



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:56 PM UTC

PDB ID : 1KOB / pdb_00001kob
Title : TWITCHIN KINASE FRAGMENT (APLYSIA), AUTOREGULATED PROTEIN KINASE DOMAIN
Authors : Kobe, B.; Heierhorst, J.; Feil, S.C.; Parker, M.W.; Benian, G.M.; Weiss, K.R.; Kemp, B.E.
Deposited on : 1996-06-28
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

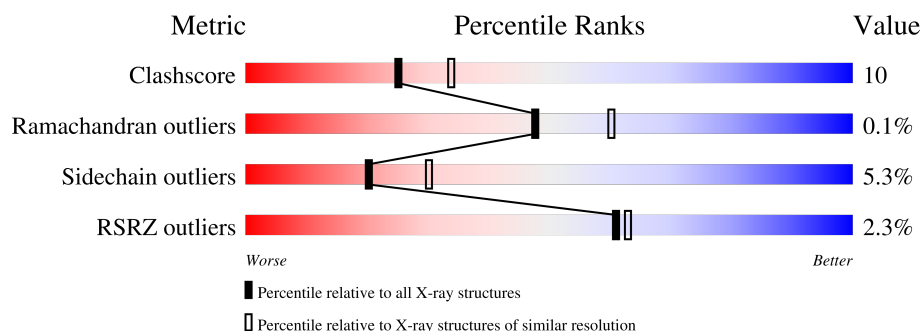
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	387	3% 66% 22% • 9%
1	B	387	% 65% 23% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6071 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.

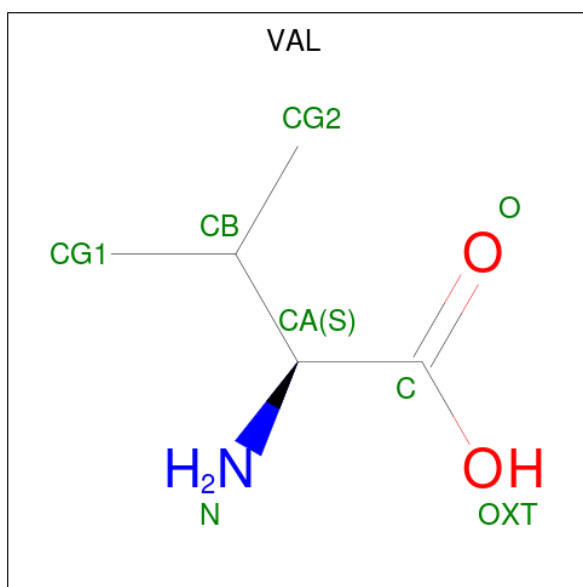
- Molecule 1 is a protein called TWITCHIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2869	1840	479	539	11			
1	B	352	Total	C	N	O	S	0	0	0
			2869	1840	479	539	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	SER	ARG	conflict	UNP Q16980
A	18	TYR	HIS	conflict	UNP Q16980
A	49	VAL	CYS	conflict	UNP Q16980
A	80	VAL	GLU	conflict	UNP Q16980
A	122	GLU	ASP	conflict	UNP Q16980
A	379	LYS	VAL	conflict	UNP Q16980
A	380	LEU	ARG	conflict	UNP Q16980
B	12	SER	ARG	conflict	UNP Q16980
B	18	TYR	HIS	conflict	UNP Q16980
B	49	VAL	CYS	conflict	UNP Q16980
B	80	VAL	GLU	conflict	UNP Q16980
B	122	GLU	ASP	conflict	UNP Q16980
B	379	LYS	VAL	conflict	UNP Q16980
B	380	LEU	ARG	conflict	UNP Q16980

- Molecule 2 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$).

