



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:25 PM GMT

PDB ID : 4E4V
Title : The crystal structure of the dimeric human importin alpha 1 at 2.5 angstrom resolution.
Authors : Hang, P.C.; Miknis, Z.M.; Franke, W.A.; Umland, T.C.; Schultz, L.W.
Deposited on : 2012-03-13
Resolution : 2.53 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

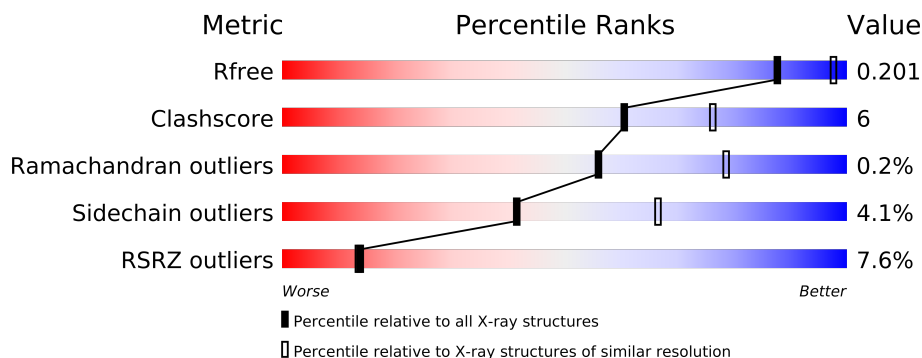
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.53 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}	66092	3240 (2.54-2.50)
Clashscore	79885	4080 (2.54-2.50)
Ramachandran outliers	78287	3990 (2.54-2.50)
Sidechain outliers	78261	3992 (2.54-2.50)
RSRZ outliers	66119	3241 (2.54-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	485	
1	B	485	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	A	601	-	X
2	GOL	A	603	-	X
2	GOL	A	605	-	X
2	GOL	A	607	-	X
2	GOL	A	608	-	X
2	GOL	B	601	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	B	602	-	X
2	GOL	B	603	-	X
2	GOL	B	604	-	X
2	GOL	B	605	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13702 atoms, of which 6849 are hydrogens and 0 are deuterium.

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 Importin subunit alpha-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	433	Total	C	H	N	O	S	0	2	0
			6658	2101	3359	554	632	12			
1	B	433	Total	C	H	N	O	S	0	1	0
			6660	2096	3366	554	631	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	MET	-	EXPRESSION TAG	UNP P52292
A	46	GLY	-	EXPRESSION TAG	UNP P52292
A	47	SER	-	EXPRESSION TAG	UNP P52292
A	48	SER	-	EXPRESSION TAG	UNP P52292
A	49	HIS	-	EXPRESSION TAG	UNP P52292
A	50	HIS	-	EXPRESSION TAG	UNP P52292
A	51	HIS	-	EXPRESSION TAG	UNP P52292
A	52	HIS	-	EXPRESSION TAG	UNP P52292
A	53	HIS	-	EXPRESSION TAG	UNP P52292
A	54	SER	-	EXPRESSION TAG	UNP P52292
A	55	SER	-	EXPRESSION TAG	UNP P52292
A	56	GLY	-	EXPRESSION TAG	UNP P52292
A	57	GLU	-	EXPRESSION TAG	UNP P52292
A	58	ASN	-	EXPRESSION TAG	UNP P52292
A	59	LEU	-	EXPRESSION TAG	UNP P52292
A	60	TYR	-	EXPRESSION TAG	UNP P52292
A	61	PHE	-	EXPRESSION TAG	UNP P52292
A	62	GLN	-	EXPRESSION TAG	UNP P52292
A	63	GLY	-	EXPRESSION TAG	UNP P52292
A	64	HIS	-	EXPRESSION TAG	UNP P52292
A	65	MET	-	EXPRESSION TAG	UNP P52292
A	66	LEU	-	EXPRESSION TAG	UNP P52292
A	67	ASP	-	EXPRESSION TAG	UNP P52292
A	68	ALA	-	EXPRESSION TAG	UNP P52292
A	69	LEU	-	EXPRESSION TAG	UNP P52292

