Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:43 PM GMT

PDB ID	:	1LQG
Title	:	ESCHERICHIA COLI URACIL-DNA GLYCOSYLASE COMPLEX WITH URACIL-DNA GLYCOSYLASE INHIBITOR PROTEIN
Authors	:	Saikrishnan, K.; Sagar, M.B.; Ravishankar, R.; Roy, S.; Purnapatre, K.; Handa, P.; Varshney, U.; Vijayan, M.
Deposited on	:	2002-05-10
Resolution	:	2.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

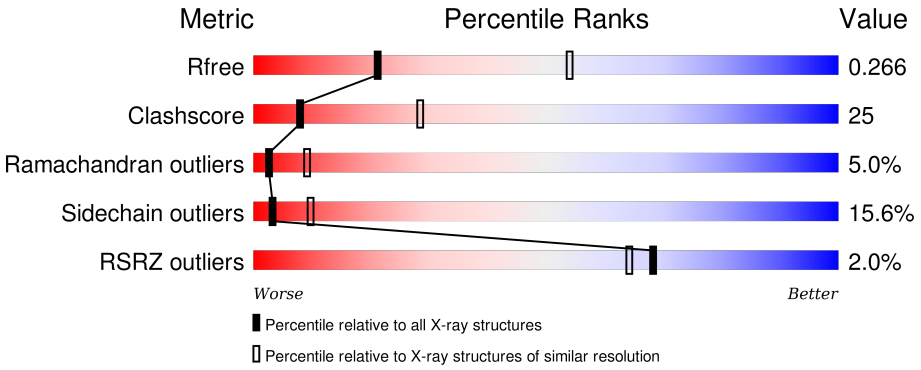
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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.

Mol	Chain	Length	Quality of chain
1	A	229	51% 37% 11%
1	B	229	3% 52% 34% 11%
2	C	84	51% 33% 13%
2	D	84	2% 54% 29% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4765 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 URACIL-DNA GLYCOSYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1755	1128	312	312	3			
1	B	224	Total	C	N	O	S	0	0	0
			1749	1127	311	308	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP P12295
B	1	MET	-	CLONING ARTIFACT	UNP P12295

- Molecule 2 is a protein called URACIL-DNA GLYCOSYLASE INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	73	Total	C	N	O	S	0	0	0
			567	358	88	118	3			
2	D	70	Total	C	N	O	S	0	0	0
			538	341	84	110	3			

- Molecule 3 is water.

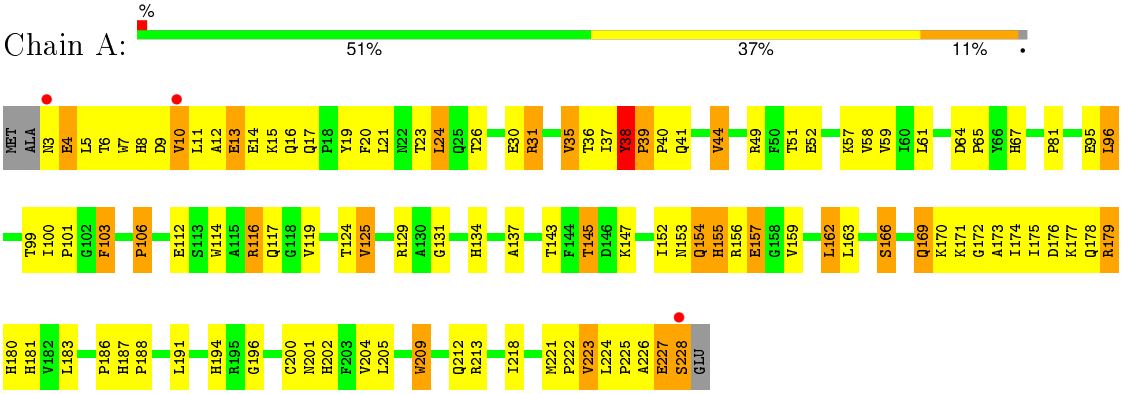
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total	O	0	0
			71	71		
3	B	51	Total	O	0	0
			51	51		
3	C	23	Total	O	0	0
			23	23		
3	D	11	Total	O	0	0
			11	11		

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.