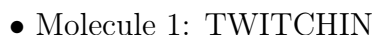


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	165	Total	O	0	0
			165	165		
3	B	161	Total	O	0	0
			161	161		

- Molecule 1: TWITCHIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.30Å 87.80Å 152.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 40.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.30) 88.1 (40.00-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.65Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.200 , 0.282 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	8.6	Xtriage
Anisotropy	1.609	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 98.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6071	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.79	1/2942 (0.0%)	1.17	30/3981 (0.8%)
1	B	0.78	1/2942 (0.0%)	1.15	32/3981 (0.8%)
All	All	0.79	2/5884 (0.0%)	1.16	62/7962 (0.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	MET	SD-CE	-7.44	1.60	1.79
1	B	165	MET	SD-CE	-7.05	1.61	1.79

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	LYS	CA-C-N	8.97	129.54	119.32
1	A	176	LYS	C-N-CA	8.97	129.54	119.32
1	A	193	ILE	N-CA-C	8.32	121.07	112.83
1	A	313	SER	N-CA-C	-8.22	103.24	113.18
1	B	202	ASN	CA-C-N	8.07	128.52	119.32
1	B	202	ASN	C-N-CA	8.07	128.52	119.32
1	A	265	CYS	N-CA-C	7.57	121.68	111.24
1	A	316	THR	N-CA-C	7.33	121.53	112.59
1	A	278	SER	N-CA-C	7.30	120.60	110.01
1	B	38	VAL	CA-C-N	7.06	127.48	119.93
1	B	38	VAL	C-N-CA	7.06	127.48	119.93
1	B	65	GLY	N-CA-C	7.04	119.30	110.29
1	A	319	ILE	N-CA-C	-6.96	101.22	107.56
1	A	266	ASP	CB-CA-C	6.83	120.29	110.79
1	B	327	ILE	CB-CA-C	-6.45	103.31	112.22
1	B	192	ILE	N-CA-C	-6.42	99.04	108.54
1	B	193	ILE	N-CA-C	6.41	118.31	112.29
1	A	107	HIS	CA-C-N	6.36	126.57	119.32
1	A	107	HIS	C-N-CA	6.36	126.57	119.32
1	B	49	VAL	CB-CA-C	-6.34	103.86	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ASP	N-CA-C	-6.34	96.78	107.99
1	B	292	GLU	CA-C-N	6.32	126.52	119.32
1	B	292	GLU	C-N-CA	6.32	126.52	119.32
1	A	358	ARG	CA-C-N	6.31	126.06	119.05
1	A	358	ARG	C-N-CA	6.31	126.06	119.05
1	B	69	ARG	N-CA-C	-6.29	101.17	110.48
1	B	372	LYS	N-CA-C	6.29	124.20	110.80
1	B	331	ILE	N-CA-C	6.23	116.98	110.62
1	B	353	SER	N-CA-C	-6.23	104.94	112.54
1	B	248	SER	N-CA-C	-6.12	102.07	109.72
1	A	373	GLU	N-CA-C	5.99	118.67	108.90
1	A	272	ASP	N-CA-C	5.95	117.57	111.14
1	B	203	PRO	N-CA-C	5.95	122.61	113.75
1	A	196	GLY	N-CA-C	5.86	120.92	113.24
1	A	38	VAL	N-CA-C	-5.82	102.39	108.15
1	A	38	VAL	CA-C-N	5.75	125.76	119.90
1	A	38	VAL	C-N-CA	5.75	125.76	119.90
1	B	358	ARG	CA-C-N	5.67	125.35	119.05
1	B	358	ARG	C-N-CA	5.67	125.35	119.05
1	A	271	GLU	N-CA-C	5.60	118.58	111.69
1	B	344	ALA	N-CA-C	5.59	118.09	111.33
1	A	318	ARG	N-CA-C	5.57	118.43	110.24
1	B	220	GLU	CB-CA-C	-5.48	102.03	110.81
1	A	292	GLU	CA-C-N	5.47	124.93	119.24
1	A	292	GLU	C-N-CA	5.47	124.93	119.24
1	A	248	SER	N-CA-C	-5.44	101.36	109.42
1	A	340	ALA	CA-C-N	5.39	125.29	119.85
1	A	340	ALA	C-N-CA	5.39	125.29	119.85
1	A	266	ASP	N-CA-C	-5.37	98.26	107.61
1	B	318	ARG	N-CA-C	5.37	118.23	110.28
1	B	190	VAL	N-CA-C	5.29	116.47	108.96
1	B	207	VAL	CB-CA-C	-5.28	102.78	110.81
1	B	362	TYR	N-CA-C	5.28	119.41	112.92
1	B	73	LYS	N-CA-C	5.28	122.04	110.80
1	B	361	GLU	N-CA-C	5.28	117.94	111.82
1	B	273	ALA	N-CA-C	5.25	118.78	112.38
1	B	142	GLU	N-CA-C	5.22	116.97	111.28
1	B	234	TRP	N-CA-C	-5.17	105.72	111.36
1	A	353	SER	N-CA-C	-5.16	106.49	112.89
1	A	203	PRO	N-CA-C	5.12	123.03	112.47
1	B	200	LYS	N-CA-C	-5.01	102.86	110.28
1	B	30	TYR	N-CA-C	5.01	118.12	110.20

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	2869	0	2812	60	0
1	B	2869	0	2812	51	0
2	A	7	0	8	1	0
3	A	165	0	0	8	0
3	B	161	0	0	7	0
All	All	6071	0	5632	110	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 10.

