



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:58 AM UTC

PDB ID : 2IEH / pdb_00002ieh
Title : Crystal structure of human kinesin Eg5 in complex with (R)-mon97, a new monastrol-based inhibitor that binds as (R)-enantiomer
Authors : Garcia-Saez, I.; Kozielski, F.
Deposited on : 2006-09-19
Resolution : 2.70 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	:	?? (??), CSD ??CSD?? (???)
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

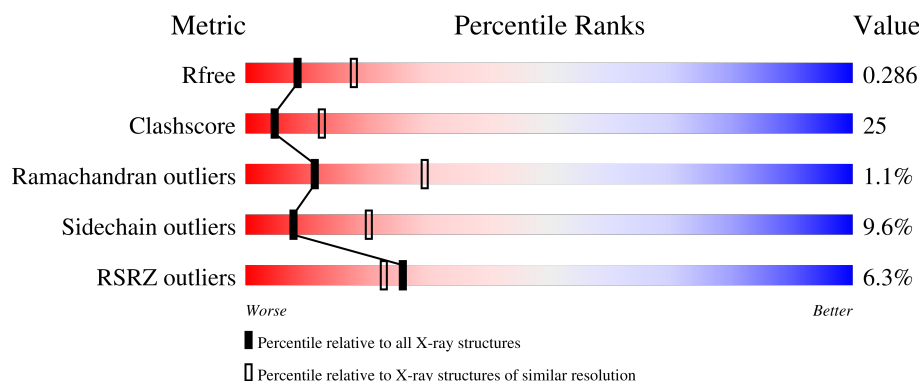
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	367	5% 47% 35% 7% 9%
1	B	367	6% 54% 30% 6% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PG4	A	606	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5607 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 Kinesin-like protein KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	2	0
			2644	1655	462	517	10			
1	B	335	Total	C	N	O	S	0	0	0
			2630	1647	458	515	10			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

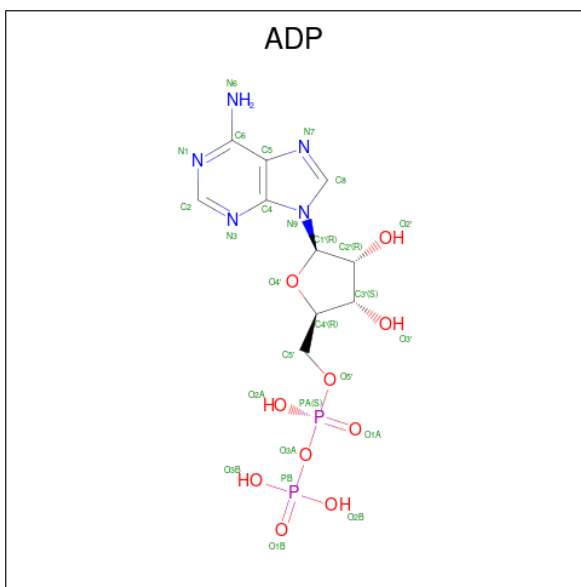
- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

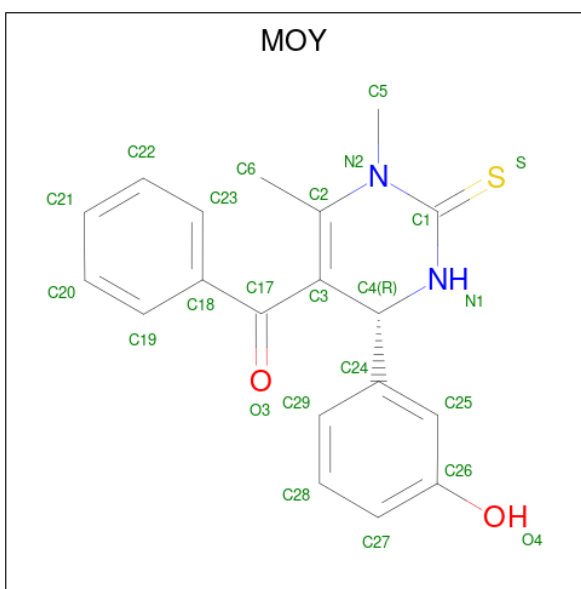
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is [(4R)-4-(3-HYDROXYPHENYL)-1,6-DIMETHYL-2-THIOXO-1,2,3,4-TETRAHYDROPYRIMIDIN-5-YL](PHENYL)METHANONE (CCD ID: MOY) (formula: C₁₉H₁₈N₂O₂S).