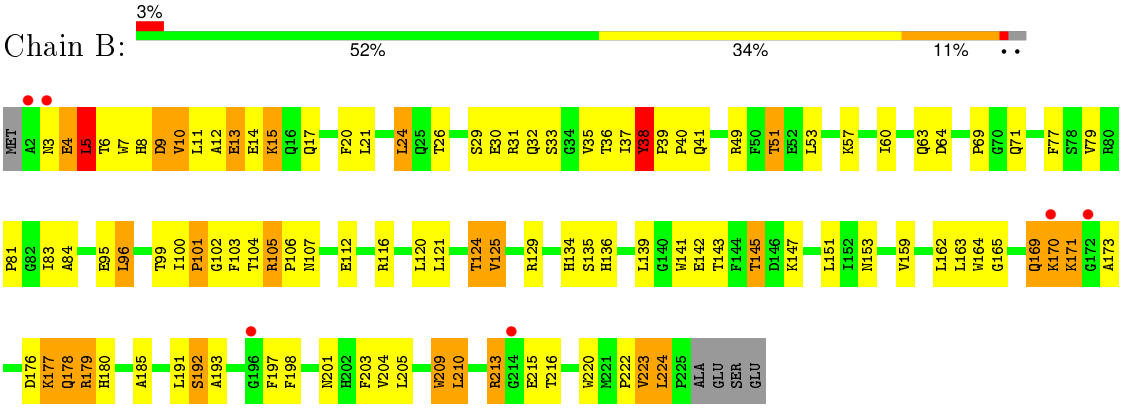
- Molecule 1: URACIL-DNA GLYCOSYLASE

Chain A:



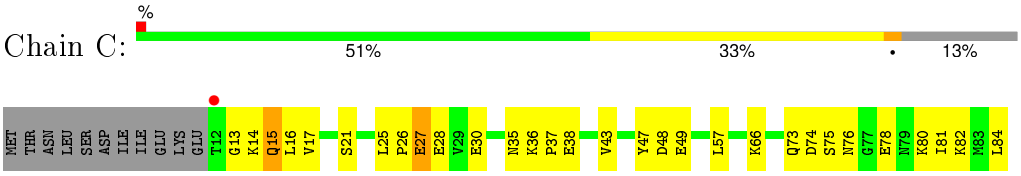
- Molecule 1: URACIL-DNA GLYCOSYLASE

Chain B:



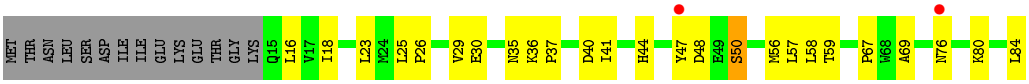
- Molecule 2: URACIL-DNA GLYCOSYLASE INHIBITOR

Chain C:



- Molecule 2: URACIL-DNA GLYCOSYLASE INHIBITOR

Chain D:


MET
THR
ASN
LEU
SER
ASP
ILE
ILE
GLU
LYS
GLU
THR
GLY
LYS
Q15
L16
V17
I18
L23
M24
L25
P26
V29
E30
N35
K36
P37
D40
I41
H44
Y47
D48
E49
S50
M56
L57
L58
T59
P67
W68
A69
N76
K80
L84

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.16Å 89.90Å 141.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.76 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.6 (20.00-2.90) 92.6 (19.76-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	6.22 (at 2.79Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.183 , 0.277 0.177 , 0.266	Depositor DCC
R_{free} test set	969 reflections (6.88%)	DCC
Wilson B-factor (Å^2)	37.1	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 88.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 15459 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4765	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.55	0/1811	0.79	1/2475 (0.0%)
1	B	0.53	0/1805	0.76	1/2466 (0.0%)
2	C	0.59	0/575	0.84	1/780 (0.1%)
2	D	0.51	0/546	0.75	0/743
All	All	0.54	0/4737	0.78	3/6464 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	38	TYR	N-CA-C	7.28	130.65	111.00
1	A	38	TYR	N-CA-C	6.48	128.50	111.00
2	C	16	LEU	N-CA-C	-5.81	95.31	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	38	TYR	Sidechain
1	B	38	TYR	Sidechain

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	1755	0	1671	105	0
1	B	1749	0	1682	95	0
2	C	567	0	555	17	0
2	D	538	0	528	13	0
3	A	71	0	0	1	0
3	B	51	0	0	2	0
3	C	23	0	0	1	0
3	D	11	0	0	1	0
All	All	4765	0	4436	224	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 25.

