



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 06:05 PM BST

PDB ID : 6RJV
Title : The X-ray structure of the Gold/Serum Albumin adduct obtained upon reaction of the protein with AuL12, a gold(III) dithiocarbamate complex
Authors : Merlino, A.; Giorgio, A.; Ferraro, G.
Deposited on : 2019-04-29
Resolution : 3.21 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

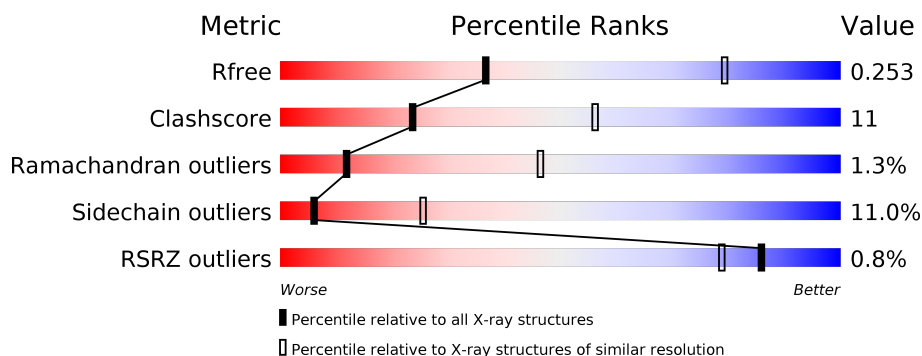
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	583	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 69% 26% . </div> </div>
1	B	583	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 65% 29% 5% </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	601	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9321 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	581	Total	C	N	O	S	0	0	0
			4637	2927	779	892	39			
1	B	581	Total	C	N	O	S	0	0	0
			4637	2927	779	892	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	THR	ALA	conflict	UNP P02769
B	190	THR	ALA	conflict	UNP P02769

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Au	0	0
			1	1		
3	A	1	Total	Au	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		

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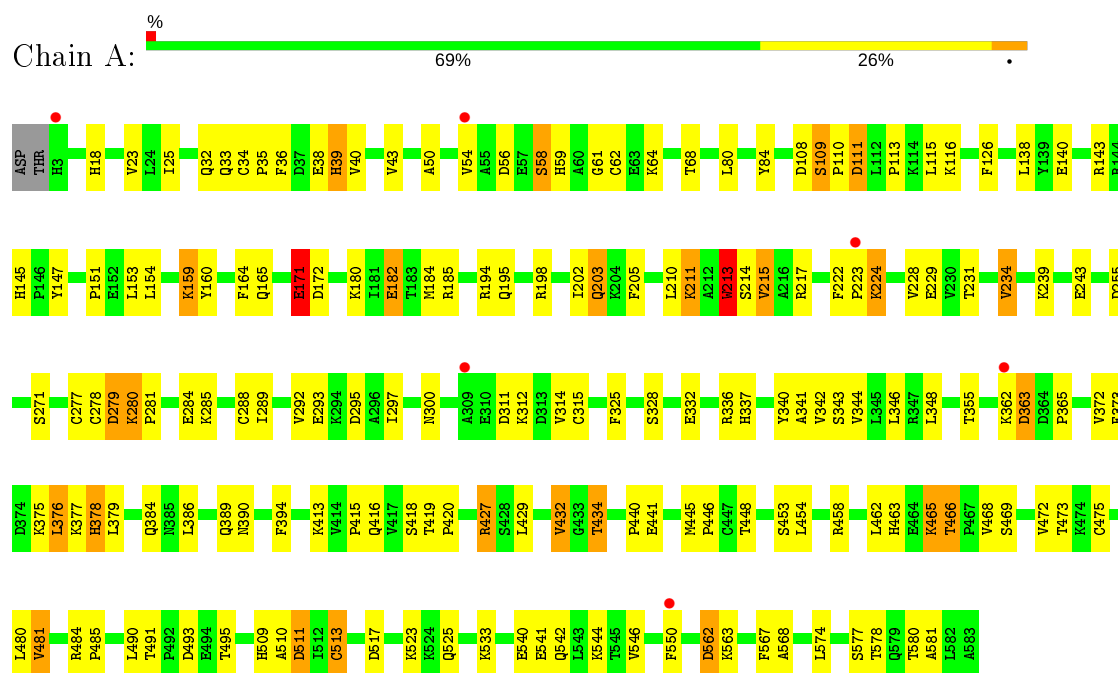
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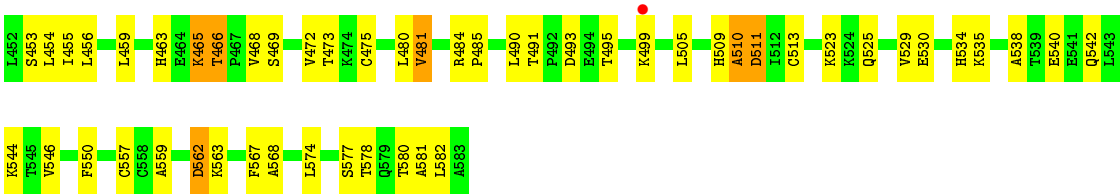
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	22	Total	O	0	0
			22	22		

