Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:47 PM GMT

PDB ID	:	4JHZ
Title	:	Structure of E. coli beta-Glucuronidase bound with a novel, potent inhibitor 2-[4-(1,3-benzodioxol-5-ylmethyl)piperazin-1-yl]-N-[(1S,2S,5S)-2,5-dimethoxy cyclohexyl]acetamide
Authors	:	Roberts, A.B.; Wallace, B.D.; Redinbo, M.R.
Deposited on	:	2013-03-05
Resolution	:	2.83 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:

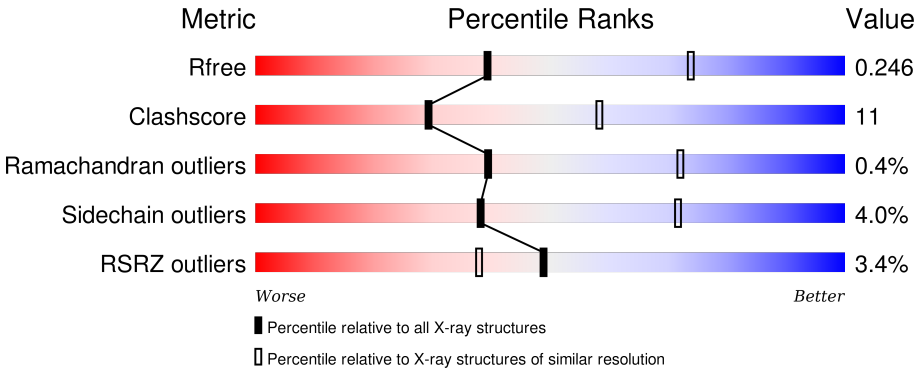
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.83 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	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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	603	3% 78% 19%
1	B	603	4% 76% 21%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9613 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.

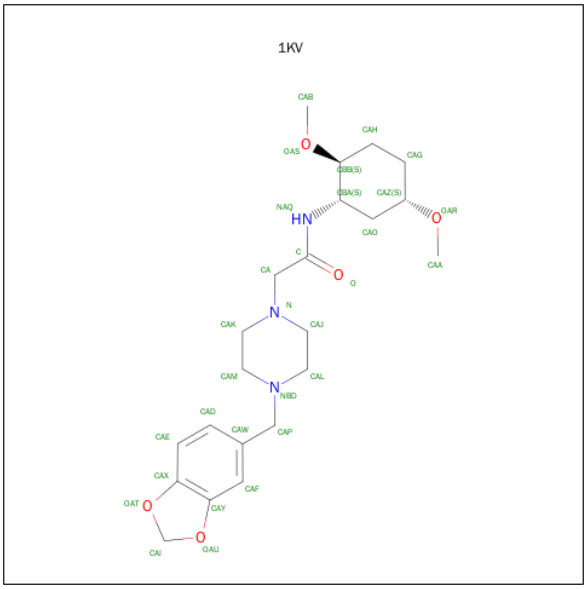
- Molecule 1 is a protein called Beta-glucuronidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	Se	0	0	0
			4746	3013	816	895	9	13			
1	B	596	Total	C	N	O	S	Se	0	0	0
			4683	2971	811	880	8	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P05804
A	0	HIS	-	EXPRESSION TAG	UNP P05804
B	-1	SER	-	EXPRESSION TAG	UNP P05804
B	0	HIS	-	EXPRESSION TAG	UNP P05804

- Molecule 2 is 2-[4-(1,3-BENZODIOXOL-5-YLMETHYL)PIPERAZIN-1-YL]-N-[(1S,2S,5S)-2,5-DIMETHOXYCYCLOHEXYL]ACETAMIDE (three-letter code: 1KV) (formula: $C_{22}H_{33}N_3O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	22	3	5		
2	B	1	Total	C	N	O	0	0
			30	22	3	5		

- Molecule 3 is water.

