ASP	2.5
1	A	418	CYS	2.5
1	A	615	CYS	2.5
1	A	644	ARG	2.3
1	A	622	PHE	2.3
1	A	617	GLY	2.2
1	A	667	THR	2.2
1	A	188	TYR	2.1
1	A	666	SER	2.1
1	A	631	PHE	2.1
1	A	602	ARG	2.1
1	A	360	VAL	2.1
1	A	621	LEU	2.0
1	A	427	PHE	2.0
1	A	600	ILE	2.0

## 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, 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(Å <sup>2</sup> )	Q<0.9
6	RU	A	705	1/1	0.82	0.17	122,122,122,122	1
5	ACT	A	704	4/4	0.92	0.12	43,45,46,47	0
3	MLI	A	702	7/7	0.93	0.09	32,35,40,43	0
4	GOL	A	703	6/6	0.93	0.11	35,36,39,40	0
7	CL	A	706	1/1	0.93	0.08	53,53,53,53	0
2	FE	A	701	1/1	1.00	0.02	38,38,38,38	0

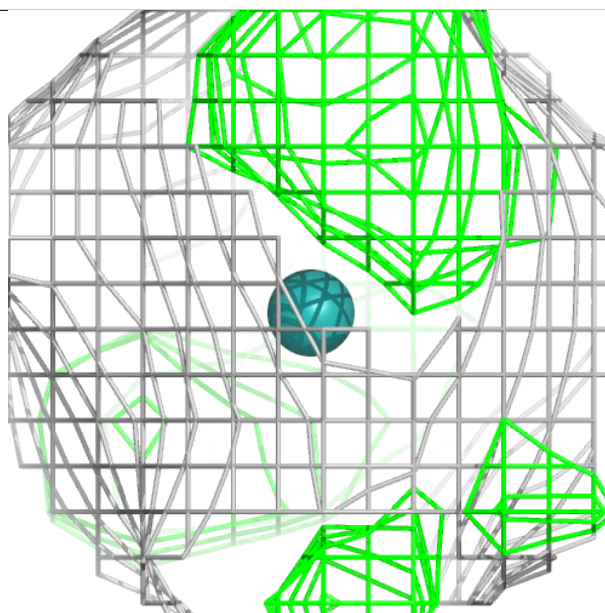
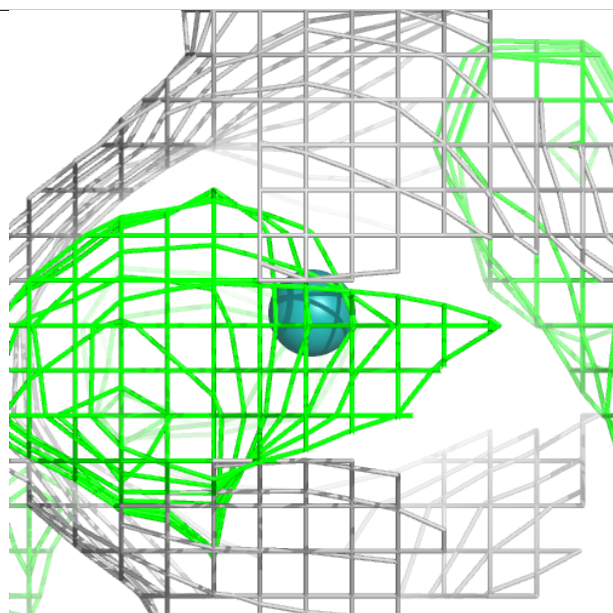
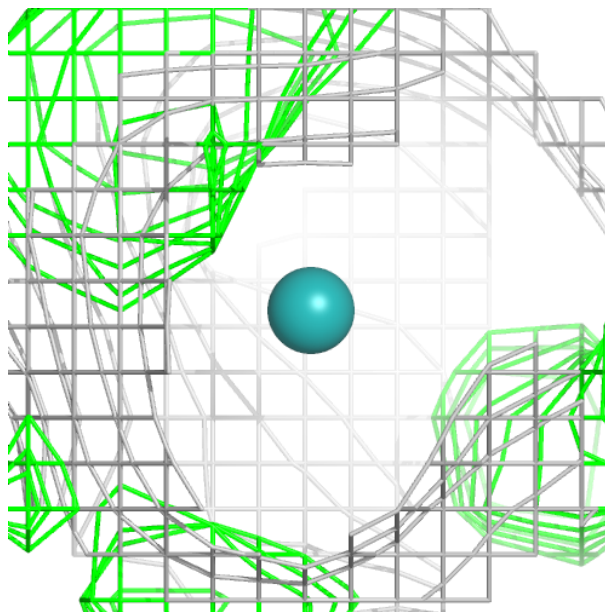
The following is a graphical depiction of the model fit to experimental electron density of all



instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

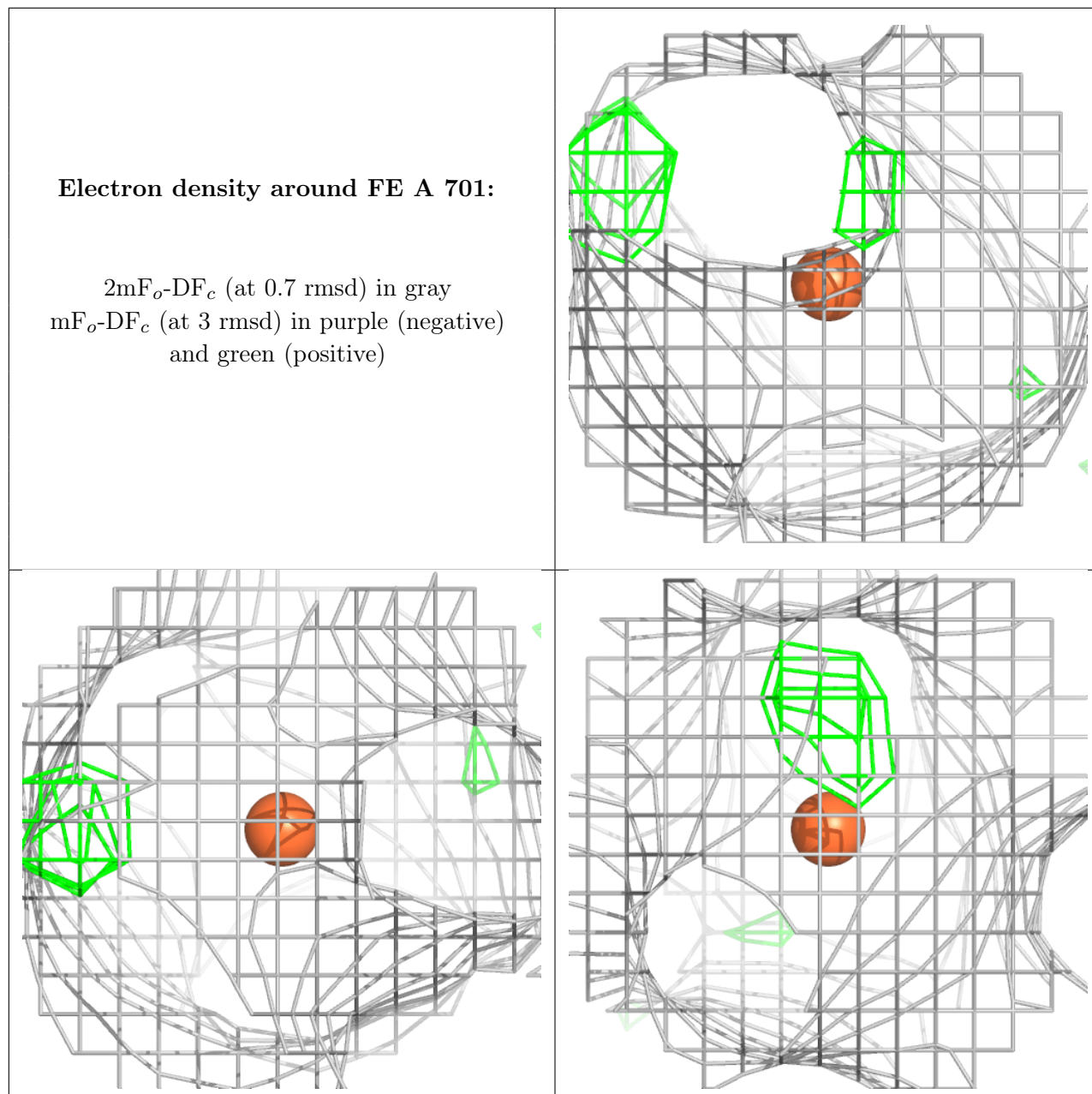
**Electron density around RU A 705:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FE A 701:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.