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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.38Å 44.61Å 142.61Å 90.00° 114.00° 90.00°	Depositor
Resolution (Å)	130.28 – 3.21 130.28 – 3.21	Depositor EDS
% Data completeness (in resolution range)	98.6 (130.28-3.21) 98.6 (130.28-3.21)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.190 , 0.253 0.189 , 0.253	Depositor DCC
R_{free} test set	985 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	97.4	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 79.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9321	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AU

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	0.43	1/4732 (0.0%)	0.87	9/6389 (0.1%)
1	B	0.39	0/4732	0.85	4/6389 (0.1%)
All	All	0.41	1/9464 (0.0%)	0.86	13/12778 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	390	ASN	CG-ND2	10.37	1.58	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	TRP	CA-CB-CG	9.16	131.10	113.70
1	A	171	GLU	CB-CG-CD	-8.51	91.22	114.20
1	B	213	TRP	CA-CB-CG	8.14	129.17	113.70
1	A	427	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	A	171	GLU	CB-CA-C	-6.37	97.66	110.40
1	B	171	GLU	CB-CG-CD	-6.33	97.11	114.20
1	A	427	ARG	NE-CZ-NH1	-6.09	117.25	120.30
1	A	390	ASN	CB-CG-ND2	-5.89	102.56	116.70
1	A	378	HIS	CA-CB-CG	5.66	123.22	113.60
1	B	149	TYR	CB-CG-CD1	5.62	124.38	121.00
1	A	378	HIS	N-CA-CB	-5.45	100.80	110.60
1	B	378	HIS	CB-CA-C	5.38	121.17	110.40
1	A	427	ARG	CD-NE-CZ	5.17	130.83	123.60

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	4637	0	4552	95	0
1	B	4637	0	4552	111	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	21	0	0	1	0
4	B	22	0	0	0	0
All	All	9321	0	9104	204	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 11.

