W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:53 PM GMT

PDB ID	:	4JU6
Title	:	Crystal structure of hcv ns5b polymerase in complex with compound 24
Authors	:	Coulombe, R.
Deposited on	:	2013-03-24
Resolution	:	2.20 Å(reported)

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

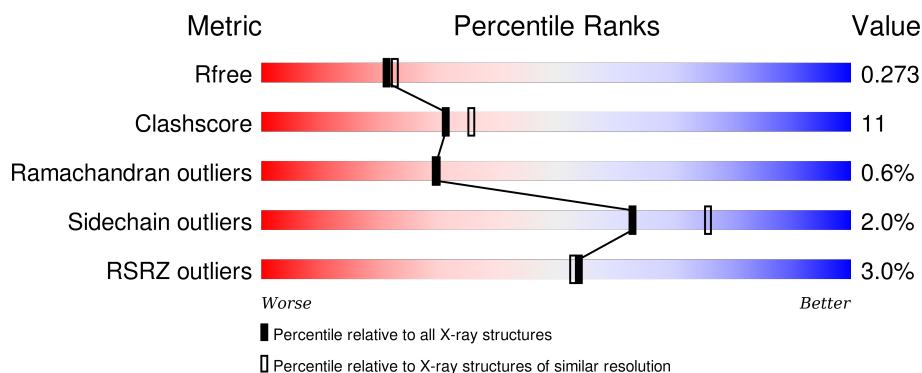|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.20 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	Percentile Ranks	Value
Rfree		0.273
Clashscore		11
Ramachandran outliers		0.6%
Sidechain outliers		2.0%
RSRZ outliers		3.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	576	77% 19% ••
1	B	576	6% 70% 26% ••

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8989 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4358	2745	770	811	32			
1	B	558	Total	C	N	O	S	0	0	0
			4346	2737	768	809	32			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	571	HIS	-	EXPRESSION TAG	UNP O92972
A	572	HIS	-	EXPRESSION TAG	UNP O92972
A	573	HIS	-	EXPRESSION TAG	UNP O92972
A	574	HIS	-	EXPRESSION TAG	UNP O92972
A	575	HIS	-	EXPRESSION TAG	UNP O92972
A	576	HIS	-	EXPRESSION TAG	UNP O92972
B	571	HIS	-	EXPRESSION TAG	UNP O92972
B	572	HIS	-	EXPRESSION TAG	UNP O92972
B	573	HIS	-	EXPRESSION TAG	UNP O92972
B	574	HIS	-	EXPRESSION TAG	UNP O92972
B	575	HIS	-	EXPRESSION TAG	UNP O92972
B	576	HIS	-	EXPRESSION TAG	UNP O92972

- Molecule 2 is 2-{[(TRANS-4-METHYLCYCLOHEXYL)CARBONYL](PROPAN-2-YL)AMINO}-5-PHENOXYBENZOIC ACID (three-letter code: 1O6) (formula: $C_{24}H_{29}NO_4$).
