



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:20 AM UTC

PDB ID : 4E4V / pdb_00004e4v
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 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)
Xtrriage (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

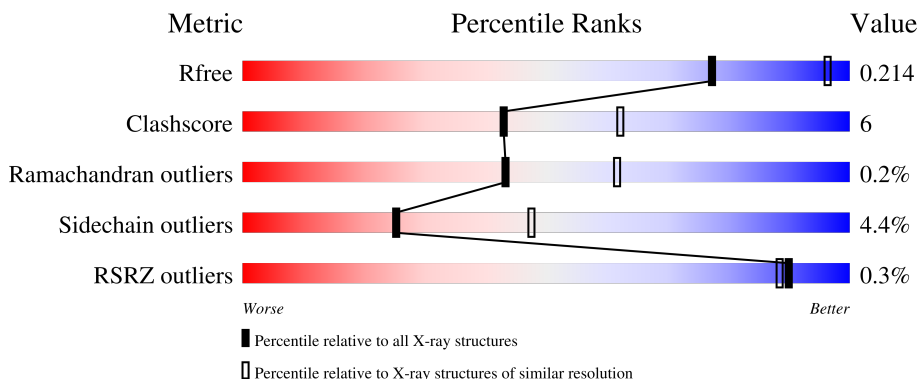
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (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 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	485	 74% 14% • 11%
1	B	485	 76% 13% • 11%

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	GOL	A	603	-	-	X	-

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 13702 atoms, of which 6849 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 Importin subunit alpha-2.

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

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

Continued on next page...

Continued from previous page...

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

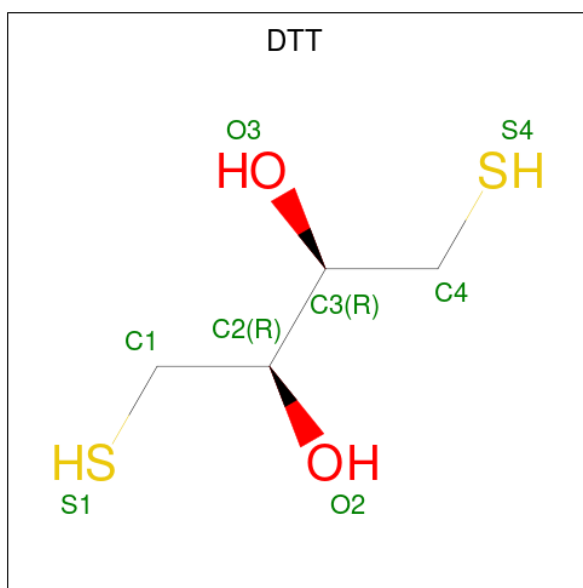
- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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 (CCD ID: DTT) (formula:

C₄H₁₀O₂S₂).



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

- Molecule 4 is water.

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

4 Data and refinement statistics i

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	7.23 (at 2.54Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.155 , 0.203 0.170 , 0.214	Depositor DCC
R_{free} test set	1971 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtrriage
Anisotropy	0.358	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.015 for -h,-l,-k 0.008 for l,-k,h	Xtrriage
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

Xtrriage'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.

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: DTT, GOL

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	0.88	1/3363 (0.0%)	1.00	6/4589 (0.1%)
1	B	0.81	0/3355	0.98	7/4578 (0.2%)
All	All	0.84	1/6718 (0.0%)	0.99	13/9167 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	ILE	CA-C	5.37	1.57	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	SER	CA-C-N	-6.58	112.04	119.28
1	A	134	SER	C-N-CA	-6.58	112.04	119.28
1	A	243	ALA	CA-C-N	6.12	126.68	120.38
1	A	243	ALA	C-N-CA	6.12	126.68	120.38
1	B	246	ILE	N-CA-C	5.79	116.53	110.62
1	B	72	GLY	N-CA-C	-5.61	106.16	112.33
1	B	295	VAL	CA-C-N	-5.41	113.33	119.28
1	B	295	VAL	C-N-CA	-5.41	113.33	119.28
1	A	101	ARG	CG-CD-NE	-5.33	100.27	112.00
1	B	249	VAL	CB-CA-C	-5.24	105.18	112.04
1	B	346	ASN	CA-C-N	-5.21	114.25	119.56
1	B	346	ASN	C-N-CA	-5.21	114.25	119.56
1	A	295	VAL	O-C-N	5.17	123.73	120.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3299	3359	3372	49	0
1	B	3294	3366	3361	35	0
2	A	48	64	64	6	0
2	B	30	40	40	2	0
3	A	8	10	10	0	0
3	B	8	10	10	1	0
4	A	87	0	0	4	2
4	B	79	0	0	5	1
All	All	6853	6849	6857	84	2

