



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:07 AM UTC

PDB ID : 9H49 / pdb_00009h49
Title : Crystal structure of the adduct between human serum transferrin (apo-form) and cisplatin
Authors : Troisi, R.; Galardo, F.; Ferraro, G.; Sica, F.; Merlino, A.
Deposited on : 2024-10-17
Resolution : 3.52 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

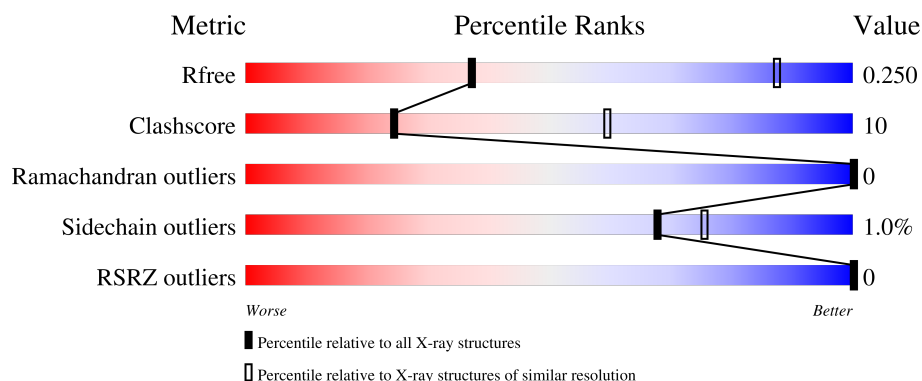
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	679	 77% 22%
1	B	679	 77% 22%

2 Entry composition [i](#)

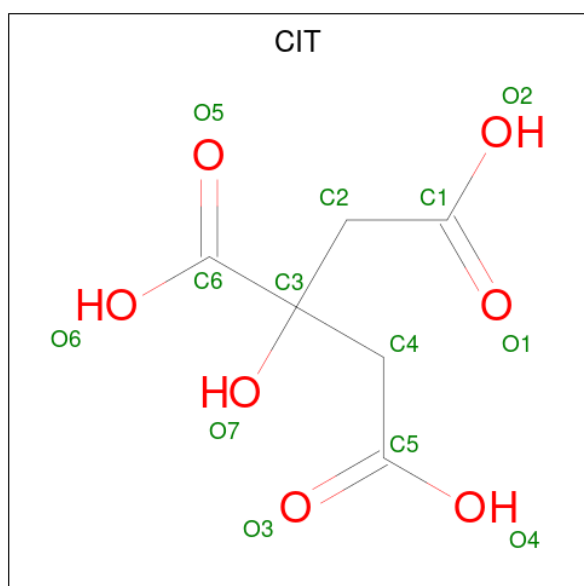
There are 5 unique types of molecules in this entry. The entry contains 10594 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			5244	3291	909	997	47			
1	B	677	Total	C	N	O	S	0	0	0
			5252	3295	910	1000	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		

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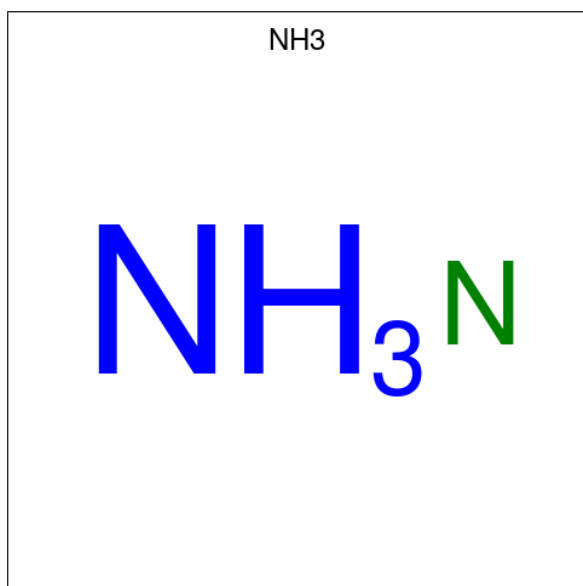
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is PLATINUM (II) ION (CCD ID: PT) (formula: Pt) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Pt	0	0
			2	2		
3	B	2	Total	Pt	0	0
			2	2		

- Molecule 4 is AMMONIA (CCD ID: NH3) (formula: H₃N).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	N	0	0
			1	1		
4	A	1	Total	N	0	0
			1	1		
4	A	1	Total	N	0	0
			1	1		
4	A	1	Total	N	0	0
			1	1		
4	B	1	Total	N	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	N	0	0
			1	1		
4	B	1	Total	N	0	0
			1	1		
4	B	1	Total	N	0	0
			1	1		

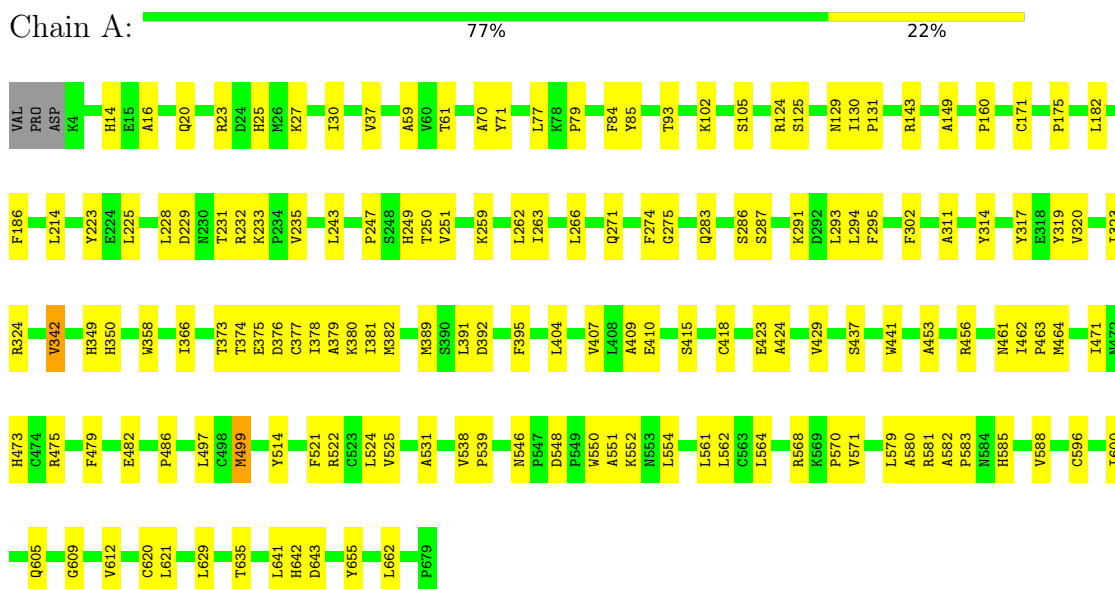
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	B	5	Total	O	0	0
			5	5		

