Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:43 PM GMT

PDB ID	:	1LOT
Title	:	CRYSTAL STRUCTURE OF THE COMPLEX OF ACTIN WITH VITAMIN D-BINDING PROTEIN
Authors	:	Head, J.F.; Swamy, N.; Ray, R.
Deposited on	:	2002-05-07
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/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:

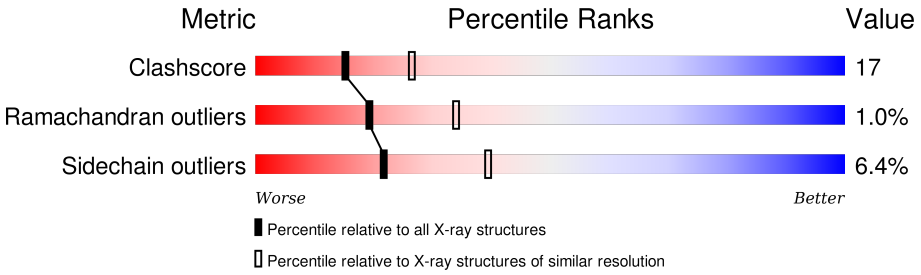
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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. 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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	458	61% 30% • 5%
2	B	375	65% 26% 5% •

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
5	GOL	A	600	-	X	-	-
5	GOL	A	610	-	X	-	-
5	GOL	A	630	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	B	620	-	X	-	-
5	GOL	B	640	-	X	-	-
5	GOL	B	650	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6387 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 Vitamin D-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3412	2141	554	686	31			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	THR	LYS	SEE REMARK 999	UNP P02774

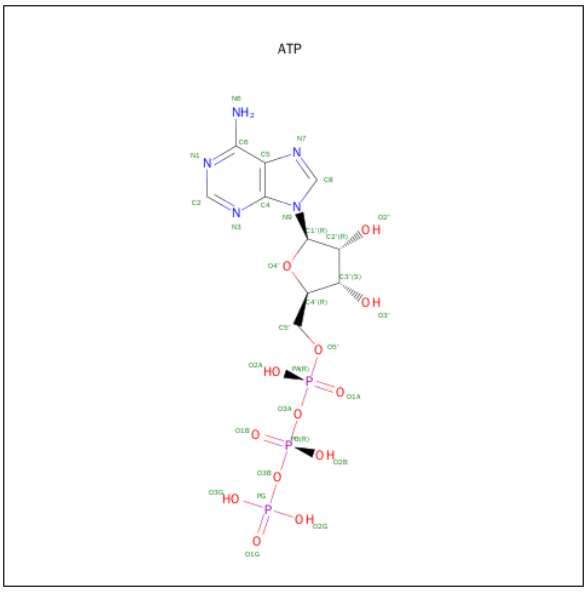
- Molecule 2 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	360	Total	C	N	O	S	0	0	0
			2820	1786	473	543	18			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

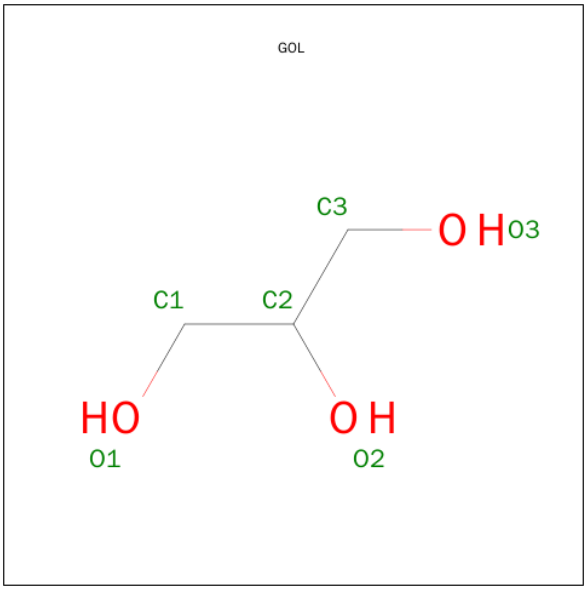
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	37	Total O 37 37	0	0
6	B	50	Total O 50 50	0	0