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 (84) 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:366:ARG:NH1	1:A:368:ASP:OD1	2.14	0.81
2:A:603:GOL:H11	1:B:480:GLU:O	1.89	0.72
1:B:257:VAL:HG22	1:B:294:VAL:CG1	2.20	0.72
1:A:257:VAL:HG22	1:A:294:VAL:CG1	2.21	0.71
1:A:426:MET:CE	1:A:444:ILE:HD11	2.21	0.71
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:A:354:GLU:HG3	4:A:757:HOH:O	1.93	0.67
1:B:101:ARG:HG2	1:B:139:GLU:OE1	1.95	0.66
1:A:176:ALA:HB3	2:A:603:GOL:H31	1.78	0.65
1:A:65:MET:HE1	4:A:744:HOH:O	1.97	0.64
1:A:101:ARG:HG2	1:A:139:GLU:OE1	1.98	0.64
1:B:101:ARG:O	1:B:105:SER:HB2	1.98	0.63
1:B:108:LYS:O	1:B:109:GLN:HG2	1.97	0.63
1:A:213:LEU:HD22	1:A:218:MET:HE1	1.82	0.62
1:A:422[A]:ILE:HD12	1:A:422[A]:ILE:H	1.63	0.61
1:A:417:VAL:HG13	1:A:422[A]:ILE:HD11	1.83	0.60
1:A:257:VAL:HG22	1:A:294:VAL:HG13	1.84	0.59
1:A:474:GLU:HA	1:A:474:GLU:OE1	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:MET:CE	1:A:444:ILE:CD1	2.85	0.55
1:B:246:ILE:HD12	1:B:285:ARG:NE	2.22	0.55
1:A:307:LEU:N	1:A:308:PRO:CD	2.70	0.54
1:B:257:VAL:HG22	1:B:294:VAL:HG13	1.86	0.54
1:B:138:PHE:CE1	1:B:181:GLN:HG2	2.42	0.54
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:325:ASP:HA	4:B:744:HOH:O	2.09	0.52
1:B:423:GLU:HB3	1:B:424:PRO:HD3	1.93	0.50
1:B:113:ASP:O	1:B:117:ARG:HG3	2.11	0.50
1:A:87:SER:O	1:A:93:GLN:NE2	2.42	0.50
1:A:306:GLU:HB3	1:A:308:PRO:HD2	1.94	0.49
1:A:108:LYS:HE3	1:B:321:VAL:O	2.13	0.49
1:A:105:SER:HB3	1:A:146:ASN:HD21	1.78	0.49
1:A:109:GLN:N	1:A:110:PRO:CD	2.76	0.48
1:A:164:ILE:HB	1:A:165:PRO:HD3	1.95	0.48
1:A:263:ASP:OD1	1:A:263:ASP:C	2.57	0.48
1:A:307:LEU:N	1:A:308:PRO:HD3	2.29	0.47
1:A:295:VAL:N	1:A:296:PRO:CD	2.76	0.47
1:B:108:LYS:O	1:B:109:GLN:CG	2.61	0.47
1:B:477:GLN:OE1	1:B:489:LEU:HD13	2.15	0.47
1:A:431:ALA:O	1:A:437:ILE:HD11	2.14	0.47
1:A:417:VAL:HG13	1:A:463:MET:HE1	1.96	0.47
1:B:207:ASP:HB2	1:B:208:PRO:HD3	1.96	0.47
1:B:290:VAL:HG13	1:B:330:VAL:HG11	1.97	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:A:243:ALA:HB1	1:A:244:PRO:HD2	1.97	0.45
1:B:121:ILE:N	1:B:122:PRO:HD2	2.31	0.45
1:A:309:ILE:O	1:A:312:PRO:HD2	2.17	0.45
1:B:257:VAL:HG13	1:B:294:VAL:HG12	1.99	0.45
1:A:257:VAL:HG22	1:A:294:VAL:HG11	1.95	0.45
1:A:105:SER:HB3	1:A:146:ASN:ND2	2.32	0.44
1:B:238:ARG:O	1:B:239:ASN:HB2	2.17	0.44
1:B:207:ASP:HB2	1:B:208:PRO:CD	2.49	0.43
1:A:423:GLU:HB3	1:A:424:PRO:HD3	2.00	0.43
1:A:358:THR:HA	4:A:720:HOH:O	2.17	0.43
1:B:74:VAL:O	1:B:74:VAL:HG12	2.19	0.43
1:A:371:GLN:HE22	2:A:608:GOL:C1	2.31	0.43
1:A:371:GLN:HE22	2:A:608:GOL:H11	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ILE:HB	1:B:165:PRO:HD3	2.01	0.42
1:A:71:GLN:HA	1:A:98:GLN:OE1	2.19	0.42
1:A:207:ASP:HB2	1:A:208:PRO:HD3	2.01	0.42
1:A:226:LEU:HD12	1:A:226:LEU:HA	1.86	0.42
1:A:215:VAL:HB	1:A:216:PRO:CD	2.49	0.42
1:A:108:LYS:HE2	1:B:323:GLY:O	2.20	0.42
1:A:426:MET:HE1	1:A:444:ILE:CD1	2.50	0.42
1:B:240:LYS:HE3	1:B:240:LYS:HB3	1.90	0.42
1:B:302:LEU:HD21	1:B:314:LEU:HA	2.01	0.42
1:A:213:LEU:HD22	1:A:218:MET:CE	2.48	0.42
1:B:307:LEU:N	1:B:308:PRO:CD	2.82	0.42
1:A:436:ILE:HD13	1:A:436:ILE:HA	1.86	0.41
1:B:386:LEU:HD23	1:B:424:PRO:HB2	2.03	0.41
1:A:250:GLU:HG3	1:A:288:MET:CE	2.50	0.41
1:B:101:ARG:HD3	1:B:142:TRP:CD2	2.56	0.41
1:A:101:ARG:HG3	1:A:102:LYS:N	2.34	0.41
1:A:404:TYR:C	1:A:404:TYR:CD2	2.98	0.41
1:A:134:SER:N	1:A:135:PRO:CD	2.84	0.41
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.91	0.41
1:B:311:THR:HB	1:B:312:PRO:CD	2.50	0.40
1:A:213:LEU:HG	1:A:229:LEU:HD21	2.03	0.40
1:B:261:HIS:HD2	4:B:740:HOH:O	2.03	0.40
1:A:253:LEU:HB2	1:A:254:PRO:HD3	2.04	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	Interatomic distance (Å)	Clash overlap (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 [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	433/485 (89%)	420 (97%)	13 (3%)	0	100	100
1	B	432/485 (89%)	423 (98%)	7 (2%)	2 (0%)	24	41
All	All	865/970 (89%)	843 (98%)	20 (2%)	2 (0%)	43	62