All (204) 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:341:ALA:HB2	1:A:446:PRO:HA	1.51	0.90
1:B:346:LEU:HB3	1:B:481:VAL:HG11	1.57	0.87
1:A:297:ILE:H	1:A:297:ILE:HD12	1.41	0.86
1:B:297:ILE:HD12	1:B:297:ILE:H	1.41	0.85
1:B:341:ALA:HB2	1:B:446:PRO:HA	1.58	0.84
1:B:50:ALA:O	1:B:54:VAL:HG23	1.81	0.80
1:A:50:ALA:O	1:A:54:VAL:HG23	1.87	0.74
1:A:195:GLN:OE1	1:A:198:ARG:NH1	2.21	0.74
1:A:427:ARG:HD2	1:A:525:GLN:OE1	1.89	0.72
1:A:346:LEU:HB3	1:A:481:VAL:HG11	1.72	0.72
1:B:35:PRO:HG2	1:B:38:GLU:HG3	1.73	0.69
1:A:35:PRO:HG2	1:A:38:GLU:HG3	1.75	0.69
1:B:509:HIS:C	1:B:511:ASP:H	1.95	0.68
1:B:223:PRO:HD2	1:B:295:ASP:HB3	1.74	0.68
1:A:341:ALA:HB3	1:A:344:VAL:HG23	1.74	0.68
1:A:550:PHE:HD1	1:A:574:LEU:HD21	1.60	0.67
1:B:332:GLU:HB3	1:B:336:ARG:HH12	1.59	0.67
1:A:332:GLU:HB3	1:A:336:ARG:HH12	1.60	0.66
1:B:341:ALA:HB3	1:B:344:VAL:HG23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ARG:HG3	1:B:342:VAL:HG21	1.78	0.65
1:B:373:PHE:HA	1:B:376:LEU:HB2	1.77	0.65
1:B:195:GLN:OE1	1:B:198:ARG:NH1	2.27	0.64
1:B:550:PHE:HD1	1:B:574:LEU:HD21	1.62	0.64
1:A:223:PRO:HD2	1:A:295:ASP:HB3	1.80	0.64
1:A:61:GLY:HA2	1:A:64:LYS:HD2	1.80	0.63
1:A:285:LYS:O	1:A:289:ILE:HG13	2.00	0.60
1:A:109:SER:OG	1:A:109:SER:O	2.12	0.60
1:A:363:ASP:O	1:A:365:PRO:HD3	2.02	0.60
1:A:108:ASP:HB2	1:A:465:LYS:CE	2.33	0.59
1:B:428:SER:HB3	1:B:455:ILE:HG12	1.84	0.58
1:A:513:CYS:O	1:B:513:CYS:O	2.22	0.58
1:B:185:ARG:HH11	1:B:185:ARG:HG2	1.69	0.58
1:B:239:LYS:O	1:B:243:GLU:HG2	2.04	0.57
1:B:207:GLU:OE2	1:B:242:LYS:HD2	2.05	0.57
1:B:151:PRO:O	1:B:154:LEU:HB2	2.05	0.57
1:A:109:SER:O	1:A:111:ASP:OD1	2.23	0.56
1:A:110:PRO:HD2	4:A:719:HOH:O	2.05	0.56
1:A:115:LEU:HD11	1:A:140:GLU:HB3	1.86	0.56
1:A:373:PHE:HA	1:A:376:LEU:HB2	1.87	0.56
1:B:109:SER:O	1:B:111:ASP:OD1	2.22	0.56
1:A:214:SER:HB3	1:A:234:VAL:HG22	1.88	0.56
1:A:355:THR:HG21	1:A:372:VAL:HG23	1.88	0.56
1:A:36:PHE:O	1:A:40:VAL:HG23	2.07	0.54
1:A:25:ILE:HD11	1:A:138:LEU:HD22	1.90	0.54
1:A:151:PRO:O	1:A:154:LEU:HB2	2.08	0.54
1:B:36:PHE:O	1:B:40:VAL:HG23	2.07	0.54
1:B:346:LEU:HB3	1:B:481:VAL:CG1	2.33	0.54
1:B:182:GLU:OE1	1:B:182:GLU:HA	2.07	0.54
1:B:61:GLY:HA2	1:B:64:LYS:HD2	1.90	0.53
1:A:211:LYS:O	1:A:215:VAL:HG23	2.08	0.53
1:B:211:LYS:O	1:B:215:VAL:HG23	2.08	0.53
1:B:26:ALA:HB2	1:B:249:LEU:HD12	1.91	0.53
1:B:378:HIS:HD2	1:B:378:HIS:O	1.91	0.53
1:A:280:LYS:HB3	1:A:284:GLU:HB3	1.91	0.53
1:A:386:LEU:HD23	1:A:389:GLN:OE1	2.08	0.53
1:A:394:PHE:HZ	1:A:434:THR:HG23	1.73	0.53
1:B:387:ILE:HD12	1:B:388:LYS:N	2.24	0.53
1:B:108:ASP:HB2	1:B:465:LYS:CE	2.39	0.52
1:B:280:LYS:HB3	1:B:284:GLU:HB3	1.90	0.52
1:B:108:ASP:HB2	1:B:465:LYS:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:HG3	1:A:342:VAL:HG21	1.91	0.52
1:B:115:LEU:HD11	1:B:140:GLU:HB3	1.92	0.52
1:A:222:PHE:HD1	1:A:271:SER:HB2	1.75	0.52
1:B:346:LEU:CB	1:B:481:VAL:HG11	2.37	0.52
1:B:61:GLY:O	1:B:64:LYS:HB2	2.09	0.52
1:A:239:LYS:O	1:A:243:GLU:HG2	2.10	0.52
1:B:142:ALA:HB2	1:B:153:LEU:HD21	1.91	0.51
1:B:222:PHE:HD1	1:B:271:SER:HB2	1.76	0.51