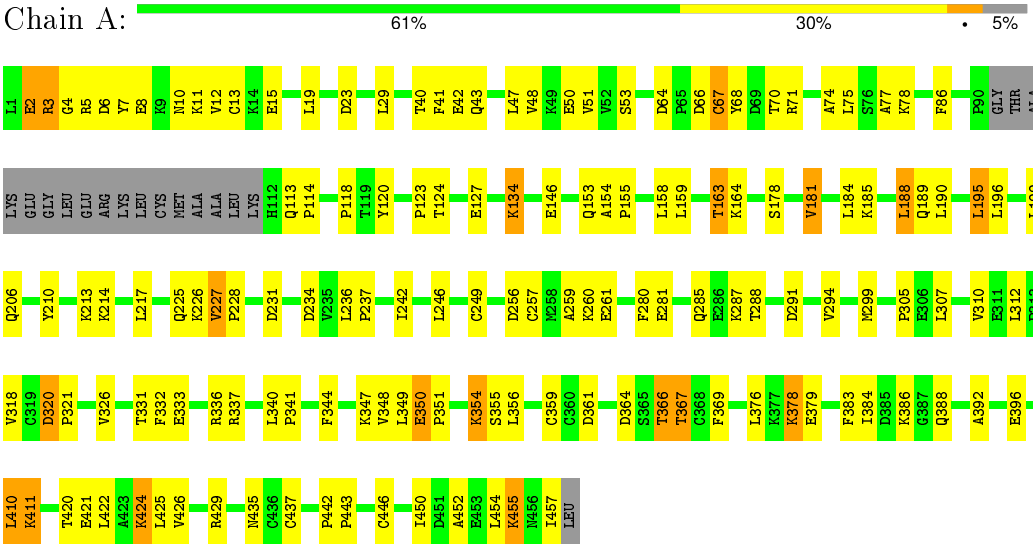
3 Residue-property plots (i)

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.

Note EDS was not executed.

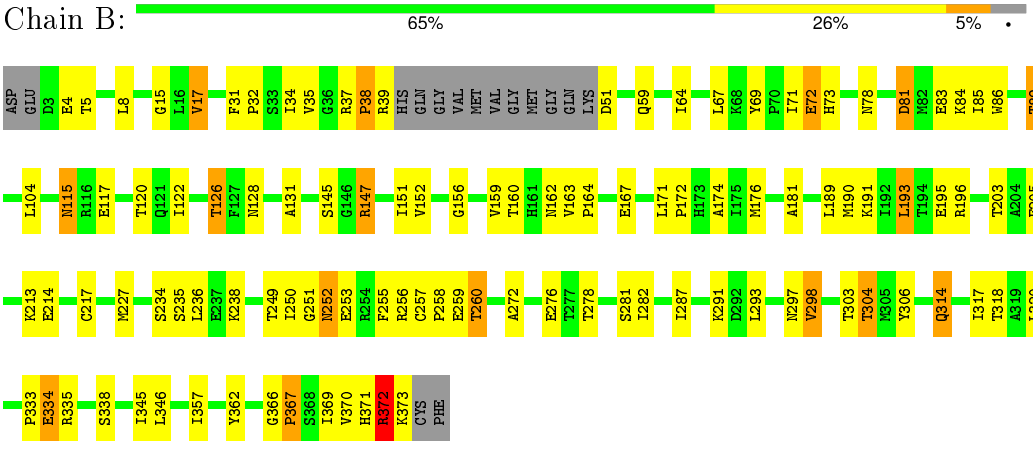
- Molecule 1: Vitamin D-binding protein

Chain A:



- Molecule 2: Actin, alpha skeletal muscle

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.17Å 87.34Å 159.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	95.8 (50.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.226 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6387	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, HIC, ATP

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	0.36	0/3478	0.59	1/4707 (0.0%)
2	B	0.37	0/2867	0.63	0/3885
All	All	0.37	0/6345	0.61	1/8592 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	CYS	N-CA-C	5.08	124.73	111.00

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	3412	0	3340	123	0
2	B	2820	0	2786	102	0
3	B	1	0	0	0	0
4	B	31	0	12	1	0
5	A	18	0	12	1	0
5	B	18	0	12	0	0
6	A	37	0	0	6	0
6	B	50	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6387	0	6162	217	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 17.