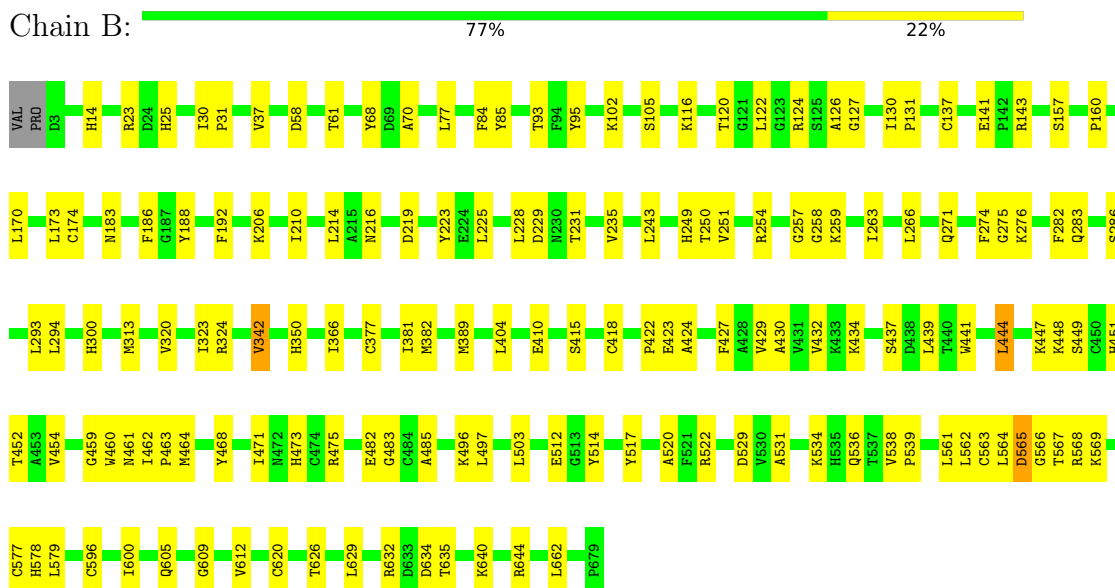
3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.18Å 103.68Å 200.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.84 – 3.52 80.84 – 3.52	Depositor EDS
% Data completeness (in resolution range)	99.2 (80.84-3.52) 99.2 (80.84-3.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.231 , 0.249 0.231 , 0.250	Depositor DCC
R_{free} test set	1177 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	141.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 125.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10594	wwPDB-VP
Average B, all atoms (Å ²)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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, PT, NH3

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	0.44	0/5363	1.00	0/7247
1	B	0.44	0/5371	1.01	0/7258
All	All	0.44	0/10734	1.01	0/14505

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5244	0	5068	98	0
1	B	5252	0	5072	107	0
2	A	39	0	15	2	0
2	B	39	0	15	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	3	0	0	0	0
5	B	5	0	0	0	0
All	All	10594	0	10170	205	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 10.