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Chain	Residue	Modelled	Actual	Comment	Reference
A	486	ARG	LYS	ENGINEERED MUTATION	UNP P52292
B	45	MET	-	EXPRESSION TAG	UNP P52292
B	46	GLY	-	EXPRESSION TAG	UNP P52292
B	47	SER	-	EXPRESSION TAG	UNP P52292
B	48	SER	-	EXPRESSION TAG	UNP P52292
B	49	HIS	-	EXPRESSION TAG	UNP P52292
B	50	HIS	-	EXPRESSION TAG	UNP P52292
B	51	HIS	-	EXPRESSION TAG	UNP P52292
B	52	HIS	-	EXPRESSION TAG	UNP P52292
B	53	HIS	-	EXPRESSION TAG	UNP P52292
B	54	SER	-	EXPRESSION TAG	UNP P52292
B	55	SER	-	EXPRESSION TAG	UNP P52292
B	56	GLY	-	EXPRESSION TAG	UNP P52292
B	57	GLU	-	EXPRESSION TAG	UNP P52292
B	58	ASN	-	EXPRESSION TAG	UNP P52292
B	59	LEU	-	EXPRESSION TAG	UNP P52292
B	60	TYR	-	EXPRESSION TAG	UNP P52292
B	61	PHE	-	EXPRESSION TAG	UNP P52292
B	62	GLN	-	EXPRESSION TAG	UNP P52292
B	63	GLY	-	EXPRESSION TAG	UNP P52292
B	64	HIS	-	EXPRESSION TAG	UNP P52292
B	65	MET	-	EXPRESSION TAG	UNP P52292
B	66	LEU	-	EXPRESSION TAG	UNP P52292
B	67	ASP	-	EXPRESSION TAG	UNP P52292
B	68	ALA	-	EXPRESSION TAG	UNP P52292
B	69	LEU	-	EXPRESSION TAG	UNP P52292
B	486	ARG	LYS	ENGINEERED MUTATION	UNP P52292

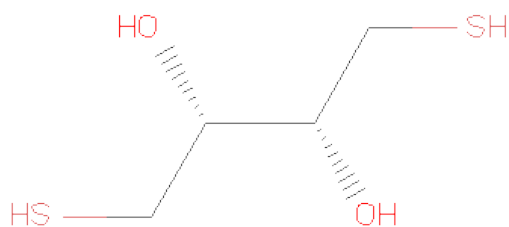
- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula:

C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	S	0	0
			18	4	10	2	2		
3	B	1	Total	C	H	O	S	0	0
			18	4	10	2	2		

- Molecule 4 is water.

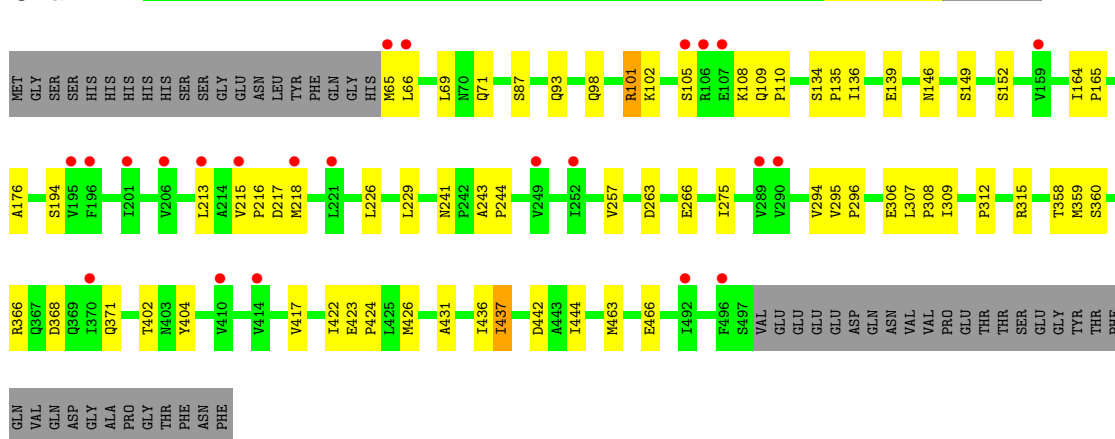
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	79	Total	O	0	0
			79	79		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