All (217) 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:40:THR:HB	1:A:43:GLN:HG3	1.44	0.96
1:A:435:ASN:HA	2:B:287:ILE:HD11	1.53	0.90
2:B:72:GLU:HG3	2:B:73:HIC:HZ3	1.51	0.88
2:B:257:CYS:O	2:B:260:THR:HG23	1.76	0.84
2:B:72:GLU:HB3	2:B:73:HIC:HD2	1.62	0.82
1:A:333:GLU:O	1:A:337:ARG:HD2	1.80	0.82
2:B:152:VAL:HG22	2:B:298:VAL:HG22	1.59	0.82
1:A:317:ASP:HB3	1:A:326:VAL:HG11	1.61	0.81
1:A:333:GLU:HG3	1:A:337:ARG:HH12	1.44	0.80
1:A:199:LEU:HD21	1:A:294:VAL:HG12	1.62	0.80
1:A:333:GLU:HG3	1:A:337:ARG:NH1	1.98	0.79
1:A:314:THR:O	1:A:318:VAL:HG23	1.83	0.78
2:B:120:THR:OG1	2:B:370:VAL:HG11	1.84	0.78
2:B:257:CYS:HB3	2:B:258:PRO:HD3	1.66	0.76
1:A:350:GLU:HB3	1:A:351:PRO:HD3	1.67	0.75
1:A:366:THR:O	1:A:367:THR:HG23	1.87	0.73
1:A:40:THR:HG22	1:A:42:GLU:H	1.54	0.71
1:A:420:THR:O	1:A:424:LYS:HD2	1.92	0.70
1:A:67:CYS:O	1:A:70:THR:N	2.26	0.69
1:A:351:PRO:O	1:A:354:LYS:HG3	1.93	0.68
2:B:190:MET:HG2	2:B:209:VAL:HG21	1.74	0.67
2:B:164:PRO:HG3	2:B:281:SER:OG	1.96	0.65
1:A:452:ALA:O	1:A:455:LYS:HE3	1.96	0.64
1:A:310:VAL:HG23	1:A:337:ARG:HD3	1.79	0.64
2:B:122:ILE:O	2:B:126:THR:HG23	1.98	0.64
1:A:378:LYS:HD2	1:A:379:GLU:N	2.14	0.63
1:A:332:PHE:O	1:A:336:ARG:HG2	1.98	0.63
2:B:333:PRO:HD2	2:B:334:GLU:OE2	1.99	0.62
2:B:272:ALA:HB1	2:B:276:GLU:HB2	1.81	0.62
1:A:450:ILE:O	1:A:454:LEU:HB2	1.99	0.62
1:A:47:LEU:O	1:A:51:VAL:HG23	2.00	0.62
1:A:4:GLY:O	1:A:5:ARG:HB2	1.99	0.62
1:A:195:LEU:CD1	2:B:167:GLU:HG3	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:ARG:O	2:B:214:GLU:HG3	2.00	0.62
1:A:408:GLU:O	1:A:411:LYS:HG2	2.00	0.61
2:B:189:LEU:O	2:B:193:LEU:HB2	1.99	0.61
1:A:312:LEU:HG	1:A:356:LEU:HD11	1.84	0.60
1:A:8:GLU:HB2	6:A:647:HOH:O	2.02	0.60
2:B:85:ILE:O	2:B:89:THR:HG22	2.02	0.59
1:A:384:ILE:O	1:A:388:GLN:HG3	2.02	0.58
2:B:72:GLU:HB3	2:B:73:HIC:CD2	2.32	0.58
2:B:234:SER:C	2:B:236:LEU:H	2.07	0.58
1:A:446:CYS:O	1:A:450:ILE:HG13	2.03	0.58
2:B:252:ASN:O	2:B:256:ARG:HG3	2.04	0.57
1:A:4:GLY:C	1:A:6:ASP:H	2.07	0.57
1:A:67:CYS:SG	1:A:68:TYR:N	2.77	0.57
2:B:17:VAL:HG11	2:B:31:PHE:CE2	2.40	0.57
1:A:364:ASP:OD1	1:A:367:THR:HG21	2.05	0.56
2:B:191:LYS:O	2:B:195:GLU:HG3	2.05	0.56
2:B:227:MET:CE	2:B:256:ARG:HD3	2.36	0.56
1:A:4:GLY:HA3	1:A:7:TYR:HB2	1.86	0.56
1:A:231:ASP:O	1:A:234:ASP:HB2	2.05	0.56
2:B:203:THR:O	2:B:206:ARG:HB3	2.05	0.56
1:A:217:LEU:HD12	1:A:331:THR:HG21	1.88	0.56
2:B:252:ASN:N	2:B:252:ASN:HD22	2.04	0.55
2:B:85:ILE:O	2:B:89:THR:CG2	2.55	0.55