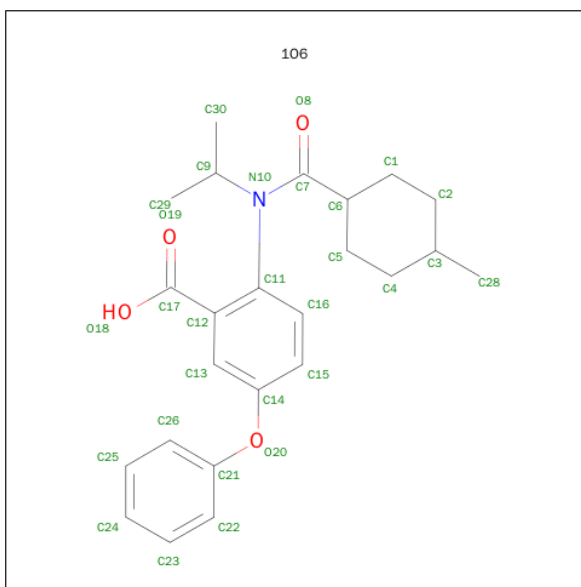
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 29	C 24	N 1	O 4	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	157	Total 157	O 157	0	0
4	B	97	Total 97	O 97	0	0

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: Genome polyprotein
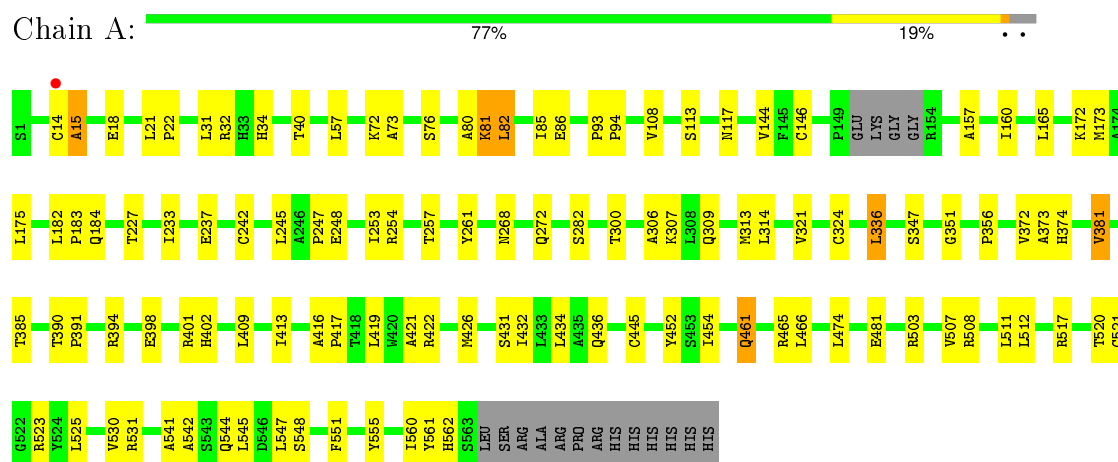
- Molecule 1: Genome polyprotein
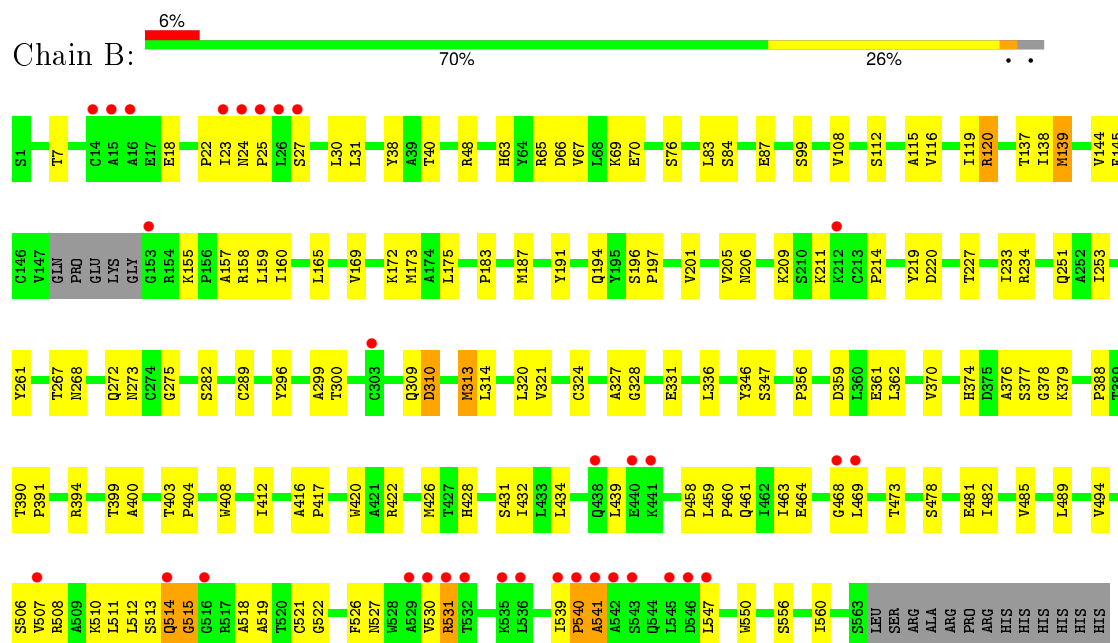
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.84Å 108.07Å 135.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 49.69 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.20) 98.5 (49.69-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.20Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.237 , 0.296 0.245 , 0.273	Depositor DCC
R_{free} test set	7925 reflections (11.21%)	DCC
Wilson B-factor (Å²)	36.0	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.33 , 39.5	EDS
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 78622 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8989	wwPDB-VP
Average B, all atoms (Å²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 1O6, MG

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	0.39	0/4453	0.65	2/6044 (0.0%)
1	B	0.40	0/4440	0.63	0/6025
All	All	0.40	0/8893	0.64	2/12069 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	351	GLY	N-CA-C	-5.48	99.41	113.10
1	A	31	LEU	CA-CB-CG	5.32	127.55	115.30

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	4358	0	4371	73	0
1	B	4346	0	4359	118	0
2	A	29	0	28	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	157	0	0	3	0
4	B	97	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8989	0	8758	188	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (188) 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:81:LYS:O	1:A:82:LEU:HB3	1.70	0.87
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.58	0.85
1:B:531:ARG:HH11	1:B:531:ARG:H	1.24	0.85
1:B:506:SER:O	1:B:510:LYS:HG3	1.78	0.82
1:A:465:ARG:NH1	1:A:545:LEU:O	2.19	0.75
1:B:515:GLY:HA2	1:B:519:ALA:HB2	1.70	0.72
1:B:461:GLN:HG2	1:B:541:ALA:HB3	1.72	0.71
1:A:248:GLU:HG3	4:A:738:HOH:O	1.94	0.68