All (224) 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:201:ASN:HB3	1:A:204:VAL:HG12	1.43	1.01
1:B:191:LEU:O	1:B:191:LEU:HG	1.68	0.90
1:A:201:ASN:HB3	1:A:204:VAL:CG1	2.03	0.87
1:A:227:GLU:O	1:A:228:SER:HB2	1.75	0.87
1:B:104:THR:HG23	1:B:105:ARG:H	1.39	0.87
1:B:165:GLY:O	1:B:169:GLN:HG2	1.77	0.85
1:B:11:LEU:O	1:B:15:LYS:HD3	1.78	0.83
1:A:173:ALA:O	1:A:174:ILE:HD13	1.80	0.81
1:A:157:GLU:OE1	1:A:213:ARG:NH2	2.14	0.81
1:B:163:LEU:HB3	1:B:169:GLN:HA	1.63	0.81
1:A:194:HIS:HB2	3:A:282:HOH:O	1.82	0.79
1:A:124:THR:HA	1:A:145:THR:HG21	1.65	0.77
1:B:223:VAL:HG13	1:B:224:LEU:N	1.99	0.77
1:A:64:ASP:HB3	1:A:125:VAL:HG13	1.66	0.76
1:A:6:THR:HG23	1:A:52:GLU:OE1	1.87	0.74
1:A:6:THR:HB	1:A:8:HIS:CD2	2.21	0.74
1:B:3:ASN:O	1:B:4:GLU:HB2	1.85	0.74
1:A:30:GLU:O	1:A:35:VAL:HG13	1.87	0.73
1:A:201:ASN:CB	1:A:204:VAL:HG12	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:TYR:O	1:B:39:PRO:C	2.27	0.71
1:A:173:ALA:C	1:A:174:ILE:HD13	2.11	0.70
1:A:67:HIS:HB2	1:A:131:GLY:H	1.56	0.70
1:B:7:TRP:O	1:B:11:LEU:HB2	1.93	0.69
1:B:159:VAL:H	1:B:180:HIS:HD2	1.39	0.69
1:B:4:GLU:O	1:B:5:LEU:HB2	1.91	0.68
1:B:191:LEU:HB2	2:D:56:MET:SD	2.33	0.68
1:A:9:ASP:C	1:A:11:LEU:H	1.97	0.68
1:B:153:ASN:HA	1:B:180:HIS:CE1	2.29	0.68
1:A:153:ASN:ND2	1:A:175:ILE:HG23	2.10	0.67
1:A:163:LEU:HB3	1:A:169:GLN:HA	1.78	0.65
1:A:119:VAL:HG22	1:A:218:ILE:HD13	1.77	0.65
1:A:100:ILE:HG23	1:A:103:PHE:HB2	1.79	0.65
1:A:186:PRO:HG2	1:A:196:GLY:HA3	1.79	0.64
1:B:112:GLU:OE2	1:B:116:ARG:HD2	1.97	0.64
1:B:11:LEU:O	1:B:15:LYS:HB2	1.98	0.63
1:A:8:HIS:ND1	1:A:8:HIS:C	2.52	0.63
2:C:30:GLU:HA	2:C:35:ASN:O	1.98	0.63
1:A:201:ASN:O	1:A:204:VAL:HG12	1.99	0.63
1:B:223:VAL:CG1	1:B:224:LEU:N	2.62	0.63
1:A:99:THR:O	1:A:101:PRO:HD3	1.99	0.63
1:B:5:LEU:HD23	1:B:53:LEU:HG	1.80	0.62
1:B:210:LEU:O	1:B:213:ARG:HG3	1.99	0.62
1:A:30:GLU:HB3	1:A:37:ILE:HD11	1.81	0.62
1:A:6:THR:CG2	1:A:7:TRP:N	2.63	0.62
1:B:213:ARG:HG2	1:B:213:ARG:HH11	1.64	0.62
1:B:124:THR:HG22	1:B:145:THR:HG21	1.82	0.62
1:B:99:THR:O	1:B:101:PRO:HD3	2.00	0.61
1:B:107:ASN:ND2	1:B:107:ASN:O	2.33	0.61
1:B:38:TYR:O	1:B:40:PRO:N	2.34	0.61
1:A:176:ASP:HB3	1:A:179:ARG:HB2	1.82	0.61
1:A:95:GLU:OE2	1:A:200:CYS:O	2.19	0.61
1:A:30:GLU:CB	1:A:37:ILE:HD11	2.31	0.61
2:D:26:PRO:HA	2:D:37:PRO:HG2	1.82	0.60
1:A:201:ASN:HB2	1:A:205:LEU:HD13	1.82	0.60
1:A:153:ASN:HD22	1:A:175:ILE:HG23	1.65	0.60
1:A:6:THR:HG22	1:A:7:TRP:N	2.14	0.60