All (2) Ramachandran outliers are listed below:

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

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	367/410 (90%)	350 (95%)	17 (5%)	24	45
1	B	366/410 (89%)	351 (96%)	15 (4%)	27	50
All	All	733/820 (89%)	701 (96%)	32 (4%)	25	47

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	85	ILE
1	A	101	ARG
1	A	136	ILE
1	A	152	SER
1	A	246	ILE
1	A	275	ILE
1	A	359	MET
1	A	360	SER
1	A	402	THR
1	A	404	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	435	LYS
1	A	436	ILE
1	A	437	ILE
1	A	442	ASP
1	A	466	GLU
1	B	70	ASN
1	B	87	SER
1	B	88	SER
1	B	115	ILE
1	B	152	SER
1	B	194	SER
1	B	202	LYS
1	B	247	ASP
1	B	291	LYS
1	B	349	THR
1	B	350	ASN
1	B	382	LEU
1	B	436	ILE
1	B	461	SER
1	B	494	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	ASN
1	A	261	HIS
1	A	350	ASN
1	A	479	HIS
1	B	375	ASN
1	B	479	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	602	-	5,5,5	0.26	0	5,5,5	0.79	0
3	DTT	B	606	-	7,7,7	0.72	0	4,8,8	1.19	1 (25%)
2	GOL	A	603	-	5,5,5	0.52	0	5,5,5	1.44	1 (20%)
2	GOL	B	601	-	5,5,5	0.45	0	5,5,5	0.42	0
2	GOL	A	605	-	5,5,5	0.41	0	5,5,5	0.44	0
2	GOL	A	608	-	5,5,5	0.48	0	5,5,5	0.62	0
2	GOL	B	603	-	5,5,5	0.33	0	5,5,5	0.41	0
2	GOL	A	606	-	5,5,5	0.33	0	5,5,5	0.19	0
2	GOL	B	605	-	5,5,5	0.46	0	5,5,5	0.28	0
2	GOL	A	604	-	5,5,5	0.44	0	5,5,5	0.23	0
2	GOL	B	604	-	5,5,5	0.39	0	5,5,5	0.43	0
2	GOL	A	601	-	5,5,5	0.42	0	5,5,5	0.35	0
3	DTT	A	609	-	7,7,7	1.07	0	4,8,8	1.29	1 (25%)
2	GOL	A	602	-	5,5,5	0.46	0	5,5,5	0.30	0
2	GOL	A	607	-	5,5,5	0.33	0	5,5,5	0.55	0