1:A:435:ASN:OD1	2:B:287:ILE:HD13	2.07	0.55
1:A:2:GLU:O	1:A:4:GLY:N	2.39	0.55
1:A:78:LYS:HB3	1:A:86:PHE:HE2	1.72	0.55
2:B:304:THR:HG23	2:B:335:ARG:HE	1.72	0.55
1:A:227:VAL:HG22	1:A:280:PHE:CE1	2.43	0.54
1:A:2:GLU:C	1:A:4:GLY:H	2.11	0.54
1:A:11:LYS:O	1:A:15:GLU:HG3	2.08	0.54
1:A:226:LYS:HE2	1:A:299:MET:O	2.08	0.54
2:B:325:MET:CE	2:B:325:MET:HA	2.39	0.53
1:A:74:ALA:O	1:A:77:ALA:HB3	2.08	0.53
1:A:195:LEU:HD11	2:B:167:GLU:HG3	1.89	0.53
1:A:350:GLU:CB	1:A:351:PRO:HD3	2.39	0.53
1:A:386:LYS:HE2	1:A:457:ILE:HD13	1.90	0.53
1:A:287:LYS:HG2	6:B:674:HOH:O	2.07	0.53
2:B:373:LYS:HG2	6:B:656:HOH:O	2.07	0.53
2:B:372:ARG:HD2	2:B:373:LYS:N	2.24	0.53
1:A:249:CYS:SG	1:A:261:GLU:HG3	2.49	0.53
2:B:37:ARG:HH11	2:B:37:ARG:HG3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LYS:HB3	6:A:646:HOH:O	2.07	0.53
1:A:120:TYR:HD1	1:A:146:GLU:HG2	1.74	0.52
1:A:354:LYS:HD2	1:A:354:LYS:C	2.30	0.52
2:B:164:PRO:HG2	2:B:174:ALA:CB	2.40	0.52
1:A:113:GLN:HG2	1:A:114:PRO:CD	2.39	0.52
1:A:40:THR:H	1:A:43:GLN:HE21	1.57	0.52
2:B:72:GLU:OE1	2:B:72:GLU:HA	2.08	0.52
1:A:113:GLN:HG2	1:A:114:PRO:HD2	1.91	0.52
1:A:316:LYS:O	1:A:320:ASP:HB2	2.09	0.51
2:B:39:ARG:HB3	2:B:64:ILE:C	2.31	0.51
2:B:152:VAL:HG22	2:B:298:VAL:CG2	2.35	0.50
1:A:210:TYR:CD1	1:A:214:LYS:HE3	2.46	0.50
1:A:210:TYR:HB3	1:A:214:LYS:HB2	1.92	0.50
1:A:305:PRO:HD2	1:A:336:ARG:O	2.11	0.50
2:B:335:ARG:HA	2:B:338:SER:OG	2.12	0.50
5:A:630:GOL:H12	6:B:685:HOH:O	2.12	0.50
1:A:195:LEU:HD13	2:B:167:GLU:HG3	1.93	0.50
2:B:86:TRP:HA	2:B:89:THR:HG23	1.93	0.50
1:A:242:ILE:O	1:A:246:LEU:HG	2.12	0.49
1:A:359:CYS:HB2	1:A:369:PHE:CZ	2.47	0.49
2:B:257:CYS:CB	2:B:258:PRO:HD3	2.41	0.49
2:B:81:ASP:O	2:B:84:LYS:HB2	2.13	0.49
2:B:190:MET:CG	2:B:209:VAL:HG21	2.41	0.49
2:B:234:SER:O	2:B:235:SER:HB2	2.12	0.49
2:B:83:GLU:OE2	2:B:126:THR:HG21	2.12	0.49
2:B:303:THR:O	2:B:303:THR:HG22	2.13	0.49
1:A:163:THR:HG22	1:A:164:LYS:N	2.28	0.49
1:A:67:CYS:O	1:A:68:TYR:C	2.51	0.49
1:A:123:PRO:O	2:B:147:ARG:NH2	2.46	0.49
2:B:164:PRO:HG2	2:B:174:ALA:HB1	1.94	0.49
1:A:155:PRO:HD2	1:A:158:LEU:HD12	1.94	0.49
2:B:35:VAL:HG21	2:B:81:ASP:HB3	1.95	0.48
1:A:184:LEU:HD23	2:B:345:ILE:HG22	1.94	0.48
2:B:151:ILE:HD11	2:B:281:SER:HB3	1.96	0.48
2:B:206:ARG:HH11	2:B:206:ARG:HG2	1.79	0.48
2:B:367:PRO:C	2:B:369:ILE:H	2.16	0.48
2:B:38:PRO:HG3	2:B:51:ASP:O	2.13	0.47
2:B:99:GLU:HA	2:B:128:ASN:O	2.13	0.47
2:B:156:GLY:O	2:B:181:ALA:HB1	2.14	0.47
2:B:115:ASN:C	2:B:115:ASN:HD22	2.17	0.47