All (205) 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:137:CYS:HA	1:B:143:ARG:HH22	1.36	0.89
1:A:283:GLN:HB2	1:A:286:SER:HB3	1.57	0.86
1:A:228:LEU:HD21	1:A:243:LEU:HA	1.62	0.81
1:B:320:VAL:O	1:B:324:ARG:HB2	1.84	0.78
1:B:569:LYS:HE2	1:B:577:CYS:HB2	1.66	0.78
1:A:229:ASP:OD1	1:A:231:THR:HG22	1.86	0.76
1:A:377:CYS:HB3	1:A:389:MET:SD	2.27	0.74
1:B:429:VAL:HA	1:B:579:LEU:HD13	1.70	0.74
1:B:137:CYS:HA	1:B:143:ARG:NH2	2.05	0.71
1:B:160:PRO:HB3	1:B:186:PHE:HD1	1.54	0.71
1:A:379:ALA:HA	1:A:382:MET:HE2	1.70	0.71
1:B:188:TYR:HB2	2:B:703:CIT:O5	1.90	0.71
1:A:84:PHE:C	1:A:85:TYR:HD1	1.98	0.70
1:B:84:PHE:C	1:B:85:TYR:HD1	2.00	0.70
1:A:561:LEU:HD23	1:A:561:LEU:H	1.56	0.69
1:A:499:MET:O	1:A:499:MET:HE2	1.92	0.69
1:B:276:LYS:HD2	1:B:300:HIS:O	1.91	0.69
1:B:228:LEU:HD21	1:B:243:LEU:HA	1.74	0.68
1:A:320:VAL:O	1:A:324:ARG:HB2	1.94	0.67
1:A:342:VAL:HG13	1:A:366:ILE:HD13	1.77	0.67
1:B:342:VAL:HG13	1:B:366:ILE:HD13	1.79	0.64
1:B:482:GLU:HB3	1:B:497:LEU:CD1	2.28	0.64
1:A:378:ILE:O	1:A:382:MET:HG3	1.97	0.64
1:A:410:GLU:HB3	1:A:635:THR:HG22	1.80	0.64
1:B:439:LEU:HD21	1:B:447:LYS:HE2	1.80	0.63
1:A:350:HIS:HB3	1:A:629:LEU:HD21	1.80	0.63
1:A:382:MET:HG2	1:A:404:LEU:HD21	1.80	0.63
1:A:37:VAL:HG22	1:A:266:LEU:HD11	1.80	0.63
1:A:538:VAL:HG11	1:A:571:VAL:HG11	1.81	0.63
1:B:229:ASP:OD1	1:B:231:THR:HG22	1.98	0.63
1:B:609:GLY:O	1:B:612:VAL:HG12	1.99	0.62
1:B:468:TYR:HA	1:B:471:ILE:HG22	1.82	0.62
1:B:410:GLU:HB3	1:B:635:THR:HG22	1.81	0.62
1:A:561:LEU:HD22	1:A:571:VAL:HA	1.83	0.61
1:A:376:ASP:O	1:A:380:LYS:HG2	2.00	0.61
1:B:283:GLN:HB2	1:B:286:SER:HB3	1.84	0.60
1:B:564:LEU:C	1:B:566:GLY:H	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:SER:OG	1:A:291:LYS:HA	2.02	0.59
1:B:561:LEU:O	1:B:563:CYS:SG	2.61	0.59
1:B:605:GLN:O	1:B:609:GLY:HA3	2.03	0.59
1:A:61:THR:CG2	1:A:294:LEU:O	2.51	0.59
1:A:283:GLN:CB	1:A:286:SER:HB3	2.32	0.58
1:B:61:THR:HB	1:B:251:VAL:HG22	1.84	0.58
1:B:432:VAL:CG1	1:B:562:LEU:HG	2.34	0.58
1:A:524:LEU:HB2	1:A:531:ALA:HB2	1.86	0.58
1:B:58:ASP:HA	1:B:254:ARG:HH21	1.67	0.58
1:B:473:HIS:CD2	1:B:475:ARG:HB2	2.39	0.58
1:B:183:ASN:HB3	1:B:186:PHE:HB2	1.86	0.57
1:A:61:THR:HG21	1:A:294:LEU:O	2.05	0.57
1:B:130:ILE:HB	1:B:131:PRO:HD3	1.87	0.57
1:B:471:ILE:C	1:B:473:HIS:H	2.13	0.57
1:A:225:LEU:HD13	1:A:235:VAL:HA	1.87	0.56
1:B:437:SER:HA	1:B:568:ARG:NH1	2.20	0.56
1:A:25:HIS:HB3	1:A:274:PHE:CZ	2.40	0.56
1:A:471:ILE:HD12	1:A:479:PHE:HB2	1.88	0.56
1:A:522:ARG:HA	1:A:525:VAL:HG22	1.88	0.56
1:B:216:ASN:HB2	1:B:219:ASP:OD1	2.06	0.56
1:A:358:TRP:CE2	1:A:621:LEU:HD11	2.41	0.55
1:A:462:ILE:HG12	1:A:580:ALA:HB3	1.88	0.55
1:A:461:ASN:HA	1:A:662:LEU:HD11	1.87	0.55
1:B:538:VAL:HB	1:B:539:PRO:HD3	1.88	0.55
1:A:642:HIS:O	1:A:643:ASP:HB2	2.07	0.54
1:A:358:TRP:CD2	1:A:621:LEU:HD11	2.43	0.54
1:B:422:PRO:HB2	1:B:644:ARG:NH1	2.23	0.54
1:A:453:ALA:HB3	1:A:456:ARG:HG2	1.88	0.54
1:B:415:SER:HB3	1:B:418:CYS:HB3	1.88	0.54
1:A:409:ALA:HB2	1:A:641:LEU:HD11	1.89	0.54
1:A:143:ARG:HA	1:A:149:ALA:HB2	1.90	0.53
1:B:434:LYS:HA	1:B:568:ARG:HH22	1.73	0.53
1:A:546:ASN:OD1	1:A:548:ASP:HB2	2.08	0.53
1:B:84:PHE:C	1:B:85:TYR:CD1	2.86	0.53
1:B:565:ASP:HB2	1:B:567:THR:HG22	1.90	0.53
1:A:609:GLY:O	1:A:612:VAL:HG12	2.09	0.53
1:B:437:SER:HA	1:B:568:ARG:HH12	1.72	0.53