1:A:32:GLN:O	1:A:143:ARG:NH2	2.40	0.51
1:B:394:PHE:HZ	1:B:434:THR:HG23	1.76	0.51
1:A:517:ASP:OD1	1:B:563:LYS:HE2	2.11	0.51
1:B:59:HIS:HB3	1:B:62:CYS:SG	2.51	0.51
1:A:277:CYS:SG	1:A:288:CYS:C	2.90	0.51
1:B:510:ALA:HA	1:B:567:PHE:CE2	2.46	0.51
1:A:332:GLU:HB3	1:A:336:ARG:NH1	2.27	0.50
1:B:540:GLU:OE1	1:B:540:GLU:N	2.44	0.50
1:B:355:THR:HG21	1:B:372:VAL:HG23	1.93	0.50
1:A:277:CYS:C	1:A:279:ASP:H	2.16	0.50
1:B:145:HIS:O	1:B:147:TYR:N	2.45	0.49
1:B:277:CYS:SG	1:B:288:CYS:C	2.91	0.49
1:B:32:GLN:O	1:B:143:ARG:NH2	2.44	0.49
1:A:35:PRO:HG2	1:A:38:GLU:CG	2.42	0.49
1:A:415:PRO:O	1:A:533:LYS:HE2	2.13	0.49
1:A:458:ARG:NH2	1:A:462:LEU:HD21	2.27	0.49
1:B:277:CYS:C	1:B:279:ASP:H	2.16	0.49
1:B:542:GLN:O	1:B:546:VAL:HG23	2.12	0.49
1:B:429:LEU:O	1:B:432:VAL:HB	2.13	0.49
1:A:108:ASP:HB2	1:A:465:LYS:HE3	1.93	0.49
1:A:542:GLN:O	1:A:546:VAL:HG23	2.12	0.49
1:B:465:LYS:HB3	1:B:466:THR:HG22	1.94	0.49
1:A:202:ILE:HG13	1:A:203:GLN:N	2.28	0.48
1:A:394:PHE:CZ	1:A:434:THR:HG23	2.48	0.48
1:B:35:PRO:HG2	1:B:38:GLU:CG	2.41	0.48
1:A:202:ILE:HG23	1:A:210:LEU:HD22	1.95	0.48
1:A:511:ASP:O	1:A:511:ASP:OD2	2.31	0.48
1:A:34:CYS:HB2	1:A:39:HIS:CE1	2.48	0.48
1:B:378:HIS:CD2	1:B:378:HIS:O	2.66	0.48
1:A:108:ASP:HB2	1:A:465:LYS:HE2	1.95	0.48
1:A:346:LEU:HB3	1:A:481:VAL:CG1	2.39	0.48
1:A:239:LYS:NZ	1:A:255:ASP:OD2	2.45	0.48
1:A:292:VAL:HG22	1:A:293:GLU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:SER:HB3	1:B:234:VAL:HG22	1.95	0.48
1:B:211:LYS:O	1:B:214:SER:HB2	2.14	0.48
1:B:419:THR:HB	1:B:420:PRO:HD3	1.95	0.47
1:A:348:LEU:HD23	1:A:376:LEU:HD22	1.96	0.47
1:B:394:PHE:CZ	1:B:434:THR:HG23	2.49	0.47
1:A:59:HIS:HB3	1:A:62:CYS:SG	2.55	0.47
1:A:429:LEU:O	1:A:432:VAL:HB	2.13	0.47
1:B:196:ARG:HG3	1:B:196:ARG:O	2.15	0.47
1:B:25:ILE:HD11	1:B:138:LEU:HD22	1.96	0.47
1:B:151:PRO:HG3	1:B:253:ALA:HA	1.95	0.47
1:A:337:HIS:HB3	1:A:340:TYR:CD1	2.49	0.47
1:A:413:LYS:HG2	1:A:490:LEU:HB2	1.96	0.47
1:B:325:PHE:O	1:B:328:SER:HB3	2.14	0.47
1:B:202:ILE:HG23	1:B:210:LEU:HD22	1.97	0.47
1:A:510:ALA:HA	1:A:567:PHE:CE2	2.50	0.46
1:B:239:LYS:NZ	1:B:243:GLU:OE2	2.44	0.46
1:B:393:GLN:HG2	1:B:402:PHE:CD1	2.50	0.46
1:A:300:ASN:N	1:A:300:ASN:HD22	2.12	0.46
1:B:484:ARG:HB3	1:B:485:PRO:HD3	1.96	0.46
1:A:550:PHE:CD1	1:A:574:LEU:HD21	2.47	0.46
1:B:109:SER:OG	1:B:109:SER:O	2.22	0.46
1:B:285:LYS:O	1:B:289:ILE:HG13	2.15	0.46
1:A:540:GLU:OE1	1:A:540:GLU:N	2.48	0.46
1:A:463:HIS:CG	1:A:472:VAL:HG11	2.50	0.46
1:A:509:HIS:C	1:A:511:ASP:H	2.18	0.46
1:B:202:ILE:HG13	1:B:203:GLN:N	2.31	0.46
1:A:484:ARG:HB3	1:A:485:PRO:HD3	1.97	0.46
1:B:578:THR:HA	1:B:581:ALA:HB3	1.97	0.45
1:A:205:PHE:CE2	1:A:480:LEU:HD13	2.51	0.45
1:A:562:ASP:C	1:A:562:ASP:OD1	2.54	0.45
1:B:363:ASP:O	1:B:365:PRO:HD3	2.17	0.45
1:B:463:HIS:CG	1:B:472:VAL:HG11	2.52	0.45
1:A:416:GLN:HA	1:A:416:GLN:OE1	2.17	0.45
1:B:550:PHE:CD1	1:B:574:LEU:HD21	2.47	0.45
1:A:465:LYS:HB3	1:A:466:THR:HG22	1.97	0.45
1:B:148:PHE:HE2	1:B:188:VAL:HG13	1.81	0.45
1:A:311:ASP:HB3	1:A:314:VAL:HG23	1.99	0.45