1:B:96:LEU:HD13	1:B:203:PHE:CD2	2.36	0.60
1:B:37:ILE:HD13	1:B:136:HIS:HE1	1.66	0.60
1:A:96:LEU:HA	1:A:99:THR:HG22	1.85	0.59
1:A:99:THR:HG23	1:A:100:ILE:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:HIS:HB2	1:A:131:GLY:N	2.17	0.59
1:B:14:GLU:HG3	1:B:147:LYS:HG2	1.83	0.59
1:A:170:LYS:O	1:A:171:LYS:C	2.37	0.59
1:B:95:GLU:O	1:B:99:THR:HG22	2.03	0.59
1:A:170:LYS:O	1:A:172:GLY:N	2.37	0.58
1:B:40:PRO:O	1:B:41:GLN:C	2.41	0.58
1:B:163:LEU:HB3	1:B:169:GLN:CA	2.33	0.57
1:A:153:ASN:HD21	1:A:176:ASP:H	1.52	0.57
1:A:10:VAL:C	1:A:12:ALA:H	2.06	0.57
1:A:9:ASP:O	1:A:11:LEU:N	2.36	0.57
1:B:95:GLU:OE2	1:B:198:PHE:O	2.22	0.57
2:D:18:ILE:HD12	2:D:44:HIS:HB3	1.87	0.57
1:A:154:GLN:O	1:A:179:ARG:NH1	2.36	0.57
2:D:23:LEU:HD11	2:D:40:ASP:HB3	1.86	0.57
1:A:159:VAL:H	1:A:180:HIS:HD2	1.51	0.56
1:B:104:THR:HG23	1:B:105:ARG:N	2.14	0.56
1:A:153:ASN:HA	1:A:180:HIS:CE1	2.40	0.56
1:A:41:GLN:NE2	1:A:44:VAL:HG21	2.20	0.56
1:B:9:ASP:C	1:B:11:LEU:H	2.09	0.56
1:A:187:HIS:CG	1:A:188:PRO:HD2	2.41	0.56
1:B:49:ARG:HH11	1:B:49:ARG:HG2	1.71	0.56
1:A:14:GLU:HG3	1:A:147:LYS:HG2	1.87	0.55
1:A:23:THR:O	1:A:26:THR:HG22	2.07	0.55
1:A:175:ILE:HG22	1:A:176:ASP:N	2.22	0.55
1:A:64:ASP:HB3	1:A:125:VAL:CG1	2.37	0.54
2:C:84:LEU:OXT	3:C:94:HOH:O	2.18	0.54
1:B:147:LYS:HE3	1:B:151:LEU:HD11	1.89	0.54
1:A:187:HIS:ND1	1:A:188:PRO:HD2	2.23	0.54
1:B:223:VAL:HG13	1:B:224:LEU:H	1.69	0.54
1:B:147:LYS:HG3	1:B:151:LEU:HD11	1.90	0.54
1:A:9:ASP:C	1:A:11:LEU:N	2.62	0.53
2:C:73:GLN:HA	2:C:78:GLU:O	2.09	0.53
1:B:69:PRO:HD2	3:B:262:HOH:O	2.08	0.53
1:A:223:VAL:HG13	1:A:224:LEU:N	2.23	0.52
1:A:6:THR:CG2	1:A:7:TRP:H	2.21	0.52
1:B:32:GLN:HB2	3:B:243:HOH:O	2.09	0.52
1:A:64:ASP:HB2	1:A:65:PRO:HD2	1.92	0.52
1:B:3:ASN:O	1:B:4:GLU:CB	2.55	0.52
1:A:58:VAL:HG12	1:A:59:VAL:N	2.24	0.52
1:B:147:LYS:O	1:B:151:LEU:CD1	2.58	0.52
1:B:147:LYS:O	1:B:151:LEU:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:VAL:CB	1:B:151:LEU:HD21	2.40	0.52
1:A:38:TYR:O	1:A:39:PRO:C	2.46	0.51
2:C:49:GLU:CG	2:C:49:GLU:O	2.57	0.51
1:A:5:LEU:H	1:A:5:LEU:HD23	1.76	0.51
1:B:176:ASP:O	1:B:178:GLN:N	2.44	0.51
1:B:106:PRO:HG3	1:B:222:PRO:HG2	1.93	0.51
1:B:9:ASP:O	1:B:11:LEU:N	2.41	0.50
1:B:60:ILE:HB	1:B:121:LEU:HD23	1.93	0.50
1:A:153:ASN:ND2	1:A:176:ASP:H	2.08	0.50
1:B:83:ILE:CG2	1:B:84:ALA:N	2.74	0.50
1:A:201:ASN:HB3	1:A:204:VAL:HG11	1.91	0.50
1:A:177:LYS:O	1:A:180:HIS:O	2.30	0.50
1:A:179:ARG:NH2	1:B:14:GLU:OE1	2.45	0.50