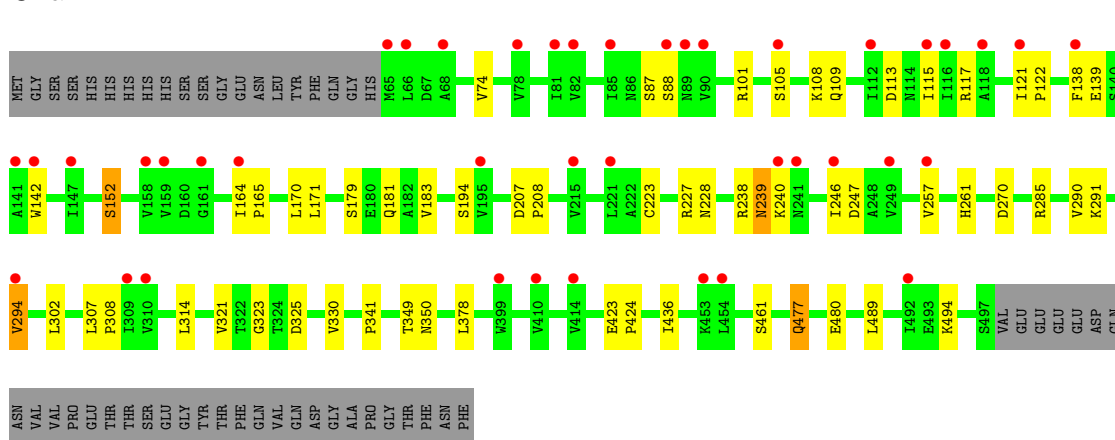
• Molecule 1: Importin subunit alpha-2

Chain A:



• Molecule 1: Importin subunit alpha-2

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.52Å 143.52Å 136.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.81 – 2.53 34.81 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.4 (34.81-2.53) 94.9 (34.81-2.53)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.57 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.155 , 0.203 0.157 , 0.201	Depositor DCC
R_{free} test set	1900 reflections (4.14%)	DCC
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 39.7	EDS
Estimated twinning fraction	0.013 for -h,-l,-k 0.006 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 47595 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13702	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: GOL, DTT