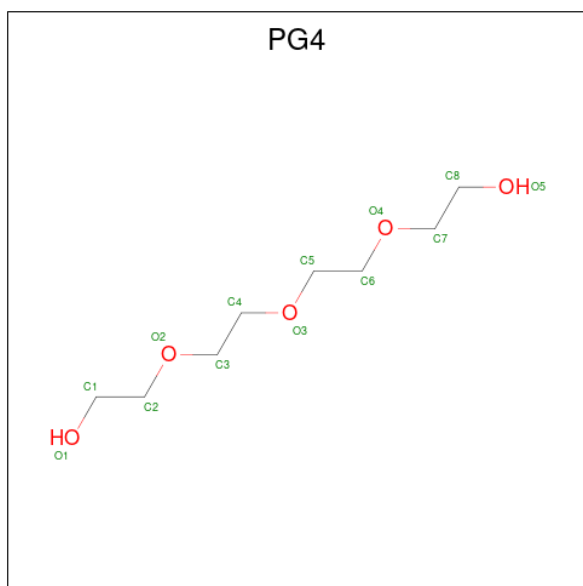
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			24	19	2	2	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			24	19	2	2	1		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).

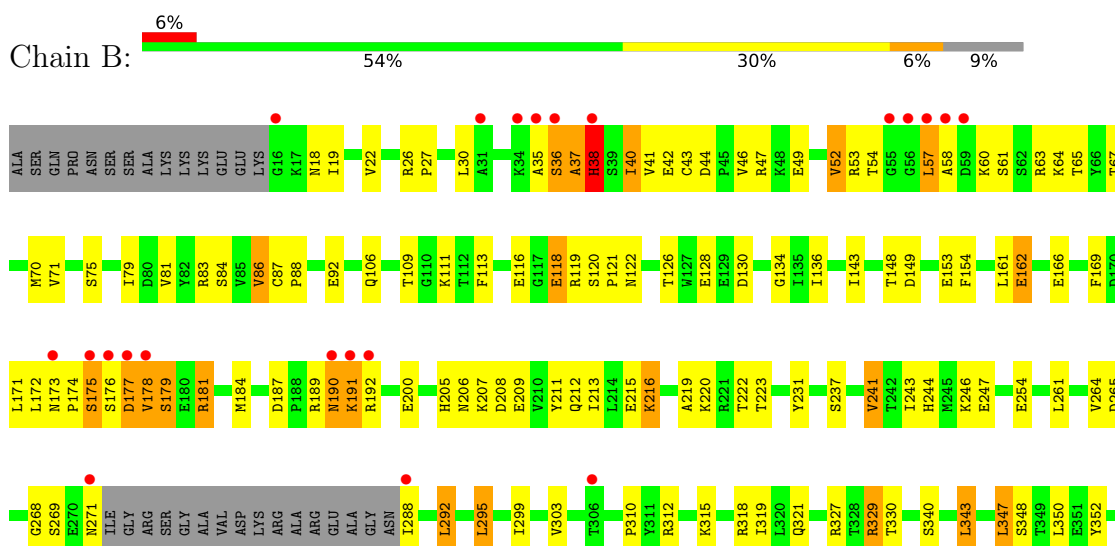


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	114	Total	O	0	0
			114	114		
8	B	100	Total	O	0	0
			100	100		

- Molecule 1: Kinesin-like protein KIF11





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.37Å 79.90Å 159.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70 25.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.00-2.70) 99.8 (25.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.281 0.239 , 0.286	Depositor DCC
R_{free} test set	2613 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5607	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7940e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, ADP, K, MOY, MG, CL

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	0.74	9/2683 (0.3%)	1.27	42/3625 (1.2%)
1	B	0.67	4/2669 (0.1%)	1.19	24/3609 (0.7%)
All	All	0.71	13/5352 (0.2%)	1.23	66/7234 (0.9%)