1:A:336:LEU:HD12	1:A:356:PRO:HD3	1.77	0.67
1:A:108:VAL:HG21	1:A:165:LEU:HD21	1.75	0.67
1:B:376:ALA:C	1:B:378:GLY:H	1.98	0.67
1:A:40:THR:HB	1:A:157:ALA:HB2	1.76	0.67
1:A:381:VAL:HG11	1:A:474:LEU:CD2	2.24	0.66
1:B:158:ARG:HH11	1:B:158:ARG:HG3	1.59	0.66
1:A:34:HIS:HB3	4:A:840:HOH:O	1.96	0.65
1:B:201:VAL:HG13	1:B:370:VAL:HG13	1.78	0.65
1:B:434:LEU:HG	1:B:439:LEU:HD11	1.78	0.65
1:B:22:PRO:HD2	1:B:400:ALA:HB1	1.76	0.65
1:A:73:ALA:O	1:A:76:SER:HB2	1.97	0.64
1:B:27:SER:OG	1:B:399:THR:HB	1.98	0.64
1:A:521:CYS:HB3	1:A:525:LEU:HD12	1.80	0.63
1:B:99:SER:HB2	1:B:165:LEU:HB3	1.81	0.63
1:B:187:MET:HE3	1:B:296:TYR:HB2	1.81	0.63
1:A:72:LYS:HD2	1:A:242:CYS:SG	2.39	0.63
1:A:81:LYS:O	1:A:82:LEU:CB	2.43	0.62
1:B:408:TRP:O	1:B:412:ILE:HG13	2.00	0.62
1:B:66:ASP:O	1:B:70:GLU:HG3	1.99	0.62
1:B:205:VAL:CG1	1:B:209:LYS:HE3	2.29	0.62
1:B:23:ILE:O	1:B:24:ASN:HB2	2.00	0.62
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.30	0.62
1:B:370:VAL:HG23	4:B:780:HOH:O	2.00	0.61
1:A:14:CYS:O	1:A:15:ALA:HB2	2.01	0.61
1:A:503:ARG:O	1:A:507:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLN:HG2	1:A:541:ALA:HB3	1.81	0.61
1:B:478:SER:O	1:B:482:ILE:HG13	2.00	0.61
1:B:434:LEU:HD11	1:B:511:LEU:CD2	2.31	0.60
1:B:22:PRO:CD	1:B:400:ALA:HB1	2.31	0.60
1:B:508:ARG:HD2	1:B:526:PHE:O	2.02	0.60
1:B:506:SER:OG	1:B:510:LYS:HE3	2.01	0.60
1:B:158:ARG:NH1	1:B:158:ARG:HG3	2.14	0.58
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.85	0.58
1:B:84:SER:OG	1:B:87:GLU:HG3	2.05	0.56
1:B:531:ARG:HH11	1:B:531:ARG:N	2.01	0.56
1:A:419:LEU:HD21	2:A:601:1O6:H20	1.87	0.55
1:A:531:ARG:HB2	1:A:531:ARG:NH1	2.22	0.55
1:B:512:LEU:C	1:B:514:GLN:H	2.09	0.55
1:B:38:TYR:CZ	1:B:145:PHE:HB2	2.41	0.55
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.88	0.55
1:B:336:LEU:HD23	1:B:356:PRO:HD3	1.89	0.55
1:B:31:LEU:HD12	1:B:31:LEU:O	2.07	0.55
1:A:85:ILE:HG12	1:A:173:MET:SD	2.47	0.55
1:A:300:THR:HA	1:A:313:MET:CE	2.37	0.54
1:B:539:ILE:HG23	1:B:540:PRO:HD2	1.89	0.54
1:A:381:VAL:HG11	1:A:474:LEU:HD21	1.89	0.54
1:B:458:ASP:OD1	1:B:461:GLN:OE1	2.27	0.53
1:B:115:ALA:O	1:B:119:ILE:HG13	2.09	0.52
1:B:376:ALA:O	1:B:378:GLY:N	2.43	0.52