2:B:120:THR:OG1	2:B:370:VAL:CG1	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:CYS:O	1:A:261:GLU:HG2	2.14	0.47
1:A:64:ASP:OD1	1:A:66:ASP:HB3	2.15	0.47
1:A:124:THR:OG1	1:A:127:GLU:HG3	2.14	0.47
2:B:15:GLY:O	2:B:32:PRO:HA	2.14	0.47
1:A:442:PRO:HA	1:A:443:PRO:HD3	1.70	0.47
2:B:318:THR:HA	2:B:327:ILE:HD12	1.96	0.47
1:A:29:LEU:HA	1:A:48:VAL:HG21	1.96	0.47
2:B:31:PHE:CE1	2:B:93:GLU:HG3	2.49	0.47
2:B:156:GLY:HA3	4:B:500:ATP:PG	2.55	0.47
1:A:206:GLN:NE2	6:A:652:HOH:O	2.47	0.47
1:A:196:LEU:HD21	1:A:259:ALA:HA	1.97	0.47
1:A:50:GLU:O	1:A:53:SER:HB3	2.15	0.47
1:A:225:GLN:NE2	6:A:635:HOH:O	2.43	0.47
1:A:285:GLN:O	2:B:372:ARG:HA	2.14	0.46
1:A:199:LEU:HD21	1:A:294:VAL:CG1	2.38	0.46
2:B:372:ARG:HD2	2:B:372:ARG:C	2.35	0.46
2:B:317:ILE:HG22	2:B:327:ILE:HD13	1.97	0.46
1:A:178:SER:HB3	1:A:181:VAL:HG13	1.97	0.46
1:A:281:GLU:O	1:A:285:GLN:HG3	2.15	0.46
1:A:307:LEU:HB3	1:A:337:ARG:HH21	1.80	0.46
1:A:6:ASP:HB3	1:A:10:ASN:ND2	2.31	0.46
1:A:67:CYS:O	1:A:70:THR:HB	2.16	0.46
1:A:154:ALA:HB2	1:A:201:ASN:HB2	1.97	0.46
2:B:152:VAL:O	2:B:162:ASN:HA	2.15	0.46
2:B:318:THR:HA	2:B:327:ILE:CD1	2.46	0.46
1:A:120:TYR:CD1	1:A:146:GLU:HG2	2.50	0.45
1:A:40:THR:H	1:A:43:GLN:NE2	2.14	0.45
2:B:69:TYR:CD1	2:B:69:TYR:N	2.84	0.45
1:A:422:LEU:O	1:A:426:VAL:HG23	2.16	0.45
1:A:256:ASP:O	1:A:260:LYS:HB2	2.16	0.45
1:A:40:THR:HG22	1:A:41:PHE:N	2.31	0.45
1:A:383:PHE:CD1	1:A:454:LEU:HD21	2.52	0.45
2:B:334:GLU:CD	2:B:334:GLU:H	2.20	0.45
1:A:118:PRO:HB2	2:B:291:LYS:HE2	1.99	0.45
2:B:131:ALA:HA	2:B:357:ILE:O	2.17	0.45
1:A:396:GLU:CD	1:A:396:GLU:H	2.21	0.45
1:A:185:LYS:O	1:A:189:GLN:HG3	2.16	0.45
1:A:408:GLU:HA	1:A:411:LYS:HE2	1.98	0.45
1:A:159:LEU:O	1:A:163:THR:HB	2.17	0.45
2:B:213:LYS:O	2:B:217:CYS:HB2	2.17	0.45
1:A:356:LEU:HG	1:A:376:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:ILE:HG22	2:B:253:GLU:HG2	1.99	0.45
2:B:272:ALA:HB1	2:B:276:GLU:CB	2.44	0.44
2:B:104:LEU:C	2:B:104:LEU:HD23	2.36	0.44
1:A:424:LYS:HA	1:A:424:LYS:HE3	1.98	0.44
1:A:406:LEU:O	1:A:410:LEU:HB2	2.17	0.44
1:A:288:THR:HG23	1:A:291:ASP:OD2	2.18	0.44
1:A:310:VAL:CG2	1:A:337:ARG:HD3	2.46	0.44
1:A:195:LEU:O	1:A:199:LEU:HB2	2.17	0.44
2:B:278:THR:O	2:B:282:ILE:HG13	2.18	0.44
2:B:72:GLU:CG	2:B:73:HIC:HZ3	2.35	0.44
2:B:372:ARG:O	2:B:373:LYS:O	2.35	0.44
1:A:340:LEU:HD21	1:A:344:PHE:HB3	2.00	0.44
2:B:213:LYS:HD2	2:B:306:TYR:OH	2.17	0.44
2:B:39:ARG:HH11	2:B:39:ARG:HG2	1.82	0.44
1:A:236:LEU:N	1:A:237:PRO:CD	2.81	0.44