All (110) 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:130:LEU:HD22	1:A:183:GLU:HA	1.56	0.86
1:B:312:HIS:HB3	1:B:315:LEU:HD12	1.66	0.75
1:A:321:SER:HB3	3:A:498:HOH:O	1.85	0.74
1:A:49:VAL:HG21	1:A:124:VAL:HG21	1.69	0.74
1:B:56:LEU:HD11	1:B:71:VAL:HG23	1.71	0.72
1:A:324:TYR:HD1	1:A:327:ILE:HD11	1.55	0.72
1:B:162:LEU:HD12	1:B:165:MET:HE3	1.73	0.71
1:A:312:HIS:HB3	1:A:315:LEU:HD12	1.74	0.69
1:B:368:TYR:HB2	3:B:394:HOH:O	1.92	0.68
1:A:138:ARG:HG3	1:A:182:CYS:SG	2.33	0.68
1:A:147:SER:O	1:A:151:VAL:HG23	1.95	0.67
1:B:59:LEU:HD22	1:B:343:PRO:HD2	1.77	0.66
1:B:94:THR:OG1	1:B:357:HIS:HE1	1.78	0.65
1:B:57:GLU:OE2	1:B:69:ARG:HD3	1.97	0.64
1:B:67:VAL:HG23	1:B:349:ALA:HB2	1.80	0.64
1:B:49:VAL:HG21	1:B:124:VAL:HG21	1.79	0.63
1:B:23:ILE:HG21	1:B:29:PHE:HE2	1.63	0.63
1:A:355:ARG:HG3	1:A:362:TYR:CG	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:TYR:CD1	1:A:327:ILE:HD11	2.34	0.62
1:A:49:VAL:CG2	1:A:124:VAL:HG21	2.30	0.62
1:B:105:LEU:HD22	1:B:165:MET:HG2	1.80	0.62
1:A:162:LEU:HD12	1:A:165:MET:HE3	1.82	0.61
1:A:374:ALA:O	2:A:388:VAL:HG23	2.02	0.60
1:B:80:VAL:HG23	1:B:129:PHE:HD1	1.67	0.59
1:A:319:ILE:HG23	1:A:323:ARG:HH11	1.67	0.59
1:A:207:VAL:HG21	1:A:369:PHE:CE2	2.39	0.57
1:A:82:LYS:HE3	1:A:348:ILE:O	2.04	0.57
1:B:37:TYR:CZ	1:B:77:ARG:HD2	2.39	0.57
1:B:138:ARG:HG3	1:B:182:CYS:SG	2.45	0.56
1:B:347:ARG:HD3	3:B:540:HOH:O	2.08	0.54
1:A:94:THR:OG1	1:A:357:HIS:CE1	2.60	0.54
1:A:114:HIS:HE1	3:A:440:HOH:O	1.90	0.54
1:A:355:ARG:HD2	3:A:457:HOH:O	2.07	0.54
1:B:110:LEU:HD22	1:B:195:PHE:CZ	2.42	0.54
1:B:49:VAL:CG2	1:B:124:VAL:HG21	2.38	0.54
1:B:258:THR:O	1:B:262:VAL:HG23	2.07	0.53
1:B:171:VAL:HG22	1:B:229:PHE:CD1	2.42	0.53
1:A:342:GLN:O	1:A:342:GLN:HG3	2.07	0.53
1:A:147:SER:HA	1:A:319:ILE:HG12	1.91	0.53
1:A:222:VAL:HG12	1:A:263:LYS:HE3	1.91	0.53
1:A:90:LEU:HG	1:B:224:ARG:O	2.09	0.52
1:B:334:LYS:HE2	3:B:410:HOH:O	2.07	0.52
1:A:145:LYS:HG2	1:A:318:ARG:HE	1.74	0.52
1:A:223:ASP:OD1	1:A:263:LYS:HG2	2.09	0.52
1:A:181:MET:HE3	1:A:193:ILE:HD13	1.93	0.51
1:A:184:THR:OG1	1:A:187:ALA:HB2	2.11	0.51
1:B:38:VAL:HG22	3:B:499:HOH:O	2.10	0.50
1:A:92:LYS:O	1:A:96:LYS:HG3	2.11	0.50
1:B:136:PHE:HD2	3:B:478:HOH:O	1.93	0.50
1:A:270:ASP:O	1:A:274:PHE:HB2	2.11	0.50
1:A:200:LYS:H	1:A:200:LYS:CD	2.25	0.49
1:B:171:VAL:HG22	1:B:229:PHE:CE1	2.47	0.49
1:A:309:LYS:O	1:A:309:LYS:HG2	2.12	0.49
1:A:225:GLU:HB3	1:A:226:PRO:HD2	1.95	0.49
1:B:147:SER:HA	1:B:319:ILE:HG12	1.95	0.49
1:A:163:LYS:HD2	1:A:303:LEU:CD1	2.43	0.48
1:B:133:GLY:HA2	1:B:344:ALA:CB	2.43	0.48
1:A:153:ASN:O	1:A:157:GLN:HG3	2.14	0.48