1:A:169:GLN:O	1:A:170:LYS:C	2.50	0.50
1:A:99:THR:CG2	1:A:100:ILE:N	2.74	0.49
1:A:58:VAL:CG1	1:A:59:VAL:N	2.74	0.49
1:B:163:LEU:HD13	1:B:169:GLN:HA	1.93	0.49
1:B:30:GLU:HB2	1:B:37:ILE:HD11	1.94	0.49
2:D:25:LEU:O	2:D:29:VAL:HG23	2.12	0.49
1:B:125:VAL:HA	1:B:141:TRP:HB3	1.94	0.49
2:D:47:TYR:HE2	3:D:94:HOH:O	1.95	0.49
2:C:74:ASP:OD2	2:C:78:GLU:HB3	2.11	0.49
1:B:201:ASN:O	1:B:204:VAL:HG12	2.13	0.48
1:B:165:GLY:C	1:B:169:GLN:HG2	2.33	0.48
2:C:49:GLU:HG3	2:C:49:GLU:O	2.14	0.48
1:B:147:LYS:HG3	1:B:151:LEU:CD1	2.42	0.48
1:B:193:ALA:HA	1:B:197:PHE:HB3	1.94	0.48
1:B:191:LEU:CG	1:B:191:LEU:O	2.50	0.48
1:A:10:VAL:C	1:A:12:ALA:N	2.67	0.48
1:B:176:ASP:C	1:B:178:GLN:H	2.17	0.48
1:B:10:VAL:C	1:B:12:ALA:H	2.17	0.48
1:B:49:ARG:HG2	1:B:49:ARG:NH1	2.29	0.48
1:B:57:LYS:NZ	1:B:216:THR:HG23	2.29	0.48
2:C:15:GLN:HG3	2:C:17:VAL:HG23	1.96	0.47
1:B:29:SER:O	1:B:33:SER:HB2	2.15	0.47
1:A:179:ARG:HH22	1:B:14:GLU:CD	2.16	0.47
1:A:200:CYS:HB2	1:A:202:HIS:CD2	2.49	0.47
1:B:14:GLU:HA	1:B:17:GLN:HG2	1.96	0.47
1:B:64:ASP:HB3	1:B:125:VAL:CG1	2.45	0.47
1:B:176:ASP:HB3	1:B:179:ARG:HB2	1.97	0.46
1:B:213:ARG:HH11	1:B:213:ARG:CG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ARG:HD3	1:B:215:GLU:OE2	2.16	0.46
1:A:204:VAL:HG13	1:A:205:LEU:N	2.30	0.46
1:B:10:VAL:C	1:B:12:ALA:N	2.66	0.46
1:B:30:GLU:CB	1:B:37:ILE:HD11	2.45	0.46
1:B:63:GLN:OE1	2:D:23:LEU:HB3	2.16	0.46
1:B:153:ASN:HA	1:B:180:HIS:HE1	1.76	0.46
1:B:104:THR:O	1:B:105:ARG:HB2	2.15	0.45
1:B:153:ASN:ND2	1:B:176:ASP:H	2.15	0.45
1:A:95:GLU:O	1:A:99:THR:HG22	2.16	0.45
1:A:38:TYR:O	1:A:40:PRO:N	2.49	0.45
1:B:129:ARG:HB2	1:B:135:SER:OG	2.15	0.45
1:B:24:LEU:HD12	1:B:24:LEU:HA	1.67	0.45
1:A:3:ASN:O	1:A:4:GLU:C	2.54	0.45
2:D:30:GLU:HA	2:D:35:ASN:O	2.17	0.45
1:A:175:ILE:CG2	1:A:176:ASP:N	2.79	0.45
2:C:36:LYS:HA	2:C:37:PRO:HD3	1.87	0.45
1:A:106:PRO:HG3	1:A:222:PRO:HG2	1.99	0.45
1:A:162:LEU:HD11	1:A:183:LEU:HD12	1.99	0.45
1:A:204:VAL:CG1	1:A:205:LEU:N	2.80	0.44
1:B:53:LEU:HD12	1:B:53:LEU:O	2.17	0.44
1:A:9:ASP:OD1	1:A:11:LEU:HD13	2.17	0.44
1:A:112:GLU:O	1:A:116:ARG:HG3	2.17	0.44
1:A:201:ASN:CB	1:A:204:VAL:CG1	2.86	0.44
2:C:30:GLU:OE1	2:C:36:LYS:HE3	2.17	0.44
1:B:103:PHE:HE2	1:B:220:TRP:O	2.01	0.44
2:C:49:GLU:OE2	2:C:49:GLU:O	2.34	0.44
1:B:163:LEU:HD11	1:B:173:ALA:HB1	1.98	0.44
1:A:30:GLU:OE1	1:A:129:ARG:NH1	2.51	0.43
1:A:191:LEU:O	1:A:191:LEU:HG	2.18	0.43
1:A:30:GLU:CD	1:A:129:ARG:NH1	2.71	0.43
1:B:169:GLN:O	1:B:171:LYS:N	2.52	0.43