1:A:538:VAL:HB	1:A:539:PRO:HD3	1.90	0.53
1:B:448:LYS:HA	1:B:482:GLU:O	2.09	0.52
1:B:512:GLU:OE2	1:B:514:TYR:HB2	2.09	0.52
1:B:482:GLU:HB3	1:B:497:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:CYS:O	1:A:381:ILE:HG12	2.09	0.51
1:B:25:HIS:CE1	1:B:282:PHE:HB2	2.45	0.51
1:A:581:ARG:O	1:A:582:ALA:C	2.53	0.51
1:B:461:ASN:HA	1:B:662:LEU:HD11	1.92	0.51
1:A:319:TYR:CE1	1:A:323:ILE:HD13	2.45	0.51
1:B:482:GLU:HB3	1:B:497:LEU:HD11	1.93	0.51
1:B:160:PRO:HB3	1:B:186:PHE:CD1	2.42	0.51
1:B:517:TYR:CZ	1:B:534:LYS:HE3	2.47	0.50
1:B:254:ARG:NH1	1:B:257:GLY:O	2.45	0.50
1:A:130:ILE:HB	1:A:131:PRO:HD3	1.93	0.50
1:B:422:PRO:HG3	1:B:640:LYS:O	2.11	0.50
1:A:271:GLN:O	1:A:275:GLY:HA3	2.11	0.49
1:B:225:LEU:HD13	1:B:235:VAL:HG12	1.92	0.49
1:A:84:PHE:C	1:A:85:TYR:CD1	2.86	0.49
1:A:429:VAL:CG1	1:A:561:LEU:HB2	2.43	0.49
1:A:462:ILE:N	1:A:463:PRO:HD2	2.27	0.49
1:B:124:ARG:HB3	2:B:702:CIT:H22	1.94	0.49
1:B:473:HIS:HD2	1:B:475:ARG:HB2	1.75	0.49
1:A:583:PRO:HD3	1:A:655:TYR:CE1	2.48	0.48
1:A:125:SER:HA	1:A:129:ASN:HB2	1.95	0.48
1:A:464:MET:HE2	1:A:464:MET:HA	1.94	0.48
1:A:514:TYR:HE1	1:A:522:ARG:HG2	1.78	0.48
1:B:259:LYS:O	1:B:263:ILE:HD12	2.13	0.48
1:B:214:LEU:HD11	1:B:223:TYR:HE2	1.79	0.48
1:B:596:CYS:O	1:B:600:ILE:HG12	2.14	0.48
1:B:157:SER:HB2	1:B:170:LEU:HA	1.95	0.48
1:B:432:VAL:HG13	1:B:568:ARG:HH21	1.78	0.48
1:A:16:ALA:O	1:A:20:GLN:HG3	2.13	0.48
1:A:561:LEU:H	1:A:561:LEU:CD2	2.23	0.48
1:A:124:ARG:HD2	2:A:703:CIT:H42	1.94	0.48
1:B:116:LYS:HD3	1:B:173:LEU:HD11	1.96	0.48
1:B:126:ALA:HA	1:B:130:ILE:HD12	1.94	0.48
1:B:23:ARG:HA	1:B:37:VAL:HB	1.96	0.48
1:B:632:ARG:O	1:B:635:THR:HG23	2.13	0.48
1:B:422:PRO:HB2	1:B:644:ARG:HH11	1.78	0.47
1:A:102:LYS:HB2	1:A:105:SER:HB3	1.95	0.47
1:A:605:GLN:O	1:A:609:GLY:HA3	2.14	0.47
1:B:61:THR:CG2	1:B:294:LEU:O	2.63	0.47
1:A:407:VAL:O	1:A:641:LEU:HB2	2.15	0.47
1:A:596:CYS:O	1:A:600:ILE:HG12	2.14	0.47
1:A:349:HIS:HB2	2:A:701:CIT:O7	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:VAL:HG11	1:A:554:LEU:HD13	1.96	0.47
1:B:561:LEU:O	1:B:577:CYS:SG	2.73	0.47
1:A:392:ASP:HA	1:A:585:HIS:CD2	2.49	0.46
1:B:377:CYS:O	1:B:381:ILE:HG12	2.15	0.46
1:A:342:VAL:CG1	1:A:366:ILE:HD13	2.42	0.46
1:A:561:LEU:HD21	1:A:570:PRO:O	2.15	0.46
1:B:448:LYS:HG2	1:B:529:ASP:OD2	2.14	0.46
1:A:482:GLU:HB3	1:A:497:LEU:HD13	1.97	0.46
1:B:452:THR:OG1	1:B:459:GLY:HA3	2.16	0.46
1:A:61:THR:HB	1:A:251:VAL:HG22	1.97	0.46
1:B:95:TYR:CD1	1:B:206:LYS:HD2	2.51	0.46
1:B:449:SER:O	1:B:483:GLY:HA2	2.16	0.46
1:A:79:PRO:HB3	1:A:250:THR:HG21	1.98	0.45
1:A:473:HIS:CE1	1:A:475:ARG:HB2	2.51	0.45
1:B:424:ALA:HB2	1:B:644:ARG:HH22	1.82	0.45
1:A:437:SER:HA	1:A:568:ARG:NH1	2.30	0.45
1:A:441:TRP:HA	1:A:562:LEU:HD21	1.99	0.45
1:A:522:ARG:NH2	1:A:550:TRP:NE1	2.64	0.45
1:B:382:MET:HB3	1:B:404:LEU:HD21	1.97	0.45
1:B:14:HIS:HB3	1:B:293:LEU:HD21	1.99	0.45
1:B:626:THR:OG1	1:B:629:LEU:HD11	2.16	0.45
1:A:232:ARG:O	1:A:233:LYS:HG2	2.17	0.45
1:A:160:PRO:HB3	1:A:186:PHE:HD1	1.81	0.45
1:A:259:LYS:HB3	1:A:262:LEU:HB2	1.99	0.45
1:A:404:LEU:HB3	1:A:588:VAL:HG13	1.97	0.45
1:A:453:ALA:HA	1:A:486:PRO:HD2	1.99	0.44
1:A:551:ALA:O	1:A:552:LYS:C	2.59	0.44
1:B:377:CYS:HB3	1:B:389:MET:SD	2.57	0.44
1:B:68:TYR:CG	1:B:323:ILE:HD12	2.51	0.44
1:B:313:MET:HG3	1:B:382:MET:HE2	1.99	0.44