1:A:268:ASN:ND2	1:A:272:GLN:HB2	2.25	0.52
1:B:374:HIS:HA	1:B:379:LYS:O	2.10	0.51
1:B:233:ILE:HD13	1:B:261:TYR:O	2.10	0.51
1:B:428:HIS:O	1:B:432:ILE:HG13	2.10	0.51
1:B:515:GLY:CA	1:B:519:ALA:HB2	2.39	0.51
1:B:227:THR:HB	1:B:347:SER:O	2.10	0.51
1:B:489:LEU:HD22	1:B:494:VAL:HB	1.91	0.51
1:A:108:VAL:CG2	1:A:165:LEU:HD21	2.41	0.50
1:B:24:ASN:N	1:B:25:PRO:HD3	2.26	0.50
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.94	0.50
1:A:254:ARG:HG2	1:B:251:GLN:NE2	2.27	0.49
1:A:465:ARG:HG2	1:A:542:ALA:O	2.12	0.49
1:B:361:GLU:HG3	1:B:370:VAL:O	2.13	0.49
1:B:187:MET:HE2	1:B:296:TYR:CD2	2.47	0.49
1:B:359:ASP:HB3	1:B:362:LEU:CD1	2.43	0.49
1:A:461:GLN:HG2	1:A:541:ALA:CB	2.43	0.49
1:B:328:GLY:HA3	1:B:331:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:CYS:O	1:A:14:CYS:SG	2.70	0.49
1:B:390:THR:HB	1:B:391:PRO:HD3	1.95	0.48
1:B:434:LEU:HD11	1:B:511:LEU:HD21	1.95	0.48
1:A:175:LEU:HD21	1:A:253:ILE:HG12	1.95	0.48
1:B:359:ASP:HB3	1:B:362:LEU:HD12	1.94	0.48
1:A:434:LEU:HD11	1:A:511:LEU:HG	1.95	0.48
1:A:555:TYR:CD1	1:A:560:ILE:HG13	2.49	0.48
1:B:508:ARG:HG3	1:B:522:GLY:O	2.13	0.48
1:B:30:LEU:HD22	1:B:428:HIS:CD2	2.48	0.48
1:B:183:PRO:HG3	1:B:289:CYS:SG	2.53	0.48
1:B:273:ASN:ND2	1:B:275:GLY:H	2.11	0.48
1:A:93:PRO:HG3	1:A:561:TYR:HB2	1.96	0.47
1:A:14:CYS:O	1:A:15:ALA:CB	2.60	0.47
1:B:7:THR:HG23	1:B:275:GLY:HA2	1.94	0.47
1:B:388:PRO:HB3	1:B:420:TRP:CD2	2.49	0.47
1:B:40:THR:HB	1:B:157:ALA:HB2	1.97	0.47
1:A:268:ASN:HD21	1:A:272:GLN:HB2	1.80	0.47
1:A:237:GLU:HG3	1:A:257:THR:OG1	2.14	0.47
1:A:300:THR:HA	1:A:313:MET:HE3	1.97	0.47
1:A:390:THR:HB	1:A:391:PRO:HD3	1.96	0.47
1:B:300:THR:HA	1:B:313:MET:HE2	1.96	0.47
1:B:211:LYS:NZ	1:B:310:ASP:O	2.44	0.47
1:B:416:ALA:HB3	1:B:417:PRO:HD3	1.97	0.47
1:B:527:ASN:O	1:B:530:VAL:HG22	2.14	0.47
1:B:201:VAL:HG13	1:B:370:VAL:CG1	2.45	0.46
1:B:403:THR:HA	1:B:404:PRO:HD3	1.78	0.46
1:B:481:GLU:O	1:B:485:VAL:HG23	2.16	0.46
1:B:172:LYS:HE3	1:B:560:ILE:HD13	1.97	0.46
1:A:512:LEU:HD21	1:A:523:ARG:HG2	1.98	0.46
1:A:21:LEU:HD12	1:A:22:PRO:HD2	1.98	0.46
1:B:376:ALA:C	1:B:378:GLY:N	2.64	0.46
1:B:201:VAL:O	1:B:205:VAL:HG23	2.14	0.46