1:A:114:TRP:O	1:A:119:VAL:HG23	2.18	0.43
1:B:170:LYS:O	1:B:171:LYS:C	2.56	0.43
1:A:159:VAL:O	1:A:180:HIS:HB3	2.18	0.43
1:A:181:HIS:HB2	1:A:209:TRP:CZ2	2.53	0.43
1:A:30:GLU:HB2	1:A:37:ILE:HD11	1.99	0.43
2:C:47:TYR:CG	2:C:48:ASP:N	2.87	0.43
1:A:13:GLU:C	1:A:15:LYS:H	2.22	0.43
2:C:25:LEU:HB3	2:C:26:PRO:HD2	2.00	0.43
1:B:209:TRP:O	1:B:210:LEU:C	2.57	0.43
1:B:51:THR:HG23	1:B:120:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:GLN:O	1:B:79:VAL:HA	2.19	0.42
2:C:81:ILE:HG22	2:C:82:LYS:N	2.34	0.42
1:A:187:HIS:CE1	1:A:188:PRO:HD2	2.54	0.42
1:B:64:ASP:HB3	1:B:125:VAL:HG13	2.02	0.42
2:D:48:ASP:OD1	2:D:50:SER:OG	2.36	0.42
1:A:179:ARG:NH2	1:B:14:GLU:CD	2.73	0.42
1:A:41:GLN:HE22	1:A:44:VAL:HG21	1.84	0.42
1:A:6:THR:HG23	1:A:7:TRP:H	1.85	0.42
1:A:163:LEU:HB3	1:A:169:GLN:CA	2.48	0.42
1:A:57:LYS:HE3	1:A:117:GLN:O	2.19	0.42
1:A:9:ASP:O	1:A:9:ASP:CG	2.57	0.42
1:B:151:LEU:HD12	1:B:151:LEU:N	2.34	0.42
1:A:152:ILE:O	1:A:156:ARG:HB2	2.19	0.42
1:A:24:LEU:HD12	1:A:24:LEU:HA	1.83	0.42
1:B:64:ASP:CB	1:B:125:VAL:HG13	2.50	0.42
1:B:139:LEU:HD12	1:B:139:LEU:N	2.35	0.42
1:B:15:LYS:HG3	1:B:20:PHE:CE2	2.55	0.42
1:A:223:VAL:CG1	1:A:224:LEU:N	2.83	0.42
1:A:166:SER:HB2	2:C:28:GLU:CD	2.40	0.41
1:A:100:ILE:HA	1:A:101:PRO:HD2	1.83	0.41
1:B:164:TRP:HA	1:B:185:ALA:O	2.20	0.41
1:B:153:ASN:HD21	1:B:176:ASP:H	1.68	0.41
1:A:96:LEU:HD12	1:A:100:ILE:HG22	2.02	0.41
2:C:38:GLU:HG3	2:C:38:GLU:O	2.20	0.41
1:A:64:ASP:CB	1:A:125:VAL:HG13	2.44	0.41
1:A:11:LEU:O	1:A:15:LYS:HG3	2.21	0.41
1:A:154:GLN:HB3	1:A:155:HIS:ND1	2.35	0.41
1:B:32:GLN:HG2	1:B:33:SER:N	2.35	0.41
1:A:31:ARG:HG2	1:A:37:ILE:HD12	2.02	0.41
2:D:44:HIS:HE1	2:D:59:THR:OG1	2.04	0.41
1:B:96:LEU:O	1:B:100:ILE:HG23	2.21	0.41
2:D:67:PRO:HB3	2:D:84:LEU:HD13	2.03	0.41
2:C:21:SER:HA	2:C:43:VAL:O	2.21	0.41
2:C:27:GLU:H	2:C:27:GLU:HG2	1.54	0.41
1:B:20:PHE:CE2	1:B:24:LEU:HD22	2.56	0.41
1:A:19:TYR:CG	1:A:20:PHE:N	2.89	0.41
1:B:112:GLU:OE2	1:B:116:ARG:NH1	2.35	0.41
2:D:41:ILE:HA	2:D:41:ILE:HD13	1.92	0.41
2:D:58:LEU:HD12	2:D:69:ALA:HB3	2.02	0.41
1:A:112:GLU:HG2	1:A:112:GLU:O	2.21	0.40
1:A:15:LYS:HA	1:A:20:PHE:CD1	2.57	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	224/229 (98%)	177 (79%)	36 (16%)	11 (5%)	3 10
1	B	222/229 (97%)	174 (78%)	33 (15%)	15 (7%)	1 4
2	C	71/84 (84%)	62 (87%)	7 (10%)	2 (3%)	6 24
2	D	68/84 (81%)	62 (91%)	5 (7%)	1 (2%)	13 42
All	All	585/626 (94%)	475 (81%)	81 (14%)	29 (5%)	3 9