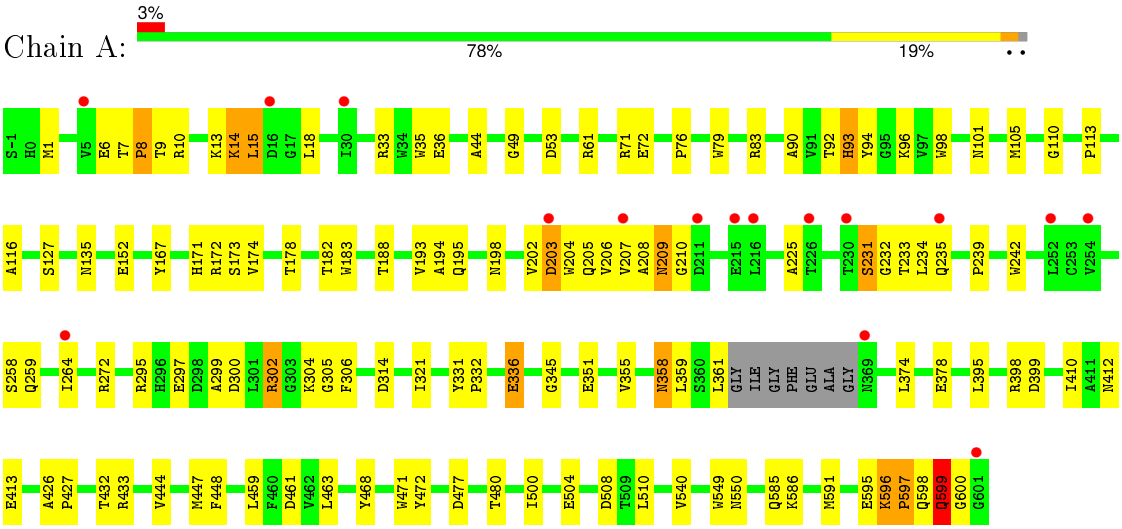
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	82	Total	O	0	0
			82	82		
3	B	42	Total	O	0	0
			42	42		

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.

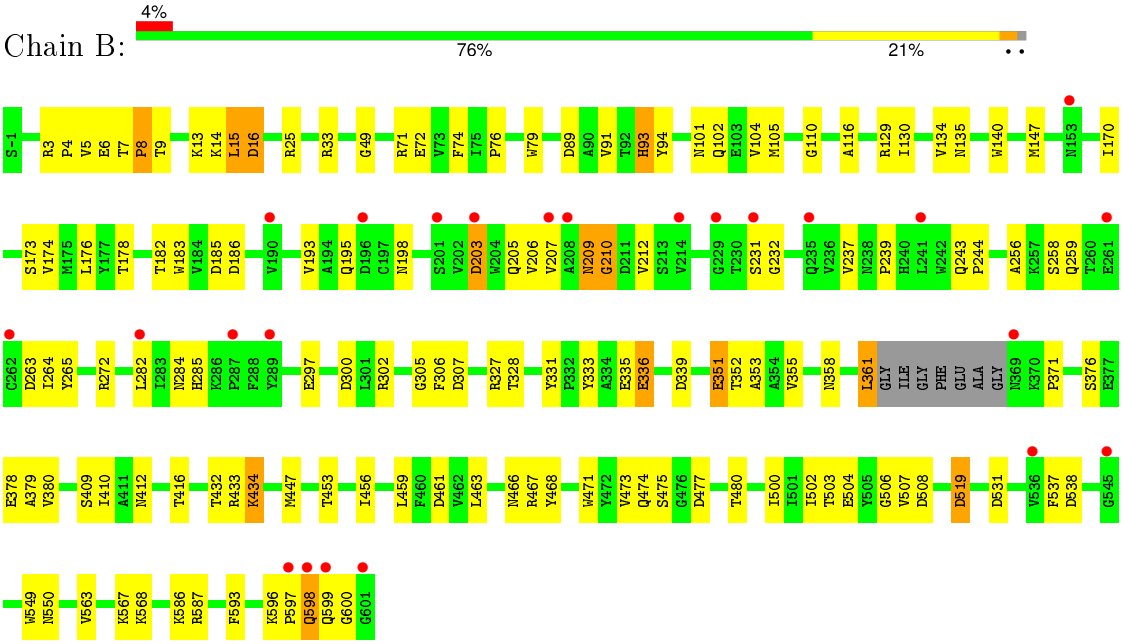
- Molecule 1: Beta-glucuronidase

Chain A:



- Molecule 1: Beta-glucuronidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.31Å 77.41Å 126.29Å 90.00° 124.84° 90.00°	Depositor
Resolution (Å)	46.51 – 2.83 48.11 – 2.83	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.51-2.83) 96.4 (48.11-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.196 , 0.247 0.201 , 0.246	Depositor DCC
R_{free} test set	1605 reflections (5.48%)	DCC
Wilson B-factor (Å^2)	56.1	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 31648 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9613	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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