1:B:205:VAL:HG13	1:B:209:LYS:HE3	1.98	0.46
1:A:416:ALA:HB3	1:A:417:PRO:HD3	1.98	0.46
1:A:233:ILE:HD13	1:A:261:TYR:O	2.16	0.46
1:B:336:LEU:CD2	1:B:356:PRO:HD3	2.46	0.46
1:B:314:LEU:HB3	1:B:321:VAL:HG13	1.97	0.46
1:B:346:TYR:O	1:B:347:SER:HB3	2.16	0.46
1:B:112:SER:O	1:B:116:VAL:HG23	2.15	0.45
1:B:556:SER:HB2	4:B:746:HOH:O	2.16	0.45
1:B:48:ARG:HG2	1:B:159:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ASN:HD21	1:B:272:GLN:HB2	1.82	0.45
1:B:197:PRO:O	1:B:201:VAL:HG23	2.16	0.45
1:B:63:HIS:O	1:B:67:VAL:HG23	2.17	0.45
1:B:547:LEU:O	1:B:550:TRP:HB2	2.16	0.45
1:A:306:ALA:O	1:A:307:LYS:HB2	2.17	0.45
1:B:359:ASP:HB3	1:B:362:LEU:HG	1.99	0.44
1:B:211:LYS:HB2	1:B:214:PRO:HB3	1.99	0.44
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.47	0.44
1:A:227:THR:HB	1:A:347:SER:O	2.17	0.44
1:B:512:LEU:C	1:B:514:GLN:N	2.70	0.44
1:B:83:LEU:HB2	1:B:173:MET:HA	2.00	0.44
1:A:434:LEU:CD1	1:A:507:VAL:HG13	2.47	0.44
1:B:327:ALA:O	1:B:331:GLU:HB2	2.17	0.44
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.87	0.44
1:A:517:ARG:O	1:A:520:THR:HB	2.18	0.44
1:B:22:PRO:O	1:B:25:PRO:HG3	2.18	0.44
1:A:309:GLN:O	1:A:324:CYS:HB2	2.17	0.44
1:A:247:PRO:HG3	1:B:234:ARG:HD3	1.99	0.44
1:A:80:ALA:HB3	1:A:245:LEU:HD23	2.00	0.44
1:A:466:LEU:HD22	1:A:551:PHE:HE2	1.83	0.44
1:B:431:SER:HB2	1:B:507:VAL:HG21	1.99	0.43
1:B:485:VAL:O	1:B:489:LEU:HG	2.18	0.43
1:B:160:ILE:HA	1:B:282:SER:OG	2.17	0.43
1:B:155:LYS:HB3	1:B:155:LYS:HE2	1.82	0.43
1:B:309:GLN:O	1:B:324:CYS:HB2	2.17	0.43
1:A:57:LEU:C	1:A:57:LEU:HD23	2.39	0.43
1:A:385:THR:HG21	1:A:481:GLU:OE1	2.19	0.43
1:B:196:SER:O	1:B:197:PRO:C	2.57	0.43
1:A:172:LYS:NZ	4:A:846:HOH:O	2.45	0.43
1:B:464:GLU:O	1:B:468:GLY:N	2.52	0.43
1:A:113:SER:O	1:A:117:ASN:ND2	2.52	0.43
1:B:268:ASN:ND2	1:B:272:GLN:HB2	2.33	0.43
1:B:18:GLU:HA	1:B:18:GLU:OE2	2.18	0.43
1:B:434:LEU:HD11	1:B:511:LEU:HG	2.00	0.43
1:B:187:MET:CE	1:B:296:TYR:HB2	2.48	0.43
1:A:409:LEU:O	1:A:413:ILE:HG13	2.18	0.43
1:B:299:ALA:C	1:B:313:MET:HE1	2.39	0.43
1:A:72:LYS:HB3	1:B:76:SER:HB2	2.00	0.42
1:A:422:ARG:HA	1:A:426:MET:SD	2.59	0.42
1:A:394:ARG:O	1:A:398:GLU:HG3	2.20	0.42