1:A:19:LEU:HB3	1:A:23:ASP:HB2	1.98	0.44
2:B:171:LEU:HA	2:B:172:PRO:HD2	1.87	0.43
2:B:34:ILE:HD11	2:B:59:GLN:HG2	2.00	0.43
2:B:314:GLN:HB2	2:B:314:GLN:HE21	1.56	0.43
2:B:251:GLY:N	2:B:253:GLU:OE2	2.49	0.43
2:B:120:THR:HG21	2:B:370:VAL:HG13	2.01	0.43
1:A:347:LYS:HB2	1:A:347:LYS:HE3	1.84	0.43
1:A:378:LYS:NZ	1:A:379:GLU:HG3	2.34	0.43
2:B:252:ASN:N	2:B:252:ASN:ND2	2.66	0.43
2:B:362:TYR:O	2:B:366:GLY:N	2.47	0.43
1:A:113:GLN:HG2	1:A:114:PRO:N	2.33	0.42
1:A:455:LYS:C	1:A:455:LYS:HD2	2.39	0.42
2:B:304:THR:CG2	2:B:335:ARG:HE	2.31	0.42
2:B:190:MET:HG3	2:B:209:VAL:HG11	2.01	0.42
2:B:238:LYS:O	2:B:249:THR:HA	2.18	0.42
1:A:12:VAL:HG23	1:A:13:CYS:N	2.34	0.42
1:A:228:PRO:HD2	6:A:654:HOH:O	2.18	0.42
1:A:3:ARG:NH1	6:A:667:HOH:O	2.29	0.42
1:A:153:GLN:HG2	1:A:205:SER:HA	2.01	0.42
1:A:71:ARG:HA	1:A:74:ALA:HB3	2.02	0.42
2:B:252:ASN:HD22	2:B:253:GLU:N	2.18	0.41
1:A:78:LYS:HB3	1:A:86:PHE:CE2	2.53	0.41
1:A:134:LYS:O	1:A:134:LYS:HE2	2.21	0.41
2:B:255:PHE:O	2:B:259:GLU:HB2	2.20	0.41
1:A:351:PRO:HA	1:A:354:LYS:HG3	2.03	0.41
2:B:193:LEU:HD12	2:B:193:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLU:HG2	1:A:75:LEU:HD13	2.02	0.41
2:B:159:VAL:HG22	2:B:160:THR:N	2.35	0.41
1:A:341:PRO:HG2	1:A:437:CYS:HA	2.03	0.41
1:A:188:LEU:HA	1:A:188:LEU:HD12	1.89	0.41
2:B:234:SER:C	2:B:236:LEU:N	2.73	0.41
2:B:71:ILE:O	2:B:71:ILE:HG22	2.20	0.41
2:B:37:ARG:NH1	2:B:37:ARG:HG3	2.36	0.41
1:A:354:LYS:HD2	1:A:355:SER:N	2.36	0.41
1:A:40:THR:CB	1:A:43:GLN:HE21	2.34	0.41
2:B:205:GLU:O	2:B:209:VAL:HG23	2.21	0.41
2:B:31:PHE:HB2	2:B:32:PRO:HD2	2.03	0.41
1:A:421:GLU:O	1:A:425:LEU:HD13	2.21	0.41
2:B:258:PRO:HG3	2:B:306:TYR:CE1	2.55	0.41
1:A:2:GLU:C	1:A:4:GLY:N	2.74	0.40
1:A:348:VAL:HG13	1:A:349:LEU:N	2.35	0.40
1:A:378:LYS:CE	1:A:379:GLU:HG3	2.51	0.40
1:A:320:ASP:HA	1:A:321:PRO:HD3	1.91	0.40
2:B:117:GLU:OE2	2:B:371:HIS:CE1	2.74	0.40
2:B:196:ARG:O	2:B:196:ARG:HG2	2.22	0.40
2:B:163:VAL:HA	2:B:164:PRO:HD3	1.89	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	432/458 (94%)	410 (95%)	18 (4%)	4 (1%)	21	37
2	B	355/375 (95%)	329 (93%)	22 (6%)	4 (1%)	17	31
All	All	787/833 (94%)	739 (94%)	40 (5%)	8 (1%)	19	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	392	ALA
2	B	5	THR
1	A	367	THR
1	A	366	THR
2	B	367	PRO
2	B	372	ARG
2	B	38	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	398/415 (96%)	380 (96%)	18 (4%)	34 59
2	B	305/317 (96%)	278 (91%)	27 (9%)	12 23
All	All	703/732 (96%)	658 (94%)	45 (6%)	22 39