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	B	602	-	-	0/4/4/4	-
3	DTT	B	606	-	-	6/8/8/8	-
2	GOL	A	603	-	-	2/4/4/4	-
2	GOL	B	601	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	605	-	-	2/4/4/4	-
2	GOL	A	608	-	-	1/4/4/4	-
2	GOL	B	603	-	-	2/4/4/4	-
2	GOL	A	606	-	-	2/4/4/4	-
2	GOL	B	605	-	-	1/4/4/4	-
2	GOL	A	604	-	-	4/4/4/4	-
2	GOL	B	604	-	-	4/4/4/4	-
2	GOL	A	601	-	-	2/4/4/4	-
3	DTT	A	609	-	-	6/8/8/8	-
2	GOL	A	602	-	-	2/4/4/4	-
2	GOL	A	607	-	-	2/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	GOL	O1-C1-C2	2.21	120.31	110.38
3	A	609	DTT	C3-C4-S4	2.04	120.12	114.43
3	B	606	DTT	O2-C2-C3	2.01	113.79	109.57

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	GOL	O1-C1-C2-C3
2	A	603	GOL	O1-C1-C2-C3
2	A	604	GOL	O1-C1-C2-O2
2	A	604	GOL	O1-C1-C2-C3
2	A	604	GOL	O2-C2-C3-O3
2	A	605	GOL	O1-C1-C2-C3
2	A	606	GOL	O1-C1-C2-C3
2	B	604	GOL	O1-C1-C2-C3
2	B	604	GOL	C1-C2-C3-O3
3	A	609	DTT	C1-C2-C3-O3
3	A	609	DTT	C1-C2-C3-C4
3	A	609	DTT	O2-C2-C3-O3
3	A	609	DTT	O2-C2-C3-C4
3	A	609	DTT	C2-C3-C4-S4
3	A	609	DTT	O3-C3-C4-S4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	606	DTT	C1-C2-C3-O3
3	B	606	DTT	C1-C2-C3-C4
3	B	606	DTT	O2-C2-C3-O3
3	B	606	DTT	O2-C2-C3-C4
3	B	606	DTT	C2-C3-C4-S4
3	B	606	DTT	O3-C3-C4-S4
2	A	602	GOL	O1-C1-C2-O2
2	A	601	GOL	O1-C1-C2-C3
2	A	604	GOL	C1-C2-C3-O3
2	A	607	GOL	O1-C1-C2-C3
2	B	603	GOL	O1-C1-C2-C3
2	B	605	GOL	O1-C1-C2-C3
2	A	601	GOL	O1-C1-C2-O2
2	B	604	GOL	O1-C1-C2-O2
2	B	604	GOL	O2-C2-C3-O3
2	A	603	GOL	O1-C1-C2-O2
2	A	605	GOL	O1-C1-C2-O2
2	A	606	GOL	O1-C1-C2-O2
2	B	603	GOL	O1-C1-C2-O2
2	A	607	GOL	O1-C1-C2-O2
2	A	608	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	606	DTT	1	0
2	A	603	GOL	4	0
2	A	608	GOL	2	0
2	B	605	GOL	1	0
2	B	604	GOL	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	433/485 (89%)	-0.72	2 (0%) 87 85	30, 62, 94, 120	3 (0%)
1	B	433/485 (89%)	-0.65	1 (0%) 91 90	40, 65, 109, 135	1 (0%)
All	All	866/970 (89%)	-0.69	3 (0%) 90 88	30, 63, 102, 135	4 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	497	SER	4.0
1	B	497	SER	3.5
1	A	388	LYS	3.3

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
3	DTT	A	609	8/8	0.73	0.19	83,113,152,152	0
2	GOL	B	601	6/6	0.80	0.20	81,97,114,114	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	A	603	6/6	0.80	0.12	63,87,101,105	0
2	GOL	B	605	6/6	0.82	0.15	83,102,119,122	0
2	GOL	A	606	6/6	0.84	0.11	85,102,112,115	0
2	GOL	A	604	6/6	0.84	0.14	81,108,126,130	0
2	GOL	A	601	6/6	0.85	0.22	80,99,118,118	0
2	GOL	A	605	6/6	0.85	0.14	88,106,124,124	0
2	GOL	A	602	6/6	0.87	0.16	80,97,110,112	0
2	GOL	B	604	6/6	0.89	0.16	87,107,128,129	0
2	GOL	A	608	6/6	0.90	0.13	80,96,105,110	0
2	GOL	A	607	6/6	0.91	0.14	65,88,104,116	0
2	GOL	B	603	6/6	0.92	0.10	76,95,108,115	0
3	DTT	B	606	8/8	0.92	0.11	86,103,115,116	0
2	GOL	B	602	6/6	0.95	0.11	69,83,92,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.