1:A:130:LEU:HD21	1:A:191:LYS:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:LEU:HA	1:B:165:MET:HE3	1.96	0.48
1:A:309:LYS:HE2	3:A:526:HOH:O	2.14	0.47
1:B:46:GLN:HG2	1:B:46:GLN:O	2.14	0.47
1:B:105:LEU:CD2	1:B:165:MET:HG2	2.44	0.47
1:B:248:SER:OG	1:B:251:ALA:HB2	2.14	0.47
1:B:67:VAL:CG1	1:B:80:VAL:HG13	2.44	0.47
1:A:355:ARG:HG3	1:A:362:TYR:CB	2.44	0.47
1:B:206:ILE:HD11	1:B:208:LYS:HE2	1.96	0.46
1:A:136:PHE:CD2	1:A:139:ILE:HD11	2.50	0.46
1:A:181:MET:HE3	1:A:193:ILE:CD1	2.45	0.46
1:A:54:ASP:OD1	1:A:73:LYS:HE2	2.15	0.46
1:B:94:THR:OG1	1:B:357:HIS:CE1	2.65	0.46
1:B:230:TYR:CE1	1:B:293:PRO:HB3	2.51	0.46
1:B:233:MET:SD	1:B:299:VAL:HG13	2.56	0.46
1:A:136:PHE:CD2	1:A:327:ILE:HD12	2.51	0.46
1:A:291:LYS:HE2	3:A:477:HOH:O	2.15	0.46
1:A:138:ARG:NH2	1:A:186:LYS:HD2	2.31	0.45
1:A:327:ILE:HG12	3:A:503:HOH:O	2.16	0.45
1:A:114:HIS:CE1	3:A:440:HOH:O	2.65	0.45
1:A:148:GLU:O	1:A:152:ILE:HG13	2.16	0.45
1:B:256:LEU:O	1:B:260:GLN:HG2	2.17	0.44
1:B:163:LYS:O	1:B:167:GLU:HG3	2.17	0.44
1:B:304:GLU:HA	1:B:309:LYS:HD2	1.99	0.44
1:A:176:LYS:O	1:A:179:ASN:HB2	2.18	0.44
1:B:145:LYS:HG2	1:B:318:ARG:HD2	1.99	0.44
1:A:132:GLY:O	1:A:344:ALA:HB3	2.18	0.44
1:A:256:LEU:C	1:A:256:LEU:HD23	2.43	0.44
1:A:94:THR:OG1	1:A:357:HIS:HE1	2.01	0.43
1:A:109:LYS:HA	1:A:109:LYS:HD3	1.77	0.43
1:B:37:TYR:CE2	1:B:77:ARG:HD2	2.54	0.43
1:B:34:TRP:HD1	3:B:491:HOH:O	2.01	0.43
1:B:210:THR:HB	1:B:364:ILE:HD13	2.00	0.43
1:B:232:ASP:O	1:B:235:ALA:HB3	2.19	0.42
1:A:171:VAL:HG21	1:A:369:PHE:CE1	2.54	0.42
1:B:237:GLY:HA2	1:B:288:LEU:HD12	2.00	0.42
1:B:175:ILE:HB	1:B:235:ALA:HB1	2.02	0.42
1:A:90:LEU:HD22	3:B:394:HOH:O	2.19	0.42
1:B:136:PHE:CD2	1:B:177:PRO:HB3	2.54	0.42
1:A:347:ARG:HD3	3:A:409:HOH:O	2.19	0.42
1:B:277:VAL:HG12	1:B:281:ALA:HB3	2.02	0.42
1:A:49:VAL:HG11	1:A:124:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PHE:HA	1:A:139:ILE:HG12	2.01	0.41
1:A:236:ILE:HD13	1:A:236:ILE:HA	1.80	0.41
1:A:67:VAL:HG23	1:A:349:ALA:HB2	2.02	0.41
1:B:80:VAL:HG23	1:B:129:PHE:CD1	2.51	0.41
1:A:162:LEU:HD21	1:A:232:ASP:HB3	2.02	0.41
1:B:57:GLU:H	1:B:57:GLU:HG3	1.45	0.41
1:B:110:LEU:HD22	1:B:195:PHE:HZ	1.85	0.41
1:B:67:VAL:HG13	1:B:80:VAL:HG13	2.02	0.40
1:A:200:LYS:H	1:A:200:LYS:HD2	1.87	0.40
1:A:185:LYS:HG2	1:A:185:LYS:O	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	350/387 (90%)	327 (93%)	22 (6%)	1 (0%)	36	46
1	B	350/387 (90%)	335 (96%)	15 (4%)	0	100	100
All	All	700/774 (90%)	662 (95%)	37 (5%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	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	312/343 (91%)	298 (96%)	14 (4%)	24	37
1	B	312/343 (91%)	293 (94%)	19 (6%)	17	24
All	All	624/686 (91%)	591 (95%)	33 (5%)	20	30