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	SER	C-O	11.06	1.38	1.23
1	B	37	ALA	CA-CB	-10.01	1.36	1.53
1	A	16	GLY	CA-C	7.50	1.61	1.51
1	A	16	GLY	N-CA	7.17	1.54	1.45
1	A	17	LYS	N-CA	6.23	1.54	1.46
1	A	102	PHE	CA-C	-6.09	1.45	1.52
1	A	189	ARG	CG-CD	5.84	1.70	1.52
1	A	102	PHE	CB-CG	-5.73	1.37	1.50
1	B	37	ALA	C-O	5.59	1.30	1.23
1	A	189	ARG	CB-CG	5.47	1.68	1.52
1	A	157	LYS	CB-CG	-5.28	1.36	1.52
1	B	38	HIS	CA-CB	5.14	1.60	1.53
1	A	254	GLU	N-CA	5.08	1.52	1.46

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	ALA	CA-C-N	15.84	143.84	122.77
1	B	37	ALA	C-N-CA	15.84	143.84	122.77
1	A	221	ARG	CG-CD-NE	10.46	135.00	112.00
1	A	86	VAL	N-CA-C	9.86	120.38	110.82
1	A	221	ARG	CD-NE-CZ	8.54	136.36	124.40
1	A	16	GLY	N-CA-C	-8.36	97.96	111.59
1	B	86	VAL	N-CA-C	8.10	118.14	110.53
1	B	179	SER	CA-C-N	-7.98	111.71	122.72
1	B	179	SER	C-N-CA	-7.98	111.71	122.72
1	A	135	ILE	N-CA-C	7.63	117.75	110.42
1	B	126	THR	N-CA-C	-7.51	100.84	110.53
1	B	175	SER	N-CA-C	7.27	121.84	113.19
1	A	251	ASP	N-CA-C	-6.93	104.63	113.23
1	A	187	ASP	CA-C-N	-6.73	112.88	119.87
1	A	187	ASP	C-N-CA	-6.73	112.88	119.87
1	A	211	TYR	N-CA-C	6.63	118.30	111.14
1	B	18	ASN	N-CA-C	6.63	118.86	110.24
1	A	253[A]	GLU	CA-C-N	-6.59	113.91	123.00
1	A	253[A]	GLU	C-N-CA	-6.59	113.91	123.00
1	A	253[B]	GLU	CA-C-N	-6.59	113.91	123.00
1	A	253[B]	GLU	C-N-CA	-6.59	113.91	123.00
1	A	59	ASP	N-CA-C	-6.53	104.09	111.14
1	A	177	ASP	N-CA-C	-6.45	100.67	109.95
1	A	221	ARG	NE-CZ-NH2	-6.39	113.45	119.20
1	B	179	SER	CA-CB-OG	-6.38	98.33	111.10
1	B	81	VAL	N-CA-C	-6.35	103.40	112.35
1	B	120	SER	CA-C-N	6.14	126.15	119.89
1	B	120	SER	C-N-CA	6.14	126.15	119.89
1	A	58	ALA	N-CA-C	-6.12	105.78	113.18
1	B	264	VAL	N-CA-C	6.06	117.31	108.58
1	A	210	VAL	N-CA-C	5.98	116.72	110.62
1	B	36	SER	O-C-N	5.97	130.22	122.40
1	A	15	LYS	CA-C-N	5.90	128.77	120.57
1	A	15	LYS	C-N-CA	5.90	128.77	120.57
1	A	224	ALA	N-CA-C	-5.84	106.28	113.41
1	A	264	VAL	N-CA-C	5.76	116.15	107.80
1	B	231	TYR	N-CA-C	5.76	118.02	111.11
1	A	182	LEU	N-CA-C	-5.69	102.03	110.46
1	A	102	PHE	CB-CA-C	-5.64	99.13	110.30
1	B	190	ASN	N-CA-C	5.64	117.31	109.31
1	A	113	PHE	N-CA-C	-5.63	104.83	110.97
1	A	312	ARG	N-CA-C	5.63	119.62	112.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	ALA	N-CA-C	-5.58	106.14	113.17
1	A	221	ARG	NE-CZ-NH1	5.55	127.05	121.50
1	A	189	ARG	NE-CZ-NH2	-5.55	114.21	119.20
1	A	125	TYR	N-CA-C	5.54	117.49	109.07
1	B	121	PRO	N-CA-C	5.49	119.84	111.11
1	A	171	LEU	N-CA-C	5.36	119.54	112.25
1	B	312	ARG	N-CA-C	5.36	118.92	112.38
1	B	269	SER	N-CA-C	5.29	119.60	113.20
1	A	126	THR	N-CA-C	-5.28	102.71	110.52
1	A	15	LYS	N-CA-C	5.23	125.65	111.00
1	B	362	LYS	CA-C-N	5.18	125.19	119.90
1	B	362	LYS	C-N-CA	5.18	125.19	119.90
1	A	189	ARG	CD-NE-CZ	5.12	131.57	124.40
1	A	15	LYS	CA-C-O	5.11	129.49	120.80
1	A	40	ILE	N-CA-C	-5.11	107.49	112.29
1	A	193	GLY	N-CA-C	5.05	118.96	111.18
1	A	221	ARG	CB-CG-CD	-5.04	99.70	111.30
1	A	309	VAL	CA-C-N	5.04	126.13	119.84
1	A	309	VAL	C-N-CA	5.04	126.13	119.84
1	A	209	GLU	N-CA-C	-5.02	108.19	114.56
1	A	220	LYS	CA-C-N	5.01	127.41	120.29
1	A	220	LYS	C-N-CA	5.01	127.41	120.29
1	B	136	ILE	CA-C-N	-5.00	113.58	119.84
1	B	136	ILE	C-N-CA	-5.00	113.58	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	TYR	Sidechain
1	B	36	SER	Mainchain