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	PRO
1	A	226	ALA
1	A	227	GLU
1	B	4	GLU
1	B	5	LEU
1	B	6	THR
1	B	171	LYS
2	C	15	GLN
1	A	4	GLU
1	A	103	PHE
1	A	106	PRO
1	B	10	VAL
1	B	13	GLU
1	B	38	TYR
1	B	101	PRO
1	B	177	LYS
2	D	50	SER
1	A	44	VAL
1	A	81	PRO
1	B	77	PHE

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Mol	Chain	Res	Type
1	A	10	VAL
1	B	105	ARG
1	B	170	LYS
1	B	192	SER
1	A	38	TYR
1	A	137	ALA
1	B	81	PRO
1	B	102	GLY
2	C	13	GLY

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	181/194 (93%)	149 (82%)	32 (18%)	2 7
1	B	181/194 (93%)	149 (82%)	32 (18%)	2 7
2	C	64/78 (82%)	57 (89%)	7 (11%)	8 23
2	D	61/78 (78%)	56 (92%)	5 (8%)	14 39
All	All	487/544 (90%)	411 (84%)	76 (16%)	3 10

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	16	GLN
1	A	17	GLN
1	A	21	LEU
1	A	24	LEU
1	A	31	ARG
1	A	35	VAL
1	A	36	THR
1	A	38	TYR
1	A	39	PRO
1	A	49	ARG
1	A	51	THR