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	49	VAL
1	A	57	GLU
1	A	61	SER
1	A	115	ASP
1	A	138	ARG
1	A	171	VAL
1	A	200	LYS
1	A	202	ASN
1	A	215	GLU
1	A	236	ILE
1	A	327	ILE
1	A	332	LYS
1	A	361	GLU
1	B	35	LYS
1	B	48	SER
1	B	57	GLU
1	B	80	VAL
1	B	115	ASP
1	B	119	ASP
1	B	138	ARG
1	B	180	ILE
1	B	199	THR
1	B	204	ASP
1	B	206	ILE
1	B	248	SER
1	B	271	GLU
1	B	299	VAL
1	B	304	GLU
1	B	325	ASN
1	B	327	ILE
1	B	330	LYS
1	B	360	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	97	ASN
1	A	179	ASN
1	A	260	GLN
1	A	305	HIS
1	A	312	HIS
1	A	325	ASN
1	A	357	HIS
1	A	360	GLN
1	B	46	GLN
1	B	104	GLN
1	B	300	HIS
1	B	357	HIS
1	B	360	GLN
1	B	363	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	VAL	A	388	1	4,6,7	0.89	0	6,7,9	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	VAL	A	388	1	-	3/5/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	388	VAL	C-CA-CB-CG1
2	A	388	VAL	C-CA-CB-CG2
2	A	388	VAL	N-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	388	VAL	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	352/387 (90%)	0.03	12 (3%) 48 50	8, 26, 65, 102	0
1	B	352/387 (90%)	0.01	4 (1%) 78 79	7, 25, 62, 102	0
All	All	704/774 (90%)	0.02	16 (2%) 61 63	7, 25, 65, 102	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	374	ALA	3.9
1	A	336	ALA	3.4
1	B	374	ALA	3.4
1	A	204	ASP	3.3
1	A	203	PRO	2.6
1	A	327	ILE	2.6
1	A	140	ALA	2.5
1	A	323	ARG	2.3
1	A	266	ASP	2.3
1	B	37	TYR	2.3
1	A	138	ARG	2.2
1	A	264	ARG	2.2
1	B	373	GLU	2.2
1	B	204	ASP	2.1
1	A	206	ILE	2.0
1	A	201	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	VAL	A	388	7/8	0.62	0.22	95,99,113,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.