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

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	0.35	0/4860	0.51	1/6600 (0.0%)
1	B	0.35	0/4795	0.50	1/6519 (0.0%)
All	All	0.35	0/9655	0.50	2/13119 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	210	GLY	N-CA-C	6.35	128.97	113.10
1	A	596	LYS	C-N-CD	5.67	140.30	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	599	GLN	Peptide
1	B	209	ASN	Peptide

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	4746	0	4493	107	0
1	B	4683	0	4384	104	0
2	A	30	0	33	2	0
2	B	30	0	33	1	0
3	A	82	0	0	0	0
3	B	42	0	0	3	0
All	All	9613	0	8943	209	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 (209) 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:13:LYS:NZ	1:A:15:LEU:CD2	1.72	1.48
1:A:13:LYS:NZ	1:A:15:LEU:HD22	1.23	1.39
1:A:13:LYS:HZ1	1:A:15:LEU:CD2	1.38	1.25
1:A:13:LYS:CE	1:A:15:LEU:HD22	1.74	1.17
1:A:13:LYS:HZ3	1:A:15:LEU:HD23	1.03	1.10
1:A:15:LEU:CD1	1:A:173:SER:HA	1.79	1.10
1:A:15:LEU:HD21	1:A:173:SER:OG	1.53	1.08
1:A:15:LEU:HD11	1:A:173:SER:HA	1.13	1.08
1:A:13:LYS:HZ3	1:A:15:LEU:CD2	1.48	1.01
1:B:477:ASP:OD2	1:B:480:THR:OG1	1.82	0.96
1:A:13:LYS:NZ	1:A:15:LEU:HD23	1.65	0.95
1:A:183:TRP:O	1:A:208:ALA:HB3	1.67	0.94
1:B:14:LYS:HD2	1:B:176:LEU:HD22	1.58	0.85
1:A:195:GLN:OE1	1:A:195:GLN:N	2.11	0.84
1:B:598:GLN:OE1	1:B:598:GLN:N	2.12	0.82
1:A:15:LEU:HD21	1:A:173:SER:HG	1.40	0.82
1:A:15:LEU:HD13	1:A:174:VAL:H	1.45	0.80
1:B:473:VAL:HG23	1:B:474:GLN:CD	2.03	0.79
1:B:207:VAL:HG11	1:B:256:ALA:CB	2.12	0.79
1:B:471:TRP:O	1:B:475:SER:OG	2.01	0.78
1:B:376:SER:O	1:B:380:VAL:O	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:CD2	1:A:173:SER:OG	2.30	0.78
1:A:183:TRP:O	1:A:208:ALA:CB	2.31	0.77
1:A:94:TYR:HB3	1:A:135:ASN:HB3	1.68	0.76
1:B:7:THR:HB	1:B:8:PRO:HD3	1.68	0.74
1:B:207:VAL:HG11	1:B:256:ALA:HB1	1.68	0.73
1:A:93:HIS:H	1:A:110:GLY:HA3	1.53	0.73
1:A:53:ASP:OD1	1:A:61:ARG:NH1	2.21	0.73
1:A:7:THR:HB	1:A:8:PRO:HD3	1.73	0.71
1:B:140:TRP:HE1	1:B:147:MSE:HE3	1.54	0.70
1:A:8:PRO:HG3	1:A:264:ILE:HD12	1.74	0.69
1:B:8:PRO:HG3	1:B:264:ILE:H	1.56	0.69
1:A:207:VAL:HG23	1:A:210:GLY:H	1.58	0.68
1:A:13:LYS:HZ1	1:A:15:LEU:HD22	0.99	0.68
1:A:193:VAL:HG23	1:A:194:ALA:O	1.94	0.67
1:A:207:VAL:HG23	1:A:210:GLY:N	2.10	0.67
1:A:598:GLN:O	1:A:599:GLN:HG2	1.94	0.66
1:B:102:GLN:O	1:B:104:VAL:HG13	1.95	0.66
1:B:473:VAL:HG23	1:B:474:GLN:OE1	1.94	0.66
1:A:598:GLN:C	1:A:600:GLY:HA2	2.16	0.66
1:A:599:GLN:HE21	1:A:599:GLN:CA	2.08	0.66
1:A:49:GLY:HA2	1:A:305:GLY:HA3	1.76	0.66
1:A:410:ILE:HD11	1:A:432:THR:HG21	1.79	0.65