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Mol	Chain	Res	Type
1	A	61	LEU
1	A	96	LEU
1	A	116	ARG
1	A	125	VAL
1	A	134	HIS
1	A	143	THR
1	A	145	THR
1	A	154	GLN
1	A	155	HIS
1	A	157	GLU
1	A	162	LEU
1	A	166	SER
1	A	169	GLN
1	A	178	GLN
1	A	179	ARG
1	A	209	TRP
1	A	212	GLN
1	A	221	MET
1	A	223	VAL
1	A	228	SER
1	B	5	LEU
1	B	8	HIS
1	B	9	ASP
1	B	13	GLU
1	B	15	LYS
1	B	21	LEU
1	B	24	LEU
1	B	26	THR
1	B	31	ARG
1	B	35	VAL
1	B	36	THR
1	B	38	TYR
1	B	51	THR
1	B	96	LEU
1	B	124	THR
1	B	125	VAL
1	B	134	HIS
1	B	142	GLU
1	B	143	THR
1	B	145	THR
1	B	162	LEU
1	B	169	GLN

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Mol	Chain	Res	Type
1	B	177	LYS
1	B	178	GLN
1	B	179	ARG
1	B	192	SER
1	B	205	LEU
1	B	209	TRP
1	B	210	LEU
1	B	213	ARG
1	B	223	VAL
1	B	224	LEU
2	C	14	LYS
2	C	27	GLU
2	C	57	LEU
2	C	66	LYS
2	C	75	SER
2	C	76	ASN
2	C	80	LYS
2	D	16	LEU
2	D	36	LYS
2	D	57	LEU
2	D	76	ASN
2	D	80	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	22	ASN
1	A	25	GLN
1	A	46	ASN
1	A	91	ASN
1	A	153	ASN
1	A	169	GLN
1	A	178	GLN
1	A	180	HIS
1	A	202	HIS
1	A	212	GLN
1	B	22	ASN
1	B	46	ASN
1	B	91	ASN
1	B	153	ASN
1	B	180	HIS

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Mol	Chain	Res	Type
2	C	44	HIS
2	D	15	GLN
2	D	35	ASN
2	D	44	HIS

5.3.3 RNA

There are no RNA molecules 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

There are no ligands in this entry.

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, 95^{th} 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	226/229 (98%)	-0.59	3 (1%)	79 78	3, 24, 67, 99	0
1	B	224/229 (97%)	-0.46	6 (2%)	58 52	7, 31, 73, 100	0
2	C	73/84 (86%)	-0.51	1 (1%)	78 76	4, 22, 81, 99	0
2	D	70/84 (83%)	-0.50	2 (2%)	55 49	11, 33, 72, 88	0
All	All	593/626 (94%)	-0.52	12 (2%)	68 64	3, 28, 72, 100	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	12	THR	6.8
1	B	196	GLY	4.5
1	B	2	ALA	4.2
1	B	3	ASN	4.1
1	A	228	SER	3.9
1	B	172	GLY	3.0
1	A	3	ASN	3.0
1	B	170	LYS	2.8
1	B	214	GLY	2.4
1	A	10	VAL	2.4
2	D	76	ASN	2.1
2	D	47	TYR	2.1

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.