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	134	LYS
1	A	163	THR
1	A	181	VAL
1	A	188	LEU
1	A	190	LEU
1	A	195	LEU
1	A	227	VAL
1	A	320	ASP
1	A	350	GLU
1	A	354	LYS
1	A	361	ASP
1	A	378	LYS
1	A	410	LEU
1	A	411	LYS
1	A	424	LYS

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Mol	Chain	Res	Type
1	A	429	ARG
1	A	455	LYS
2	B	4	GLU
2	B	8	LEU
2	B	17	VAL
2	B	67	LEU
2	B	72	GLU
2	B	78	ASN
2	B	81	ASP
2	B	89	THR
2	B	115	ASN
2	B	126	THR
2	B	145	SER
2	B	147	ARG
2	B	176	MET
2	B	193	LEU
2	B	210	ARG
2	B	252	ASN
2	B	260	THR
2	B	293	LEU
2	B	297	ASN
2	B	298	VAL
2	B	304	THR
2	B	314	GLN
2	B	320	LEU
2	B	325	MET
2	B	334	GLU
2	B	346	LEU
2	B	372	ARG

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

Mol	Chain	Res	Type
1	A	10	ASN
1	A	43	GLN
1	A	83	ASN
1	A	142	GLN
1	A	189	GLN
1	A	206	GLN
1	A	225	GLN
1	A	244	ASN
1	A	315	ASN

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Mol	Chain	Res	Type
1	A	388	GLN
2	B	78	ASN
2	B	111	ASN
2	B	115	ASN
2	B	252	ASN
2	B	263	GLN
2	B	297	ASN
2	B	314	GLN
2	B	360	GLN
2	B	371	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

1 non-standard protein/DNA/RNA residue is 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	HIC	B	73	2	8,11,12	0.96	1 (12%)	5,14,16	1.12	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	HIC	B	73	2	-	0/4/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	73	HIC	CZ-NE2	-2.09	1.42	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	73	HIC	4	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	$\#\|Z\| > 2$
5	GOL	A	600	-	5,5,5	4.74	5 (100%)	5,5,5	5.73	3 (60%)
5	GOL	A	610	-	5,5,5	4.77	5 (100%)	5,5,5	5.68	3 (60%)
5	GOL	A	630	-	5,5,5	4.80	5 (100%)	5,5,5	5.72	3 (60%)
4	ATP	B	500	3	24,33,33	2.11	8 (33%)	31,52,52	3.28	11 (35%)
5	GOL	B	620	-	5,5,5	4.79	5 (100%)	5,5,5	5.70	3 (60%)
5	GOL	B	640	-	5,5,5	4.76	5 (100%)	5,5,5	5.68	3 (60%)
5	GOL	B	650	-	5,5,5	4.71	5 (100%)	5,5,5	5.71	3 (60%)

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
5	GOL	A	600	-	-	0/4/4/4	0/0/0/0
5	GOL	A	610	-	-	0/4/4/4	0/0/0/0
5	GOL	A	630	-	-	0/4/4/4	0/0/0/0
4	ATP	B	500	3	-	0/18/38/38	0/3/3/3
5	GOL	B	620	-	-	0/4/4/4	0/0/0/0
5	GOL	B	640	-	-	0/4/4/4	0/0/0/0
5	GOL	B	650	-	-	0/4/4/4	0/0/0/0