1:A:15:LEU:HD13	1:A:174:VAL:N	2.11	0.64
1:A:18:LEU:HD22	1:A:44:ALA:HB1	1.80	0.63
1:B:94:TYR:HB3	1:B:135:ASN:HB3	1.79	0.63
1:A:198:ASN:HA	1:A:239:PRO:HD3	1.81	0.63
1:B:473:VAL:O	1:B:474:GLN:HB2	1.99	0.62
1:A:599:GLN:HE21	1:A:599:GLN:HA	1.64	0.62
1:B:351:GLU:HG2	1:B:409:SER:HB3	1.80	0.62
1:B:16:ASP:HB2	1:B:71:ARG:HH21	1.64	0.61
1:A:13:LYS:HZ1	1:A:15:LEU:HD21	1.53	0.61
1:A:15:LEU:HD13	1:A:173:SER:HA	1.81	0.61
1:A:463:LEU:HD23	1:A:500:ILE:HG12	1.83	0.60
1:A:361:LEU:HD22	2:A:701:1KV:H15	1.82	0.60
1:B:140:TRP:CD2	1:B:379:ALA:HA	2.36	0.60
1:B:519:ASP:OD1	1:B:519:ASP:N	2.32	0.60
1:B:49:GLY:HA2	1:B:305:GLY:HA3	1.84	0.59
1:B:477:ASP:OD2	1:B:480:THR:CB	2.49	0.59
1:A:540:VAL:O	1:A:596:LYS:NZ	2.35	0.59
1:B:207:VAL:HG11	1:B:256:ALA:HB2	1.85	0.59
1:B:71:ARG:NH1	1:B:72:GLU:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ARG:HH11	1:B:503:THR:HB	1.68	0.58
1:B:13:LYS:HB3	1:B:15:LEU:HB2	1.86	0.57
1:B:473:VAL:HG23	1:B:474:GLN:NE2	2.20	0.57
1:B:433:ARG:NH1	1:B:461:ASP:OD1	2.37	0.57
1:A:225:ALA:HB1	1:A:235:GLN:HG3	1.87	0.57
1:A:306:PHE:CZ	1:A:336:GLU:HG3	2.40	0.57
1:A:358:ASN:ND2	1:A:413:GLU:O	2.37	0.57
1:B:244:PRO:HB2	1:B:593:PHE:HE1	1.71	0.56
1:A:14:LYS:NZ	1:A:14:LYS:HB2	2.21	0.56
1:A:15:LEU:CD1	1:A:174:VAL:H	2.16	0.56
1:B:258:SER:OG	1:B:259:GLN:N	2.39	0.56
1:A:10:ARG:HE	1:B:76:PRO:HA	1.71	0.56
1:A:468:TYR:OH	1:A:504:GLU:OE1	2.20	0.55
1:B:335:GLU:N	1:B:335:GLU:OE1	2.29	0.55
1:B:91:VAL:O	1:B:110:GLY:HA2	2.06	0.55
1:B:9:THR:HG23	1:B:178:THR:O	2.06	0.55
1:B:597:PRO:C	1:B:598:GLN:OE1	2.46	0.54
1:B:563:VAL:O	1:B:567:LYS:NZ	2.40	0.54
1:A:591:MSE:HE2	1:A:597:PRO:HG3	1.90	0.53
1:B:3:ARG:O	1:B:265:TYR:OH	2.19	0.53
1:A:14:LYS:NZ	1:A:14:LYS:CB	2.72	0.53
1:B:101:ASN:OD1	1:B:129:ARG:NH2	2.42	0.53
1:B:140:TRP:CG	1:B:379:ALA:HA	2.43	0.53
1:B:15:LEU:HD11	1:B:173:SER:HA	1.90	0.53
1:A:13:LYS:HE2	1:A:15:LEU:HB2	1.90	0.53
1:B:327:ARG:NH2	1:B:412:ASN:OD1	2.41	0.53
1:B:306:PHE:CZ	1:B:336:GLU:HG3	2.44	0.53
1:B:8:PRO:HG3	1:B:264:ILE:HD12	1.92	0.52
1:B:355:VAL:HG23	1:B:412:ASN:HD22	1.74	0.52
1:B:244:PRO:HB2	1:B:593:PHE:CE1	2.44	0.52
1:A:258:SER:OG	1:A:259:GLN:N	2.42	0.51
1:A:13:LYS:HE2	1:A:15:LEU:HD22	1.83	0.51
1:A:18:LEU:CD2	1:A:44:ALA:HB1	2.40	0.51
1:A:599:GLN:CA	1:A:599:GLN:NE2	2.73	0.51
1:B:186:ASP:HB3	1:B:206:VAL:HG13	1.93	0.51
1:B:282:LEU:HD23	1:B:285:HIS:HA	1.91	0.51
1:B:15:LEU:O	1:B:16:ASP:C	2.49	0.51
1:A:33:ARG:HB3	1:A:36:GLU:HG3	1.92	0.51
1:A:205:GLN:N	1:A:205:GLN:OE1	2.44	0.51
1:A:207:VAL:O	1:A:207:VAL:HG22	2.11	0.51