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	0.66	0/3363	0.73	2/4589 (0.0%)
1	B	0.61	0/3355	0.71	1/4578 (0.0%)
All	All	0.63	0/6718	0.72	3/9167 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	101	ARG	CG-CD-NE	-5.49	100.27	111.80
1	B	294	VAL	CB-CA-C	-5.42	101.11	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3299	3359	0	44	0
1	B	3294	3366	0	37	0
2	A	48	64	0	6	0
2	B	30	40	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	10	0	0	0
3	B	8	10	0	1	0
4	A	87	0	0	3	2
4	B	79	0	0	5	1
All	All	6853	6849	0	80	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (80) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:366:ARG:NH1	1:A:368:ASP:OD1	2.14	0.81
2:A:603:GOL:H11	1:B:480:GLU:O	1.89	0.73
1:B:257:VAL:HG22	1:B:294:VAL:CG1	2.20	0.71
1:A:426:MET:CE	1:A:444:ILE:HD11	2.21	0.70
1:A:257:VAL:HG22	1:A:294:VAL:CG1	2.22	0.70
1:B:270:ASP:OD2	4:B:753:HOH:O	2.10	0.69
1:A:266:GLU:OE1	4:A:733:HOH:O	2.11	0.68
1:B:101:ARG:HG2	1:B:139:GLU:OE1	1.95	0.66
1:A:176:ALA:HB2	2:A:603:GOL:H31	1.79	0.65
1:B:108:LYS:O	1:B:109:GLN:HG2	1.95	0.64
1:A:101:ARG:HG2	1:A:139:GLU:OE1	1.97	0.64
1:A:65:MET:HE1	4:A:744:HOH:O	1.99	0.63
1:B:257:VAL:HG22	1:B:294:VAL:HG12	1.80	0.62
1:B:101:ARG:O	1:B:105:SER:HB2	2.00	0.61
1:A:241:ASN:OD1	1:B:152:SER:OG	2.19	0.60
1:A:213:LEU:HD22	1:A:218:MET:HE1	1.84	0.60
1:A:417:VAL:HG13	1:A:422[A]:ILE:HD11	1.84	0.60
1:A:257:VAL:HG22	1:A:294:VAL:HG13	1.85	0.57
1:A:426:MET:CE	1:A:444:ILE:CD1	2.85	0.55
1:A:307:LEU:N	1:A:308:PRO:CD	2.70	0.54
1:B:325:ASP:HA	4:B:744:HOH:O	2.07	0.54
1:B:138:PHE:CE1	1:B:181:GLN:HG2	2.42	0.53
1:B:246:ILE:HD12	1:B:285:ARG:NE	2.23	0.53
2:A:603:GOL:C1	1:B:480:GLU:O	2.54	0.53
3:B:606:DTT:S4	4:B:712:HOH:O	2.59	0.53
2:A:603:GOL:H12	1:B:480:GLU:HB3	1.90	0.52
1:B:113:ASP:O	1:B:117:ARG:HG3	2.10	0.51
1:B:423:GLU:HB3	1:B:424:PRO:HD3	1.93	0.50
1:B:171:LEU:CD2	1:B:183:VAL:HG21	2.42	0.50
1:A:87:SER:O	1:A:93:GLN:NE2	2.42	0.50
1:A:108:LYS:HE3	1:B:321:VAL:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:306:GLU:HB3	1:A:308:PRO:HD2	1.95	0.48
1:A:109:GLN:N	1:A:110:PRO:CD	2.76	0.48
1:A:105:SER:HB3	1:A:146:ASN:HD22	1.79	0.48
1:A:309:ILE:O	1:A:312:PRO:HD2	2.14	0.47
1:B:108:LYS:O	1:B:109:GLN:CG	2.61	0.47
1:A:295:VAL:N	1:A:296:PRO:CD	2.76	0.47
2:B:604:GOL:H31	4:B:745:HOH:O	2.15	0.47
1:B:228:ASN:ND2	2:B:605:GOL:O1	2.48	0.46
1:B:477:GLN:OE1	1:B:489:LEU:HD13	2.16	0.46
1:A:71:GLN:HA	1:A:98:GLN:OE1	2.15	0.46
1:A:431:ALA:O	1:A:437:ILE:HD13	2.15	0.46
1:A:307:LEU:N	1:A:308:PRO:HD3	2.31	0.46
1:B:121:ILE:N	1:B:122:PRO:HD2	2.31	0.46
1:A:243:ALA:HB1	1:A:244:PRO:HD2	1.97	0.46
1:B:207:ASP:HB2	1:B:208:PRO:HD3	1.98	0.45
1:B:238:ARG:O	1:B:239:ASN:HB2	2.16	0.45
1:A:417:VAL:HG13	1:A:463:MET:HE1	1.98	0.45
1:B:290:VAL:HG13	1:B:330:VAL:HG11	1.99	0.45
1:A:436:ILE:HA	1:A:436:ILE:HD12	1.82	0.45
1:A:164:ILE:HB	1:A:165:PRO:HD3	1.99	0.44
1:A:105:SER:HB3	1:A:146:ASN:ND2	2.32	0.44
1:A:226:LEU:HA	1:A:226:LEU:HD12	1.86	0.44
1:B:207:ASP:HB2	1:B:208:PRO:CD	2.48	0.44
1:A:257:VAL:HG22	1:A:294:VAL:HG11	1.97	0.43
1:A:423:GLU:HB3	1:A:424:PRO:HD3	2.00	0.43
1:A:263:ASP:C	1:A:263:ASP:OD1	2.57	0.43
1:B:257:VAL:HG13	1:B:294:VAL:HG11	2.01	0.43
1:B:240:LYS:HB3	1:B:240:LYS:HE3	1.89	0.43
1:A:371:GLN:HE22	2:A:608:GOL:C1	2.31	0.43
1:A:358:THR:HA	4:A:720:HOH:O	2.18	0.43
1:B:74:VAL:O	1:B:74:VAL:HG12	2.19	0.43
1:A:101:ARG:HG3	1:A:102:LYS:N	2.33	0.42
1:B:307:LEU:N	1:B:308:PRO:CD	2.82	0.42
1:B:101:ARG:HD3	1:B:142:TRP:CD2	2.55	0.41
1:A:108:LYS:HE2	1:B:323:GLY:O	2.20	0.41
1:A:371:GLN:HE22	2:A:608:GOL:H11	1.85	0.41
1:B:164:ILE:HB	1:B:165:PRO:HD3	2.02	0.41
1:A:215:VAL:HB	1:A:216:PRO:CD	2.50	0.41
1:A:426:MET:HE1	1:A:444:ILE:CD1	2.51	0.41
1:A:213:LEU:HD22	1:A:218:MET:CE	2.49	0.41
1:A:213:LEU:HG	1:A:229:LEU:HD21	2.03	0.41
1:A:134:SER:N	1:A:135:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:341:PRO:HD3	1:B:378:LEU:HD23	2.02	0.41
1:B:170:LEU:HA	1:B:170:LEU:HD23	1.95	0.41
1:B:302:LEU:HD21	1:B:314:LEU:HA	2.03	0.40
1:B:261:HIS:HD2	4:B:740:HOH:O	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:763:HOH:O	4:A:763:HOH:O[8_555]	1.66	0.54
4:A:750:HOH:O	4:B:763:HOH:O[3_444]	2.01	0.19