1:A:23:VAL:HG12	1:A:43:VAL:HG22	1.98	0.45
1:A:578:THR:HA	1:A:581:ALA:HB3	1.98	0.45
1:B:33:GLN:HE21	1:B:33:GLN:HB2	1.50	0.45
1:A:145:HIS:O	1:A:147:TYR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:SER:OG	1:B:421:THR:OG1	2.23	0.45
1:B:562:ASP:OD1	1:B:562:ASP:C	2.55	0.45
1:A:138:LEU:HD23	1:A:153:LEU:HG	2.00	0.44
1:A:277:CYS:O	1:A:279:ASP:N	2.49	0.44
1:A:325:PHE:O	1:A:328:SER:HB3	2.16	0.44
1:B:171:GLU:HG2	1:B:172:ASP:H	1.82	0.44
1:A:363:ASP:C	1:A:365:PRO:HD3	2.38	0.44
1:B:413:LYS:HG2	1:B:490:LEU:HB2	2.00	0.44
1:B:297:ILE:H	1:B:297:ILE:CD1	2.13	0.44
1:B:557:CYS:C	1:B:559:ALA:H	2.21	0.44
1:A:182:GLU:HA	1:A:182:GLU:OE1	2.15	0.44
1:B:126:PHE:CZ	1:B:165:GLN:HA	2.53	0.44
1:B:39:HIS:O	1:B:43:VAL:HG23	2.17	0.44
1:B:194:ARG:HA	1:B:454:LEU:HD22	1.98	0.44
1:B:509:HIS:O	1:B:511:ASP:N	2.47	0.44
1:A:61:GLY:O	1:A:64:LYS:HB2	2.18	0.44
1:A:346:LEU:CB	1:A:481:VAL:HG11	2.45	0.44
1:A:126:PHE:CZ	1:A:165:GLN:HA	2.52	0.44
1:B:535:LYS:HG3	1:B:582:LEU:HD23	1.98	0.43
1:B:332:GLU:HB3	1:B:336:ARG:NH1	2.28	0.43
1:B:505:LEU:HD22	1:B:530:GLU:HG3	2.01	0.43
1:B:525:GLN:O	1:B:529:VAL:HG23	2.18	0.43
1:B:300:ASN:HD22	1:B:300:ASN:N	2.16	0.43
1:A:202:ILE:HG13	1:A:203:GLN:H	1.82	0.43
1:A:171:GLU:HB3	1:A:172:ASP:H	1.31	0.43
1:A:297:ILE:CD1	1:A:297:ILE:H	2.14	0.43
1:A:194:ARG:HA	1:A:454:LEU:HD22	1.99	0.43
1:B:510:ALA:HA	1:B:567:PHE:CD2	2.53	0.43
1:A:213:TRP:HA	1:A:346:LEU:HD11	2.00	0.43
1:B:178:LEU:HD23	1:B:181:ILE:HD11	1.99	0.43
1:A:160:TYR:CZ	1:A:164:PHE:HE2	2.37	0.42
1:A:419:THR:HB	1:A:420:PRO:HD3	2.00	0.42
1:A:541:GLU:HG2	1:A:541:GLU:H	1.67	0.42
1:B:205:PHE:CE2	1:B:480:LEU:HD13	2.54	0.42
1:B:226:GLU:HB3	1:B:228:VAL:HG23	2.01	0.42
1:A:138:LEU:HD21	1:A:154:LEU:HD23	2.01	0.42
1:A:224:LYS:HB2	1:A:295:ASP:OD2	2.20	0.42
1:B:414:VAL:C	1:B:416:GLN:H	2.21	0.42
1:B:372:VAL:C	1:B:374:ASP:H	2.22	0.42
1:A:56:ASP:C	1:A:58:SER:H	2.24	0.42
1:A:562:ASP:O	1:A:563:LYS:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:LEU:HD22	1:B:222:PHE:HE2	1.85	0.41
1:B:171:GLU:HG2	1:B:172:ASP:N	2.34	0.41
1:B:350:LYS:O	1:B:353:GLU:HB3	2.19	0.41
1:B:386:LEU:HD23	1:B:389:GLN:OE1	2.20	0.41
1:B:509:HIS:C	1:B:511:ASP:N	2.67	0.41
1:B:574:LEU:O	1:B:577:SER:HB2	2.20	0.41
1:B:384:GLN:O	1:B:387:ILE:HG13	2.21	0.41
1:B:499:LYS:O	1:B:534:HIS:HA	2.21	0.41
1:B:142:ALA:HB2	1:B:153:LEU:CD2	2.50	0.41
1:B:152:GLU:O	1:B:155:TYR:HB3	2.20	0.41
1:B:451:TYR:O	1:B:455:ILE:HD12	2.21	0.41
1:B:407:ILE:HG23	1:B:529:VAL:HG22	2.02	0.41
1:A:159:LYS:HD3	1:A:159:LYS:HA	1.79	0.41
1:B:40:VAL:O	1:B:44:ASN:ND2	2.54	0.41
1:B:440:PRO:O	1:B:442:SER:N	2.54	0.41
1:B:456:LEU:O	1:B:459:LEU:HB3	2.21	0.41
1:A:80:LEU:HD12	1:A:84:TYR:CD1	2.56	0.40
1:B:443:GLU:O	1:B:446:PRO:HD2	2.21	0.40
1:B:412:ARG:NH2	1:B:538:ALA:O	2.54	0.40
1:A:574:LEU:O	1:A:577:SER:HB2	2.22	0.40
1:B:29:GLN:HG2	1:B:146:PRO:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	579/583 (99%)	527 (91%)	46 (8%)	6 (1%)	15	52
1	B	579/583 (99%)	533 (92%)	37 (6%)	9 (2%)	9	42
All	All	1158/1166 (99%)	1060 (92%)	83 (7%)	15 (1%)	12	46