1:B:410:ILE:HD11	1:B:432:THR:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:THR:HG23	1:A:178:THR:O	2.11	0.50
1:A:172:ARG:NH2	1:A:297:GLU:OE1	2.39	0.50
1:A:231:SER:OG	1:A:232:GLY:N	2.43	0.50
1:A:8:PRO:HG3	1:A:264:ILE:H	1.77	0.50
1:A:203:ASP:OD2	1:A:233:THR:HB	2.12	0.49
1:A:182:THR:HG23	1:A:209:ASN:HB2	1.95	0.49
1:B:6:GLU:HA	1:B:9:THR:O	2.11	0.49
1:B:203:ASP:OD2	1:B:203:ASP:N	2.44	0.49
1:B:74:PHE:O	3:B:836:HOH:O	2.20	0.49
1:A:355:VAL:HG23	1:A:412:ASN:HD22	1.78	0.48
1:B:15:LEU:HD13	1:B:174:VAL:H	1.79	0.48
1:A:167:TYR:HB2	1:A:304:LYS:HG3	1.95	0.48
1:B:376:SER:O	1:B:378:GLU:O	2.32	0.48
1:B:105:MSE:HE2	1:B:116:ALA:HB3	1.95	0.48
1:A:599:GLN:N	1:A:599:GLN:NE2	2.60	0.48
1:A:202:VAL:HG22	1:A:234:LEU:CD1	2.43	0.48
1:B:297:GLU:HG3	1:B:331:TYR:HE1	1.79	0.48
1:B:91:VAL:HG22	1:B:170:ILE:HG12	1.97	0.47
1:A:471:TRP:CZ2	1:A:508:ASP:HB2	2.49	0.47
1:A:477:ASP:OD2	1:A:480:THR:OG1	2.29	0.47
1:B:147:MSE:HE1	1:B:371:PRO:HD3	1.95	0.47
1:A:92:THR:OG1	1:A:171:HIS:ND1	2.46	0.47
1:A:433:ARG:NH2	1:A:459:LEU:O	2.48	0.47
1:B:205:GLN:OE1	1:B:205:GLN:N	2.48	0.47
1:A:598:GLN:C	1:A:599:GLN:HG2	2.35	0.47
1:B:16:ASP:HB2	1:B:71:ARG:NH2	2.30	0.47
1:B:198:ASN:HA	1:B:239:PRO:HD3	1.96	0.47
1:A:398:ARG:HD2	1:A:399:ASP:OD1	2.16	0.46
1:A:90:ALA:HB3	1:A:172:ARG:HD2	1.97	0.46
1:A:599:GLN:N	1:A:600:GLY:CA	2.78	0.46
1:B:549:TRP:HA	1:B:550:ASN:HA	1.63	0.46
1:A:96:LYS:HE3	1:A:98:TRP:CZ2	2.51	0.46
1:B:416:THR:HG21	1:B:456:ILE:HG12	1.98	0.46
1:B:471:TRP:CZ2	1:B:508:ASP:HB2	2.51	0.45
1:B:33:ARG:HB2	1:B:33:ARG:NH1	2.31	0.45
1:B:327:ARG:NH1	1:B:503:THR:HB	2.29	0.45
1:B:434:LYS:HD2	1:B:434:LYS:HA	1.78	0.45
1:A:586:LYS:HE3	1:A:586:LYS:HB2	1.47	0.45
1:A:598:GLN:C	1:A:599:GLN:CG	2.85	0.45
1:A:14:LYS:HZ2	1:A:14:LYS:HB2	1.82	0.45
1:B:13:LYS:C	1:B:15:LEU:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ARG:NH1	1:A:461:ASP:OD2	2.50	0.45
1:B:433:ARG:NH2	1:B:459:LEU:O	2.50	0.45
1:A:33:ARG:HG2	1:A:35:TRP:CZ2	2.52	0.45
1:A:598:GLN:OE1	1:A:598:GLN:N	2.50	0.44
1:B:93:HIS:HB2	1:B:135:ASN:O	2.17	0.44
1:A:549:TRP:HA	1:A:550:ASN:HA	1.67	0.44
1:B:8:PRO:HG2	1:B:263:ASP:OD1	2.18	0.44
1:A:412:ASN:HA	1:A:444:VAL:HB	1.99	0.44
1:A:1:MSE:HE1	1:A:113:PRO:HB2	1.99	0.44
1:A:15:LEU:CD1	1:A:173:SER:CA	2.72	0.44
1:A:598:GLN:O	1:A:600:GLY:HA2	2.17	0.44
1:B:93:HIS:H	1:B:110:GLY:HA3	1.83	0.44
1:B:339:ASP:OD1	3:B:832:HOH:O	2.21	0.44
1:A:105:MSE:HG3	1:A:116:ALA:HB2	1.99	0.44
1:B:5:VAL:HG12	1:B:6:GLU:H	1.82	0.44
1:B:352:THR:HG22	1:B:353:ALA:H	1.83	0.44
1:A:6:GLU:HA	1:A:9:THR:O	2.17	0.43
1:A:1:MSE:HE3	1:A:1:MSE:HB3	1.92	0.43