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	610	GOL	C3-C2	-8.16	1.21	1.52
5	B	640	GOL	C3-C2	-8.06	1.21	1.52
5	A	600	GOL	C3-C2	-8.02	1.21	1.52
5	B	620	GOL	C3-C2	-8.02	1.21	1.52
5	A	630	GOL	C3-C2	-8.00	1.21	1.52
5	B	650	GOL	C3-C2	-7.83	1.22	1.52
4	B	500	ATP	O5'-C5'	-4.02	1.28	1.44
5	A	630	GOL	C1-C2	-3.24	1.39	1.52
5	B	620	GOL	C1-C2	-3.18	1.40	1.52
5	B	640	GOL	C1-C2	-3.17	1.40	1.52
5	B	650	GOL	C1-C2	-3.06	1.40	1.52
5	A	630	GOL	O2-C2	-3.05	1.34	1.43
5	A	600	GOL	C1-C2	-3.03	1.40	1.52
5	A	610	GOL	C1-C2	-2.99	1.40	1.52
5	B	620	GOL	O2-C2	-2.87	1.34	1.43
5	B	640	GOL	O2-C2	-2.80	1.35	1.43
5	A	610	GOL	O2-C2	-2.75	1.35	1.43
5	A	600	GOL	O2-C2	-2.64	1.35	1.43
5	B	650	GOL	O2-C2	-2.63	1.35	1.43
4	B	500	ATP	PB-O2B	-2.42	1.44	1.54
4	B	500	ATP	PB-O1B	-2.30	1.42	1.51
4	B	500	ATP	PA-O2A	-2.17	1.45	1.54
4	B	500	ATP	C8-N7	-2.10	1.30	1.34
4	B	500	ATP	C2-N3	2.18	1.36	1.32
5	A	610	GOL	O3-C3	3.23	1.56	1.42
5	B	640	GOL	O3-C3	3.30	1.56	1.42
5	A	630	GOL	O3-C3	3.36	1.56	1.42
5	B	620	GOL	O3-C3	3.36	1.56	1.42
5	A	600	GOL	O3-C3	3.39	1.57	1.42
5	B	650	GOL	O3-C3	3.58	1.57	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	500	ATP	O4'-C1'	4.31	1.46	1.41
5	B	640	GOL	O1-C1	4.41	1.61	1.42
5	A	630	GOL	O1-C1	4.48	1.61	1.42
5	A	600	GOL	O1-C1	4.51	1.61	1.42
5	B	650	GOL	O1-C1	4.52	1.61	1.42
5	A	610	GOL	O1-C1	4.53	1.61	1.42
5	B	620	GOL	O1-C1	4.54	1.61	1.42
4	B	500	ATP	C4-N3	5.45	1.43	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	500	ATP	O5'-PA-O1A	-6.95	82.63	109.62
4	B	500	ATP	O3A-PA-O5'	-5.14	89.30	102.94
4	B	500	ATP	C5'-C4'-C3'	-4.16	98.71	115.21
4	B	500	ATP	C1'-N9-C4	-3.72	121.33	126.94
4	B	500	ATP	N3-C2-N1	-3.31	126.36	128.89
4	B	500	ATP	C4'-O4'-C1'	-2.15	107.35	109.72
4	B	500	ATP	C4-C5-N7	2.34	111.63	109.48
5	B	640	GOL	O1-C1-C2	3.12	125.34	110.18
5	B	620	GOL	O1-C1-C2	3.20	125.71	110.18
5	B	650	GOL	O1-C1-C2	3.22	125.80	110.18
5	A	600	GOL	O1-C1-C2	3.24	125.91	110.18
5	A	610	GOL	O1-C1-C2	3.29	126.15	110.18
5	A	630	GOL	O1-C1-C2	3.31	126.22	110.18
4	B	500	ATP	O2A-PA-O3A	3.32	120.15	105.09
4	B	500	ATP	O2B-PB-O3B	3.60	121.44	105.09
4	B	500	ATP	O4'-C4'-C3'	4.04	113.29	105.15
5	A	600	GOL	O2-C2-C3	6.54	138.62	108.65
5	A	610	GOL	O2-C2-C3	6.54	138.66	108.65
5	A	630	GOL	O2-C2-C3	6.57	138.80	108.65
5	B	650	GOL	O2-C2-C3	6.58	138.82	108.65
5	B	640	GOL	O2-C2-C3	6.61	138.97	108.65
5	B	620	GOL	O2-C2-C3	6.61	138.98	108.65
5	A	610	GOL	O3-C3-C2	10.35	160.37	110.18
5	B	640	GOL	O3-C3-C2	10.37	160.47	110.18
5	B	620	GOL	O3-C3-C2	10.40	160.60	110.18
5	A	630	GOL	O3-C3-C2	10.44	160.81	110.18
5	B	650	GOL	O3-C3-C2	10.45	160.87	110.18
5	A	600	GOL	O3-C3-C2	10.49	161.07	110.18
4	B	500	ATP	O5'-C5'-C4'	12.00	153.37	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	630	GOL	1	0
4	B	500	ATP	1	0

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.