1:B:137:THR:HA	1:B:267:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ARG:HG2	1:B:426:MET:HE1	2.01	0.42
1:A:445:CYS:SG	1:A:454:ILE:HD12	2.59	0.42
1:A:160:ILE:HA	1:A:282:SER:OG	2.19	0.42
1:B:108:VAL:HG21	1:B:165:LEU:HD21	2.01	0.42
1:A:544:GLN:O	1:A:544:GLN:HG2	2.19	0.42
1:B:65:ARG:O	1:B:69:LYS:HG3	2.20	0.42
1:B:416:ALA:CB	1:B:463:ILE:HG23	2.50	0.42
1:B:512:LEU:O	1:B:514:GLN:N	2.53	0.42
1:A:545:LEU:HD22	1:A:547:LEU:CD1	2.50	0.42
1:B:531:ARG:NH1	1:B:531:ARG:H	2.04	0.41
1:A:18:GLU:HG3	1:A:401:ARG:NH1	2.35	0.41
1:B:459:LEU:N	1:B:460:PRO:CD	2.83	0.41
1:A:452:TYR:OH	1:A:562:HIS:HD2	2.03	0.41
1:B:515:GLY:HA2	1:B:519:ALA:CB	2.46	0.41
1:A:40:THR:HB	1:A:157:ALA:CB	2.47	0.41
1:B:120:ARG:NH1	1:B:120:ARG:HG3	2.35	0.41
1:B:138:ILE:O	1:B:139:MET:HG2	2.20	0.41
1:A:508:ARG:CZ	1:A:530:VAL:HG11	2.51	0.41
1:B:175:LEU:HD21	1:B:253:ILE:HG12	2.02	0.41
1:B:434:LEU:CD1	1:B:507:VAL:HG13	2.51	0.41
1:B:464:GLU:HG3	1:B:469:LEU:HD23	2.02	0.41
1:B:205:VAL:O	1:B:206:ASN:C	2.58	0.41
1:A:182:LEU:N	1:A:183:PRO:CD	2.83	0.41
1:A:21:LEU:HA	1:A:22:PRO:HD3	1.92	0.40
1:A:508:ARG:NH1	1:A:530:VAL:HG11	2.36	0.40
1:B:191:TYR:O	1:B:194:GLN:HG2	2.22	0.40
1:B:431:SER:HB2	1:B:507:VAL:CG2	2.51	0.40
1:A:432:ILE:O	1:A:436:GLN:HG3	2.21	0.40
1:A:421:ALA:O	1:A:426:MET:HG3	2.20	0.40
1:B:518:ALA:O	1:B:521:CYS:HB2	2.20	0.40
1:A:372:VAL:HG22	1:A:373:ALA:N	2.35	0.40
1:A:374:HIS:O	1:A:474:LEU:HA	2.22	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	555/576 (96%)	534 (96%)	19 (3%)	2 (0%)	39	42
1	B	554/576 (96%)	518 (94%)	31 (6%)	5 (1%)	21	19
All	All	1109/1152 (96%)	1052 (95%)	50 (4%)	7 (1%)	30	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ALA
1	B	377	SER
1	B	515	GLY
1	A	82	LEU
1	B	513	SER
1	B	540	PRO
1	B	541	ALA

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	477/491 (97%)	466 (98%)	11 (2%)	58	71
1	B	475/491 (97%)	467 (98%)	8 (2%)	68	81
All	All	952/982 (97%)	933 (98%)	19 (2%)	63	76

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	81	LYS
1	A	86	GLU
1	A	146	CYS
1	A	184	GLN

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Mol	Chain	Res	Type
1	A	336	LEU
1	A	381	VAL
1	A	402	HIS
1	A	431	SER
1	A	461	GLN
1	A	548	SER