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	441	GLU
1	B	510	ALA
1	A	215	VAL
1	A	441	GLU
1	A	568	ALA
1	B	128	ALA
1	B	113	PRO
1	B	281	PRO
1	B	299	GLU
1	B	568	ALA
1	A	278	CYS
1	A	281	PRO
1	B	254	ASP
1	A	113	PRO
1	B	215	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	519/521 (100%)	461 (89%)	58 (11%)	6	24
1	B	519/521 (100%)	463 (89%)	56 (11%)	6	26
All	All	1038/1042 (100%)	924 (89%)	114 (11%)	6	25

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	33	GLN
1	A	39	HIS
1	A	58	SER
1	A	68	THR
1	A	109	SER
1	A	111	ASP
1	A	116	LYS

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Mol	Chain	Res	Type
1	A	159	LYS
1	A	171	GLU
1	A	180	LYS
1	A	182	GLU
1	A	184	MET
1	A	185	ARG
1	A	203	GLN
1	A	211	LYS
1	A	213	TRP
1	A	224	LYS
1	A	228	VAL
1	A	229	GLU
1	A	231	THR
1	A	234	VAL
1	A	279	ASP
1	A	280	LYS
1	A	312	LYS
1	A	315	CYS
1	A	343	SER
1	A	362	LYS
1	A	363	ASP
1	A	375	LYS
1	A	376	LEU
1	A	377	LYS
1	A	378	HIS
1	A	379	LEU
1	A	384	GLN
1	A	418	SER
1	A	432	VAL
1	A	434	THR
1	A	440	PRO
1	A	445	MET
1	A	448	THR
1	A	453	SER
1	A	465	LYS
1	A	466	THR
1	A	468	VAL
1	A	469	SER
1	A	473	THR
1	A	475	CYS
1	A	481	VAL
1	A	491	THR