1:B:210:GLY:O	1:B:212:VAL:HG23	2.18	0.43
1:B:567:LYS:HE3	3:B:825:HOH:O	2.18	0.43
1:A:332:PRO:HG3	1:A:395:LEU:HD13	2.00	0.43
1:A:299:ALA:HB3	1:A:302:ARG:HG2	2.00	0.43
1:B:598:GLN:O	1:B:600:GLY:N	2.52	0.43
1:B:467:ARG:HD3	1:B:467:ARG:HA	1.79	0.43
1:A:426:ALA:HB3	1:A:427:PRO:HD3	2.01	0.43
1:B:243:GLN:OE1	1:B:284:ASN:ND2	2.40	0.43
1:A:295:ARG:NH2	1:A:314:ASP:OD2	2.51	0.43
1:B:328:THR:O	1:B:351:GLU:HB2	2.19	0.43
1:A:83:ARG:O	1:A:178:THR:HA	2.17	0.43
1:A:297:GLU:HG3	1:A:331:TYR:HE1	1.84	0.43
1:B:183:TRP:HE1	1:B:185:ASP:HB3	1.84	0.43
1:B:14:LYS:HZ1	1:B:130:ILE:HG13	1.84	0.42
1:B:195:GLN:N	1:B:195:GLN:OE1	2.52	0.42
1:B:182:THR:OG1	1:B:209:ASN:HB2	2.18	0.42
1:A:9:THR:O	1:A:10:ARG:HG3	2.20	0.42
1:B:502:ILE:HG13	1:B:537:PHE:CE2	2.54	0.42
1:B:466:ASN:CG	1:B:504:GLU:HB2	2.39	0.42
1:A:35:TRP:HD1	1:A:101:ASN:HA	1.84	0.42
1:B:15:LEU:HA	1:B:15:LEU:HD12	1.72	0.42
1:B:89:ASP:OD2	1:B:173:SER:HB2	2.19	0.42
1:A:361:LEU:HD11	1:A:448:PHE:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ASP:O	1:B:232:GLY:HA2	2.19	0.42
1:B:361:LEU:HD22	2:B:701:1KV:H15	2.02	0.42
1:A:472:TYR:HB3	2:A:701:1KV:H14	2.02	0.41
1:B:596:LYS:O	1:B:598:GLN:OE1	2.37	0.41
1:B:328:THR:HA	1:B:333:TYR:CZ	2.55	0.41
1:B:468:TYR:OH	1:B:504:GLU:OE1	2.36	0.41
1:A:242:TRP:CZ2	1:A:345:GLY:HA2	2.55	0.41
1:A:71:ARG:NH1	1:A:72:GLU:O	2.54	0.41
1:A:76:PRO:HG2	1:A:79:TRP:CE2	2.56	0.41
1:B:507:VAL:C	1:B:568:LYS:HG2	2.41	0.41
1:A:302:ARG:HH22	1:B:307:ASP:CG	2.24	0.41
1:B:586:LYS:HB2	1:B:586:LYS:HE3	1.81	0.41
1:A:188:THR:HB	1:A:204:TRP:HE3	1.84	0.41
1:B:463:LEU:HD23	1:B:500:ILE:HG12	2.03	0.41
1:B:94:TYR:O	1:B:134:VAL:HA	2.21	0.41
1:B:76:PRO:HG2	1:B:79:TRP:CZ2	2.56	0.41
1:B:3:ARG:HA	1:B:4:PRO:HD3	1.92	0.41
1:A:321:ILE:O	1:A:585:GLN:HA	2.21	0.41
1:A:14:LYS:CB	1:A:14:LYS:HZ3	2.33	0.41
1:B:336:GLU:HG2	1:B:336:GLU:H	1.46	0.41
1:B:231:SER:OG	1:B:232:GLY:N	2.55	0.40
1:B:506:GLY:HA3	1:B:549:TRP:O	2.22	0.40
1:B:538:ASP:OD1	1:B:587:ARG:NH2	2.54	0.40
1:A:359:LEU:HG	1:A:374:LEU:HD13	2.03	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	592/603 (98%)	553 (93%)	37 (6%)	2 (0%)	46 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	592/603 (98%)	549 (93%)	40 (7%)	3 (0%)	34 67
All	All	1184/1206 (98%)	1102 (93%)	77 (6%)	5 (0%)	39 72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	93	HIS
1	A	93	HIS
1	B	447	MSE
1	A	8	PRO
1	B	8	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	499/498 (100%)	479 (96%)	20 (4%)	38 72
1	B	482/498 (97%)	463 (96%)	19 (4%)	39 72
All	All	981/996 (98%)	942 (96%)	39 (4%)	38 72