1	B	120	ARG
1	B	139	MET
1	B	220	ASP
1	B	310	ASP
1	B	313	MET
1	B	473	THR
1	B	514	GLN
1	B	531	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	GLN
1	A	273	ASN
1	A	374	HIS
1	A	438	GLN
1	A	483	ASN
1	A	544	GLN
1	A	562	HIS
1	B	251	GLN
1	B	273	ASN
1	B	309	GLN
1	B	406	ASN
1	B	428	HIS
1	B	436	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	#$|Z| > 2$
2	1O6	A	601	-	28,31,31	2.04	10 (35%)	34,43,43	1.00	1 (2%)

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	1O6	A	601	-	-	0/20/34/34	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	1O6	C25-C26	2.08	1.43	1.38
2	A	601	1O6	C16-C15	2.12	1.42	1.38
2	A	601	1O6	C22-C21	2.16	1.43	1.38
2	A	601	1O6	C16-C11	2.16	1.43	1.39
2	A	601	1O6	C15-C14	2.28	1.43	1.38
2	A	601	1O6	C9-N10	2.30	1.53	1.49
2	A	601	1O6	C26-C21	2.61	1.43	1.38
2	A	601	1O6	C6-C7	2.86	1.56	1.51
2	A	601	1O6	C12-C11	3.22	1.45	1.41
2	A	601	1O6	C7-N10	5.78	1.44	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	1O6	C29-C9-N10	3.96	117.19	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	1O6	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	559/576 (97%)	0.02	1 (0%)	95	95	19, 34, 51, 63	0
1	B	558/576 (96%)	0.38	33 (5%)	26	25	22, 42, 60, 67	0
All	All	1117/1152 (96%)	0.20	34 (3%)	54	53	19, 37, 57, 67	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	ILE	5.2
1	B	24	ASN	5.0
1	B	530	VAL	4.9
1	B	535	LYS	4.7
1	B	531	ARG	4.2
1	B	27	SER	4.1
1	B	539	ILE	3.9
1	B	26	LEU	3.8
1	B	532	THR	3.7
1	B	507	VAL	3.6
1	B	542	ALA	3.6
1	B	529	ALA	3.6
1	B	15	ALA	3.3
1	B	14	CYS	3.2
1	B	468	GLY	3.0
1	B	541	ALA	3.0
1	B	545	LEU	2.9
1	B	540	PRO	2.8
1	B	153	GLY	2.7
1	B	536	LEU	2.6
1	A	14	CYS	2.6
1	B	440	GLU	2.5
1	B	438	GLN	2.3
1	B	516	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	16	ALA	2.3
1	B	514	GLN	2.2
1	B	469	LEU	2.2
1	B	441	LYS	2.2
1	B	25	PRO	2.1
1	B	212	LYS	2.1
1	B	303	CYS	2.1
1	B	547	LEU	2.1
1	B	546	ASP	2.1
1	B	543	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	1O6	A	601	29/29	0.91	0.16	1.93	35,40,46,47	0
3	MG	A	602	1/1	0.84	0.19	1.61	57,57,57,57	0
3	MG	B	601	1/1	0.66	0.55	-	75,75,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.