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	2644	0	2671	154	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2630	0	2656	119	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	27	0	12	2	0
5	B	27	0	12	2	0
6	A	24	0	18	1	0
6	B	24	0	18	2	0
7	A	13	0	18	20	0
8	A	114	0	0	20	0
8	B	100	0	0	12	0
All	All	5607	0	5405	275	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 (275) 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:163:ILE:HG21	8:A:720:HOH:O	1.57	1.03
1:A:171:LEU:HD22	8:A:714:HOH:O	1.59	1.00
1:B:83:ARG:HD2	8:B:705:HOH:O	1.62	0.98
1:B:70:MET:HE1	1:B:84:SER:HB3	1.43	0.98
1:B:49:GLU:HG2	1:B:67:THR:HG22	1.44	0.95
1:A:183:GLN:O	8:A:717:HOH:O	1.84	0.95
1:A:77:LYS:HD2	7:A:606:PG4:H41	1.47	0.95
1:B:191:LYS:HG3	1:B:192:ARG:HG3	1.46	0.94
1:A:197:LYS:N	8:A:717:HOH:O	2.01	0.93
1:A:221:ARG:CD	8:A:714:HOH:O	2.16	0.93
1:A:57:LEU:O	1:A:61:SER:HB3	1.68	0.92
1:A:328:THR:O	1:A:361:ASN:ND2	2.02	0.92
1:A:77:LYS:HB3	7:A:606:PG4:H81	1.54	0.90
1:B:30:LEU:HD12	8:B:679:HOH:O	1.73	0.89
1:A:245:MET:HE3	1:A:257:LYS:HB2	1.59	0.84
1:A:189:ARG:HD3	8:A:630:HOH:O	1.77	0.83
1:A:30:LEU:HD13	1:A:33[A]:ARG:NH2	1.94	0.82
1:B:153:GLU:HG2	8:B:680:HOH:O	1.78	0.82
1:A:92:GLU:HA	1:A:95:MET:HE3	1.63	0.81
1:A:78:GLN:H	7:A:606:PG4:H52	1.45	0.81
1:B:57:LEU:O	1:B:61:SER:HB3	1.81	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:CD1	1:A:33[A]:ARG:NH2	2.44	0.80
1:A:221:ARG:NE	8:A:714:HOH:O	2.12	0.80
1:B:52:VAL:HG11	1:B:347:LEU:CD1	2.11	0.80
1:A:221:ARG:HD3	8:A:714:HOH:O	1.81	0.77
1:B:87:CYS:HB3	1:B:88:PRO:HD3	1.64	0.77
1:A:97:TYR:HE2	1:A:364:GLU:HA	1.50	0.77
1:B:46:VAL:HG23	1:B:47:ARG:HG2	1.66	0.76
1:A:162:GLU:OE1	8:A:714:HOH:O	2.04	0.75
1:B:177:ASP:C	1:B:179:SER:H	1.93	0.75
1:A:218:ALA:O	1:A:221:ARG:HB3	1.87	0.75
1:A:54:THR:HG21	1:A:64:LYS:HG3	1.68	0.75
1:A:166:GLU:O	1:A:315:LYS:HE3	1.86	0.74
1:A:177:ASP:OD1	1:A:179:SER:OG	2.05	0.73