1:B:482:GLU:HG2	1:B:496:LYS:HD2	1.99	0.44
1:A:612:VAL:CG1	1:A:620:CYS:HB3	2.48	0.44
1:B:25:HIS:HB3	1:B:274:PHE:CZ	2.53	0.44
1:B:564:LEU:C	1:B:566:GLY:N	2.75	0.44
1:B:350:HIS:HB3	1:B:629:LEU:HD21	1.99	0.44
1:B:520:ALA:HB1	1:B:531:ALA:HB1	2.00	0.44
1:B:432:VAL:HG12	1:B:562:LEU:HG	2.00	0.44
1:A:70:ALA:HB1	1:A:77:LEU:HB2	1.99	0.44
1:A:14:HIS:HB3	1:A:293:LEU:HD21	2.01	0.43
1:A:247:PRO:HB3	1:A:314:TYR:CE2	2.53	0.43
1:A:462:ILE:CG2	1:A:579:LEU:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:CYS:HB2	1:B:183:ASN:HD21	1.84	0.43
1:B:271:GLN:O	1:B:275:GLY:HA3	2.19	0.43
1:A:23:ARG:O	1:A:27:LYS:HB2	2.18	0.43
1:A:423:GLU:O	1:A:424:ALA:HB3	2.18	0.43
1:A:415:SER:HB3	1:A:418:CYS:HB3	2.00	0.43
1:B:451:HIS:CD2	1:B:485:ALA:HB2	2.54	0.43
1:A:84:PHE:HB3	1:A:93:THR:HG22	2.00	0.43
1:B:61:THR:HG21	1:B:294:LEU:O	2.19	0.42
1:B:429:VAL:HG22	1:B:430:ALA:H	1.84	0.42
1:B:612:VAL:HG13	1:B:620:CYS:SG	2.58	0.42
1:A:521:PHE:O	1:A:525:VAL:HG13	2.19	0.42
1:B:534:LYS:HD3	1:B:536:GLN:CD	2.45	0.42
1:B:192:PHE:CZ	1:B:210:ILE:HD12	2.55	0.42
1:A:522:ARG:NH2	1:A:550:TRP:HE1	2.18	0.42
1:A:429:VAL:HG13	1:A:561:LEU:HB2	2.00	0.42
1:A:71:TYR:HB2	1:A:311:ALA:HB3	2.02	0.42
1:A:59:ALA:HB2	1:A:263:ILE:HG12	2.01	0.41
1:B:423:GLU:O	1:B:424:ALA:HB3	2.20	0.41
1:B:30:ILE:HG23	1:B:31:PRO:HD2	2.02	0.41
1:B:454:VAL:HG23	1:B:460:TRP:CE2	2.55	0.41
1:B:514:TYR:HE1	1:B:522:ARG:HD2	1.85	0.41
1:A:293:LEU:C	1:A:295:PHE:H	2.29	0.41
1:B:61:THR:HA	1:B:250:THR:O	2.20	0.41
1:B:84:PHE:HB3	1:B:93:THR:HG22	2.03	0.41
1:B:427:PHE:HD2	1:B:578:HIS:CB	2.34	0.41
1:B:632:ARG:HD3	1:B:634:ASP:OD2	2.20	0.41
1:A:171:CYS:HB3	1:A:175:PRO:HA	2.03	0.41
1:A:214:LEU:HD11	1:A:223:TYR:HE2	1.85	0.41
1:A:373:THR:HG22	1:A:374:THR:N	2.36	0.41
1:A:271:GLN:NE2	1:A:302:PHE:H	2.19	0.41
1:A:317:TYR:HA	1:A:320:VAL:HG22	2.01	0.41
1:A:564:LEU:HD21	1:A:579:LEU:HA	2.03	0.41
1:B:37:VAL:HG22	1:B:266:LEU:HD11	2.02	0.41
1:B:188:TYR:OH	2:B:702:CIT:C1	2.68	0.41
1:B:254:ARG:HB2	1:B:258:GLY:HA2	2.02	0.41
1:B:441:TRP:HA	1:B:444:LEU:HD13	2.03	0.41
1:A:391:LEU:HD22	1:A:395:PHE:HB3	2.03	0.40
1:B:120:THR:OG1	1:B:127:GLY:HA3	2.21	0.40
1:B:462:ILE:N	1:B:463:PRO:HD2	2.36	0.40
1:A:373:THR:HG22	1:A:375:GLU:H	1.86	0.40
1:B:102:LYS:HB2	1:B:105:SER:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ALA:HB1	1:B:77:LEU:HD12	2.03	0.40
1:B:122:LEU:C	1:B:122:LEU:HD23	2.47	0.40
1:B:471:ILE:C	1:B:473:HIS:N	2.79	0.40
1:B:464:MET:HA	1:B:464:MET:HE2	2.04	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	674/679 (99%)	625 (93%)	49 (7%)	0	100	100
1	B	675/679 (99%)	614 (91%)	61 (9%)	0	100	100
All	All	1349/1358 (99%)	1239 (92%)	110 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	569/572 (100%)	564 (99%)	5 (1%)	70	76
1	B	570/572 (100%)	564 (99%)	6 (1%)	65	75
All	All	1139/1144 (100%)	1128 (99%)	11 (1%)	68	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	182	LEU
1	A	249	HIS
1	A	342	VAL
1	A	499	MET
1	B	141	GLU
1	B	249	HIS
1	B	342	VAL
1	B	444	LEU
1	B	503	LEU
1	B	565	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	230	ASN
1	A	268	ASN
1	A	269	GLN
1	A	283	GLN
1	A	289	HIS
1	A	361	ASN
1	A	540	GLN
1	A	578	HIS
1	B	75	ASN
1	B	213	ASN
1	B	230	ASN
1	B	283	GLN
1	B	349	HIS
1	B	361	ASN
1	B	451	HIS
1	B	578	HIS
1	B	598	HIS
1	B	603	GLN