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	15	LEU
1	A	127	SER
1	A	152	GLU
1	A	203	ASP
1	A	206	VAL
1	A	209	ASN
1	A	231	SER
1	A	272	ARG
1	A	300	ASP
1	A	302	ARG

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Mol	Chain	Res	Type
1	A	336	GLU
1	A	351	GLU
1	A	358	ASN
1	A	378	GLU
1	A	447	MSE
1	A	510	LEU
1	A	595	GLU
1	A	597	PRO
1	A	599	GLN
1	B	15	LEU
1	B	16	ASP
1	B	25	ARG
1	B	193	VAL
1	B	203	ASP
1	B	237	VAL
1	B	272	ARG
1	B	300	ASP
1	B	302	ARG
1	B	336	GLU
1	B	351	GLU
1	B	358	ASN
1	B	361	LEU
1	B	434	LYS
1	B	453	THR
1	B	519	ASP
1	B	531	ASP
1	B	598	GLN
1	B	599	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	385	GLN
1	A	599	GLN
1	B	330	HIS

5.3.3 RNA

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)

2 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	1KV	A	701	-	33,33,33	2.46	11 (33%)	41,45,45	2.05	11 (26%)
2	1KV	B	701	-	33,33,33	2.54	10 (30%)	41,45,45	2.09	12 (29%)