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	433/485 (89%)	420 (97%)	13 (3%)	0	100	100
1	B	432/485 (89%)	423 (98%)	7 (2%)	2 (0%)	38	60
All	All	865/970 (89%)	843 (98%)	20 (2%)	2 (0%)	56	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	477	GLN
1	B	239	ASN

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	367/410 (90%)	350 (95%)	17 (5%)	37	60
1	B	366/410 (89%)	351 (96%)	15 (4%)	41	66
All	All	733/820 (89%)	701 (96%)	32 (4%)	41	63

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	69	LEU
1	A	136	ILE
1	A	149[A]	SER
1	A	149[B]	SER
1	A	152	SER
1	A	194	SER
1	A	217	ASP
1	A	275	ILE
1	A	315	ARG
1	A	359	MET
1	A	360	SER
1	A	402	THR
1	A	404	TYR
1	A	437	ILE
1	A	442	ASP
1	A	466	GLU
1	B	87	SER
1	B	88	SER
1	B	115	ILE
1	B	152	SER
1	B	179	SER
1	B	194	SER
1	B	223[A]	CYS
1	B	223[B]	CYS
1	B	247	ASP
1	B	291	LYS
1	B	349	THR
1	B	350	ASN
1	B	436	ILE
1	B	461	SER
1	B	494	LYS

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	86	ASN
1	A	93	GLN
1	A	137	GLN
1	A	188	ASN
1	A	367	GLN
1	A	479	HIS
1	B	188	ASN
1	B	228	ASN
1	B	371	GLN
1	B	479	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

15 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	GOL	A	601	-	5,5,5	0.34	0	5,5,5	0.43	0
2	GOL	A	602	-	5,5,5	0.42	0	5,5,5	0.20	0
2	GOL	A	603	-	5,5,5	0.40	0	5,5,5	1.39	1 (20%)
2	GOL	A	604	-	5,5,5	0.36	0	5,5,5	0.29	0
2	GOL	A	605	-	5,5,5	0.32	0	5,5,5	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	606	-	5,5,5	0.26	0	5,5,5	0.26	0
2	GOL	A	607	-	5,5,5	0.28	0	5,5,5	0.53	0
2	GOL	A	608	-	5,5,5	0.43	0	5,5,5	0.57	0
3	DTT	A	609	-	7,7,7	1.20	1 (14%)	8,8,8	1.54	1 (12%)
2	GOL	B	601	-	5,5,5	0.33	0	5,5,5	0.50	0
2	GOL	B	602	-	5,5,5	0.23	0	5,5,5	0.72	0
2	GOL	B	603	-	5,5,5	0.29	0	5,5,5	0.39	0
2	GOL	B	604	-	5,5,5	0.28	0	5,5,5	0.44	0
2	GOL	B	605	-	5,5,5	0.35	0	5,5,5	0.41	0
3	DTT	B	606	-	7,7,7	0.82	0	8,8,8	1.37	3 (37%)