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Mol	Chain	Res	Type
1	A	493	ASP
1	A	495	THR
1	A	511	ASP
1	A	513	CYS
1	A	523	LYS
1	A	544	LYS
1	A	562	ASP
1	A	580	THR
1	B	39	HIS
1	B	58	SER
1	B	68	THR
1	B	109	SER
1	B	111	ASP
1	B	159	LYS
1	B	185	ARG
1	B	203	GLN
1	B	211	LYS
1	B	213	TRP
1	B	224	LYS
1	B	228	VAL
1	B	231	THR
1	B	234	VAL
1	B	279	ASP
1	B	280	LYS
1	B	281	PRO
1	B	284	GLU
1	B	297	ILE
1	B	307	ASP
1	B	315	CYS
1	B	333	TYR
1	B	343	SER
1	B	362	LYS
1	B	363	ASP
1	B	375	LYS
1	B	376	LEU
1	B	377	LYS
1	B	378	HIS
1	B	379	LEU
1	B	381	ASP
1	B	384	GLN
1	B	418	SER
1	B	427	ARG

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Mol	Chain	Res	Type
1	B	432	VAL
1	B	434	THR
1	B	435	ARG
1	B	440	PRO
1	B	445	MET
1	B	448	THR
1	B	453	SER
1	B	465	LYS
1	B	466	THR
1	B	468	VAL
1	B	469	SER
1	B	473	THR
1	B	475	CYS
1	B	481	VAL
1	B	491	THR
1	B	493	ASP
1	B	495	THR
1	B	511	ASP
1	B	523	LYS
1	B	544	LYS
1	B	562	ASP
1	B	580	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	44	ASN
1	A	300	ASN
1	A	384	GLN
1	B	33	GLN
1	B	44	ASN
1	B	266	ASN
1	B	300	ASN
1	B	378	HIS
1	B	384	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	581/583 (99%)	-0.04	6 (1%)	82 73	76, 112, 161, 191	0
1	B	581/583 (99%)	-0.11	3 (0%)	91 86	74, 111, 156, 179	0
All	All	1162/1166 (99%)	-0.07	9 (0%)	86 79	74, 112, 160, 191	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	550	PHE	3.4
1	A	309	ALA	3.1
1	A	362	LYS	3.0
1	A	3	HIS	2.7
1	A	223	PRO	2.4
1	B	74	LEU	2.3
1	B	270	ILE	2.3
1	A	54	VAL	2.2
1	B	499	LYS	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 monosaccharides 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
2	MG	A	601	1/1	0.63	0.60	75,75,75,75	1
3	AU	B	602	1/1	0.91	0.11	119,119,119,119	1
2	MG	B	601	1/1	0.93	0.52	48,48,48,48	1
3	AU	A	602	1/1	0.98	0.12	111,111,111,111	1

6.5 Other polymers [i](#)

There are no such residues in this entry.