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	1KV	A	701	-	-	0/16/45/45	0/4/4/4
2	1KV	B	701	-	-	0/16/45/45	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	1KV	CA-C	-2.02	1.49	1.52
2	B	701	1KV	CBB-CBA	2.09	1.56	1.52
2	A	701	1KV	CAF-CAW	2.25	1.43	1.39
2	A	701	1KV	C-NAQ	2.25	1.38	1.34
2	B	701	1KV	CAF-CAW	2.27	1.43	1.39
2	A	701	1KV	CBB-CBA	2.34	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	1KV	O-C	2.45	1.28	1.23
2	A	701	1KV	O-C	2.47	1.28	1.23
2	B	701	1KV	C-NAQ	2.57	1.39	1.34
2	A	701	1KV	CAJ-N	3.23	1.55	1.46
2	B	701	1KV	CAJ-N	3.52	1.56	1.46
2	A	701	1KV	CAK-N	4.00	1.57	1.46
2	B	701	1KV	CAK-N	4.09	1.58	1.46
2	A	701	1KV	CAM-NBD	5.14	1.61	1.46
2	A	701	1KV	CAL-NBD	5.28	1.61	1.46
2	B	701	1KV	CAL-NBD	5.33	1.61	1.46
2	A	701	1KV	CA-N	5.43	1.57	1.46
2	B	701	1KV	CA-N	5.43	1.57	1.46
2	B	701	1KV	CAM-NBD	5.55	1.62	1.46
2	A	701	1KV	CAP-NBD	6.94	1.60	1.47
2	B	701	1KV	CAP-NBD	7.12	1.60	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	1KV	CAH-CAG-CAZ	-3.20	105.89	110.90
2	A	701	1KV	O-C-NAQ	-2.91	118.07	123.01
2	B	701	1KV	O-C-NAQ	-2.47	118.81	123.01
2	A	701	1KV	OAT-CAI-OAU	-2.24	104.33	108.12
2	B	701	1KV	OAT-CAI-OAU	-2.24	104.34	108.12
2	B	701	1KV	CAI-OAU-CAY	2.01	108.24	105.35
2	B	701	1KV	CAE-CAD-CAW	2.31	124.20	121.04
2	A	701	1KV	CAP-NBD-CAL	2.31	116.24	111.08
2	B	701	1KV	CAG-CAH-CBB	2.31	115.99	110.95
2	B	701	1KV	CAP-NBD-CAL	2.32	116.24	111.08
2	B	701	1KV	CA-N-CAJ	2.37	114.57	111.07
2	A	701	1KV	CAE-CAD-CAW	2.43	124.36	121.04
2	A	701	1KV	CAG-CAH-CBB	2.76	116.95	110.95
2	B	701	1KV	CA-N-CAK	2.97	115.46	111.07
2	A	701	1KV	CAO-CBA-NAQ	3.13	116.06	110.59
2	A	701	1KV	CA-N-CAK	3.15	115.72	111.07
2	A	701	1KV	CAW-CAP-NBD	3.60	120.13	113.16
2	B	701	1KV	CAW-CAP-NBD	3.65	120.22	113.16
2	B	701	1KV	CAO-CBA-NAQ	3.73	117.10	110.59
2	B	701	1KV	CA-C-NAQ	4.31	123.56	115.04
2	A	701	1KV	CA-C-NAQ	4.42	123.77	115.04
2	A	701	1KV	CBA-NAQ-C	5.74	134.25	123.61
2	B	701	1KV	CBA-NAQ-C	6.52	135.69	123.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	1KV	2	0
2	B	701	1KV	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

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	583/603 (96%)	0.02	16 (2%)	58	47	19, 51, 111, 174	0
1	B	583/603 (96%)	0.23	24 (4%)	41	30	36, 82, 133, 186	0
All	All	1166/1206 (96%)	0.12	40 (3%)	49	38	19, 70, 123, 186	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	VAL	4.9
1	B	282	LEU	3.8
1	B	229	GLY	3.3
1	B	599	GLN	3.2
1	B	196	ASP	3.2
1	B	190	VAL	2.9
1	B	207	VAL	2.8
1	B	545	GLY	2.8
1	B	261	GLU	2.7
1	B	289	TYR	2.7
1	A	252	LEU	2.7
1	A	264	ILE	2.7
1	B	153	ASN	2.6
1	B	241	LEU	2.5
1	B	235	GLN	2.5
1	A	226	THR	2.5
1	A	5	VAL	2.5
1	B	201	SER	2.5
1	B	369	ASN	2.5
1	A	30	ILE	2.4
1	A	16	ASP	2.4
1	A	369	ASN	2.4
1	A	230	THR	2.4
1	A	216	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	208	ALA	2.3
1	B	597	PRO	2.3
1	B	598	GLN	2.3
1	B	203	ASP	2.3
1	B	536	VAL	2.2
1	B	287	PRO	2.2
1	A	254	VAL	2.2
1	B	601	GLY	2.2
1	A	203	ASP	2.2
1	A	235	GLN	2.2
1	A	211	ASP	2.1
1	B	262	CYS	2.1
1	A	215	GLU	2.1
1	B	231	SER	2.1
1	A	601	GLY	2.1
1	B	214	VAL	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, 95^{th} 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	1KV	B	701	30/30	0.89	0.27	1.20	59,69,103,125	0
2	1KV	A	701	30/30	0.94	0.21	0.79	21,60,68,69	0

6.5 Other polymers (i)

There are no such residues in this entry.