5.3.3 RNA ⓘ

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](#)

Of 18 ligands modelled in this entry, 4 are monoatomic and 8 are modelled with single atom - leaving 6 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$
2	CIT	B	701	-	12,12,12	1.18	1 (8%)	17,17,17	1.10	2 (11%)
2	CIT	A	701	-	12,12,12	1.23	1 (8%)	17,17,17	1.14	2 (11%)
2	CIT	A	703	-	12,12,12	1.15	1 (8%)	17,17,17	1.16	2 (11%)
2	CIT	B	702	-	12,12,12	1.18	1 (8%)	17,17,17	1.14	2 (11%)
2	CIT	B	703	-	12,12,12	1.13	1 (8%)	17,17,17	1.21	2 (11%)
2	CIT	A	702	-	12,12,12	1.19	1 (8%)	17,17,17	1.13	2 (11%)

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	701	-	-	6/16/16/16	-
2	CIT	A	701	-	-	7/16/16/16	-
2	CIT	A	703	-	-	1/16/16/16	-
2	CIT	B	702	-	-	6/16/16/16	-
2	CIT	B	703	-	-	9/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	A	702	-	-	10/16/16/16	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	CIT	C3-C6	2.44	1.56	1.53
2	A	702	CIT	C3-C6	2.25	1.55	1.53
2	B	701	CIT	C3-C6	2.22	1.55	1.53
2	B	702	CIT	C3-C6	2.18	1.55	1.53
2	B	703	CIT	C3-C6	2.12	1.55	1.53
2	A	703	CIT	C3-C6	2.12	1.55	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	703	CIT	O5-C6-C3	-2.61	117.04	122.09
2	A	703	CIT	O5-C6-C3	-2.56	117.14	122.09
2	B	703	CIT	O6-C6-C3	2.45	117.85	113.14
2	A	703	CIT	O6-C6-C3	2.38	117.71	113.14
2	A	701	CIT	O6-C6-C3	2.33	117.61	113.14
2	B	702	CIT	O5-C6-C3	-2.28	117.68	122.09
2	B	701	CIT	O5-C6-C3	-2.26	117.71	122.09
2	A	702	CIT	O5-C6-C3	-2.23	117.77	122.09
2	A	701	CIT	O5-C6-C3	-2.23	117.78	122.09
2	A	702	CIT	O6-C6-C3	2.18	117.32	113.14
2	B	702	CIT	O6-C6-C3	2.14	117.25	113.14
2	B	701	CIT	O6-C6-C3	2.12	117.21	113.14

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	CIT	C1-C2-C3-O7
2	A	701	CIT	C1-C2-C3-C4
2	A	701	CIT	O7-C3-C6-O5
2	A	701	CIT	O7-C3-C6-O6
2	A	701	CIT	C4-C3-C6-O5
2	A	701	CIT	C4-C3-C6-O6
2	A	702	CIT	C1-C2-C3-O7
2	A	702	CIT	C1-C2-C3-C4
2	A	702	CIT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	A	702	CIT	C6-C3-C4-C5
2	A	702	CIT	O7-C3-C6-O5
2	A	702	CIT	O7-C3-C6-O6
2	A	702	CIT	C4-C3-C6-O5
2	A	702	CIT	C4-C3-C6-O6
2	B	702	CIT	C2-C3-C6-O5
2	B	702	CIT	C2-C3-C6-O6
2	B	702	CIT	O7-C3-C6-O5
2	B	702	CIT	O7-C3-C6-O6
2	B	703	CIT	C1-C2-C3-O7
2	B	703	CIT	C1-C2-C3-C4
2	B	703	CIT	C1-C2-C3-C6
2	B	703	CIT	O7-C3-C6-O5
2	B	703	CIT	O7-C3-C6-O6
2	B	703	CIT	C4-C3-C6-O5
2	B	703	CIT	C4-C3-C6-O6
2	A	702	CIT	O7-C3-C4-C5
2	A	702	CIT	C1-C2-C3-C6
2	B	701	CIT	O7-C3-C4-C5
2	A	701	CIT	C1-C2-C3-C6
2	B	701	CIT	C6-C3-C4-C5
2	B	701	CIT	C2-C3-C4-C5
2	B	702	CIT	O2-C1-C2-C3
2	B	702	CIT	O1-C1-C2-C3
2	B	701	CIT	C4-C3-C6-O5
2	B	701	CIT	C2-C3-C6-O5
2	B	701	CIT	C4-C3-C6-O6
2	B	703	CIT	C2-C3-C6-O5
2	B	703	CIT	C2-C3-C6-O6
2	A	703	CIT	C3-C4-C5-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	CIT	1	0
2	A	703	CIT	1	0
2	B	702	CIT	2	0
2	B	703	CIT	1	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	676/679 (99%)	-0.72	0 100 100	105, 155, 220, 244	0
1	B	677/679 (99%)	-0.68	0 100 100	107, 160, 218, 244	0
All	All	1353/1358 (99%)	-0.70	0 100 100	105, 157, 219, 244	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
4	NH3	B	705	1/1	0.47	0.08	224,224,224,224	1
4	NH3	B	709	1/1	0.53	0.17	166,166,166,166	1
2	CIT	B	703	13/13	0.55	0.08	186,202,207,209	0
2	CIT	B	702	13/13	0.63	0.07	169,180,196,201	0
4	NH3	B	708	1/1	0.70	0.08	209,209,209,209	1
4	NH3	A	706	1/1	0.70	0.10	243,243,243,243	1
3	PT	B	704	1/1	0.76	0.09	245,245,245,245	1