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	GOL	A	601	-	-	0/4/4/4	0/0/0/0
2	GOL	A	602	-	-	0/4/4/4	0/0/0/0
2	GOL	A	603	-	-	0/4/4/4	0/0/0/0
2	GOL	A	604	-	-	0/4/4/4	0/0/0/0
2	GOL	A	605	-	-	0/4/4/4	0/0/0/0
2	GOL	A	606	-	-	0/4/4/4	0/0/0/0
2	GOL	A	607	-	-	0/4/4/4	0/0/0/0
2	GOL	A	608	-	-	0/4/4/4	0/0/0/0
3	DTT	A	609	-	-	0/8/8/8	0/0/0/0
2	GOL	B	601	-	-	0/4/4/4	0/0/0/0
2	GOL	B	602	-	-	0/4/4/4	0/0/0/0
2	GOL	B	603	-	-	0/4/4/4	0/0/0/0
2	GOL	B	604	-	-	0/4/4/4	0/0/0/0
2	GOL	B	605	-	-	0/4/4/4	0/0/0/0
3	DTT	B	606	-	-	0/8/8/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	609	DTT	C4-C3	2.00	1.55	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	609	DTT	C3-C4-S4	3.47	120.12	114.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	606	DTT	O3-C3-C4	-2.19	105.75	109.87
2	A	603	GOL	O1-C1-C2	2.17	120.31	109.71
3	B	606	DTT	O2-C2-C3	2.03	113.79	109.83
3	B	606	DTT	O2-C2-C1	-2.02	106.08	109.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	433/485 (89%)	0.31	23 (5%) 25 26	43, 58, 86, 110	1 (0%)
1	B	433/485 (89%)	0.56	41 (9%) 8 8	38, 60, 99, 127	0
All	All	866/970 (89%)	0.43	64 (7%) 14 14	38, 59, 94, 127	1 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	VAL	4.6
1	B	240	LYS	4.6
1	B	115	ILE	4.4
1	A	201	ILE	4.4
1	A	206	VAL	4.2
1	B	88	SER	4.0
1	A	65	MET	3.9
1	B	399	TRP	3.7
1	B	195	VAL	3.7
1	B	89	ASN	3.6
1	B	82	VAL	3.6
1	B	410	VAL	3.6
1	B	85	ILE	3.5
1	B	164	ILE	3.4
1	B	78	VAL	3.3
1	B	81	ILE	3.2
1	A	492	ILE	3.2
1	B	309	ILE	3.2
1	A	195	VAL	3.2
1	A	66	LEU	3.2
1	B	414	VAL	3.2
1	B	66	LEU	3.1
1	A	218	MET	3.1
1	B	246	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	106	ARG	2.9
1	A	221	LEU	2.8
1	B	68	ALA	2.8
1	A	105	SER	2.8
1	A	410	VAL	2.8
1	B	215	VAL	2.8
1	A	252	ILE	2.8
1	B	147	ILE	2.8
1	B	454	LEU	2.8
1	B	158	VAL	2.7
1	B	65	MET	2.6
1	B	118	ALA	2.6
1	B	142	TRP	2.6
1	A	213	LEU	2.6
1	A	215	VAL	2.6
1	A	159	VAL	2.5
1	B	159	VAL	2.5
1	B	257	VAL	2.5
1	B	138	PHE	2.5
1	B	161	GLY	2.4
1	B	141	ALA	2.4
1	A	196	PHE	2.4
1	A	249	VAL	2.3
1	B	221	LEU	2.3
1	A	370	ILE	2.3
1	B	121	ILE	2.3
1	B	112	ILE	2.3
1	A	290	VAL	2.2
1	B	249	VAL	2.2
1	B	310	VAL	2.2
1	A	496	PHE	2.2
1	B	492	ILE	2.2
1	A	414	VAL	2.1
1	B	241	ASN	2.1
1	B	116	ILE	2.1
1	B	105	SER	2.1
1	B	294	VAL	2.1
1	B	453	LYS	2.1
1	A	107	GLU	2.1
1	A	289	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	A	605	6/6	0.49	9.83	88,106,124,124	0
2	GOL	A	607	6/6	0.39	8.33	65,88,104,116	0
2	GOL	A	603	6/6	0.30	4.21	63,87,101,105	0
2	GOL	B	602	6/6	0.46	3.78	69,83,92,110	0
2	GOL	B	605	6/6	0.40	3.65	83,102,119,122	0
2	GOL	A	608	6/6	0.33	3.22	80,96,105,110	0
2	GOL	A	601	6/6	0.47	3.05	80,99,118,118	0
2	GOL	B	604	6/6	0.40	2.98	87,107,128,129	0
2	GOL	B	603	6/6	0.28	2.66	76,95,108,115	0
2	GOL	B	601	6/6	0.23	2.08	81,97,114,114	0
2	GOL	A	604	6/6	0.36	1.85	81,108,126,130	0
2	GOL	A	606	6/6	0.19	1.12	85,102,112,115	0
3	DTT	A	609	8/8	0.25	0.63	83,113,152,152	0
2	GOL	A	602	6/6	0.14	0.09	80,97,110,112	0
3	DTT	B	606	8/8	0.20	-0.51	86,103,115,116	0

6.5 Other polymers ⓘ

There are no such residues in this entry.