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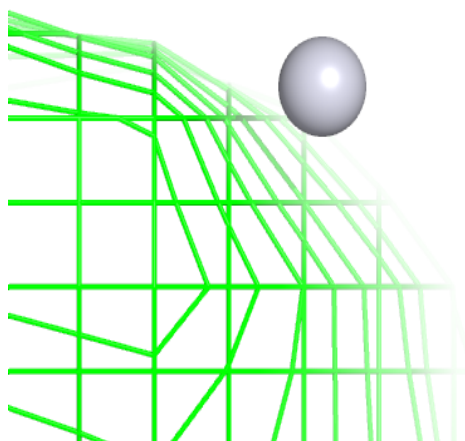
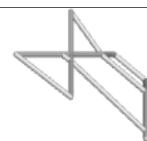
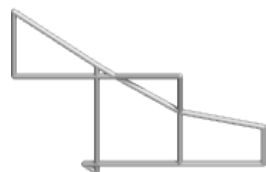
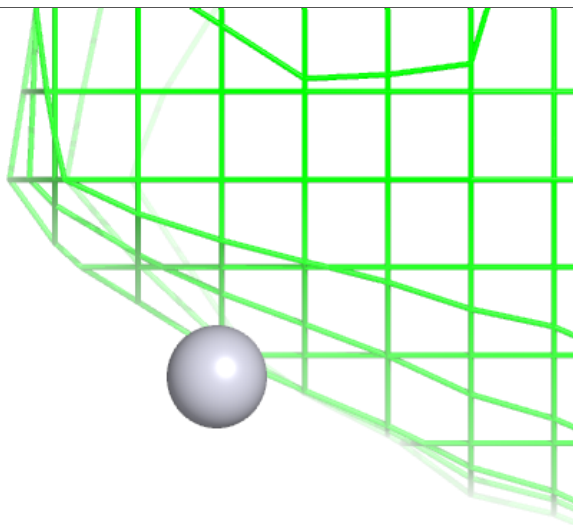
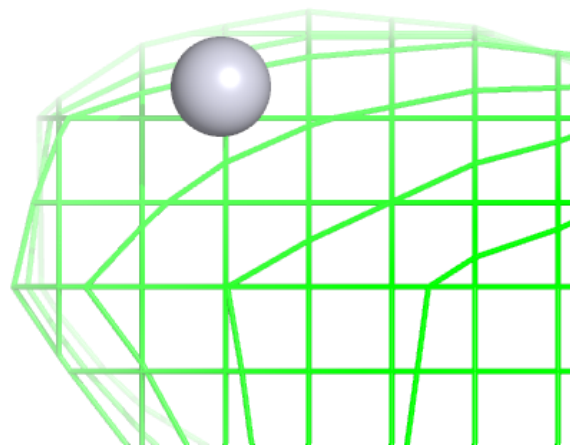
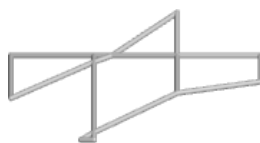
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CIT	B	701	13/13	0.77	0.06	188,204,207,210	0
4	NH3	A	709	1/1	0.78	0.12	264,264,264,264	1
2	CIT	A	703	13/13	0.81	0.07	183,191,193,199	0
2	CIT	A	702	13/13	0.83	0.05	178,185,200,206	0
2	CIT	A	701	13/13	0.85	0.08	153,179,182,182	0
4	NH3	A	705	1/1	0.86	0.12	263,263,263,263	1
3	PT	A	707	1/1	0.88	0.06	289,289,289,289	1
4	NH3	A	708	1/1	0.88	0.07	263,263,263,263	1
3	PT	A	704	1/1	0.91	0.05	275,275,275,275	1
4	NH3	B	706	1/1	0.91	0.08	235,235,235,235	1
3	PT	B	707	1/1	0.94	0.05	203,203,203,203	1

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.

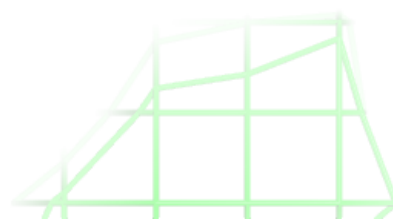
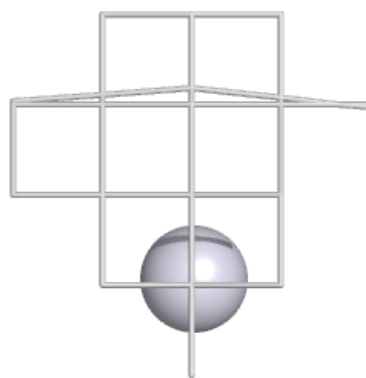
Electron density around PT B 704:

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



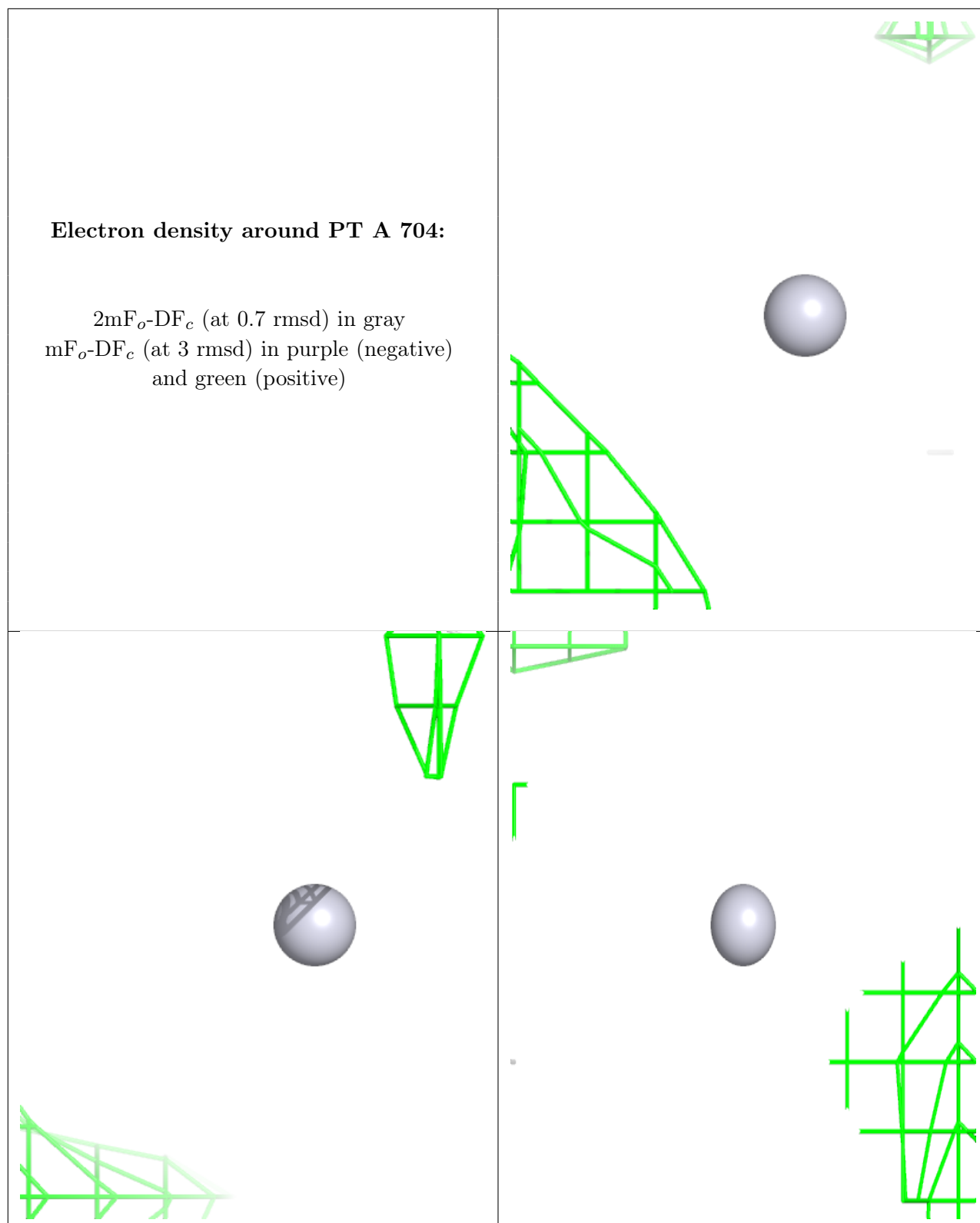
Electron density around PT A 707:

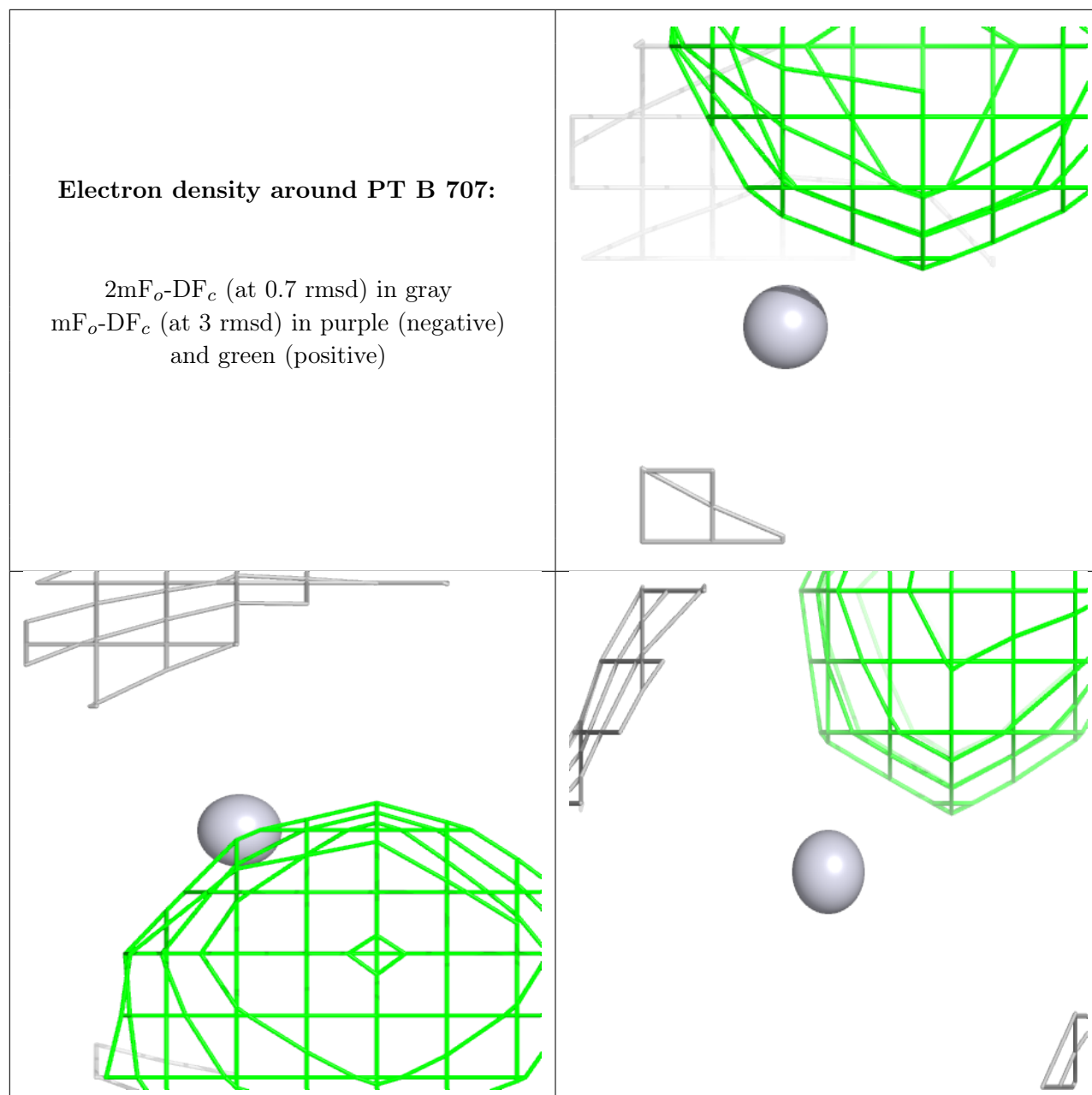
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PT A 704:

$2mF_o - DF_c$ (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.