1:B:173:ASN:HD22	1:B:200:GLU:HG2	1.53	0.73
1:B:220:LYS:NZ	8:B:698:HOH:O	2.20	0.73
1:B:177:ASP:HB3	1:B:179:SER:OG	1.89	0.73
1:A:40:ILE:O	1:A:40:ILE:HG13	1.88	0.73
1:A:78:GLN:H	7:A:606:PG4:C5	2.02	0.72
1:B:57:LEU:CD2	1:B:58:ALA:H	2.02	0.72
1:A:139:THR:O	1:A:143:ILE:HG13	1.90	0.72
1:A:351:GLU:HG2	8:A:718:HOH:O	1.90	0.72
1:A:329:ARG:HG3	8:A:703:HOH:O	1.89	0.71
1:A:131:PRO:HB2	7:A:606:PG4:C7	2.22	0.70
1:A:131:PRO:HB2	7:A:606:PG4:H71	1.73	0.69
1:A:147:LEU:HD23	1:A:154:PHE:CG	2.28	0.69
1:B:237:SER:HB3	1:B:265:ASP:HB3	1.75	0.69
1:A:299:ILE:O	1:A:303:VAL:HG22	1.93	0.69
1:A:249:THR:HB	1:A:253[A]:GLU:HG3	1.73	0.68
1:A:299:ILE:HG23	1:A:359:ILE:HD11	1.75	0.68
1:A:180:GLU:HG3	1:A:180:GLU:O	1.92	0.68
1:A:38:HIS:CD2	8:A:642:HOH:O	2.46	0.68
1:B:189:ARG:HH11	1:B:189:ARG:HG2	1.58	0.67
1:B:53:ARG:HB2	1:B:63:ARG:NH1	2.09	0.67
1:B:241:VAL:HG13	1:B:261:LEU:HB3	1.76	0.67
1:B:271:ASN:O	1:B:292:LEU:HD12	1.95	0.66
1:B:189:ARG:HG2	1:B:189:ARG:NH1	2.11	0.66
1:A:107:THR:OG1	1:A:270:GLU:OE2	2.14	0.66
1:B:52:VAL:HG11	1:B:347:LEU:HD11	1.77	0.66
1:B:119:ARG:NH2	1:B:130:ASP:OD2	2.29	0.66
1:A:40:ILE:HG21	1:A:340:SER:HA	1.76	0.66
5:A:600:ADP:N1	7:A:606:PG4:H31	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLU:C	1:A:255:LEU:HD23	2.22	0.65
1:B:61:SER:OG	8:B:696:HOH:O	2.07	0.65
1:B:327:ARG:HD3	1:B:364:GLU:HB3	1.77	0.65
1:A:33[A]:ARG:NH2	8:A:664:HOH:O	2.27	0.64
1:A:320:LEU:O	1:A:324:LEU:HD12	1.98	0.64
1:B:54:THR:HG21	1:B:64:LYS:HG2	1.79	0.64
1:B:22:VAL:CG1	1:B:70:MET:HB2	2.28	0.63
1:B:22:VAL:HG12	1:B:70:MET:HB2	1.80	0.63
1:B:327:ARG:HG3	1:B:327:ARG:HH11	1.63	0.63
1:A:249:THR:HG22	1:A:250:ILE:N	2.13	0.63
1:A:40:ILE:HD12	1:A:343:LEU:HD13	1.81	0.62
1:A:74:ALA:O	7:A:606:PG4:H11	2.00	0.62
1:B:54:THR:CG2	1:B:64:LYS:HG2	2.30	0.62
1:A:30:LEU:HD11	1:A:33[A]:ARG:NH2	2.15	0.61
1:A:249:THR:HG22	1:A:250:ILE:H	1.65	0.61
1:B:177:ASP:CB	1:B:179:SER:OG	2.49	0.61
1:A:351:GLU:OE1	8:A:713:HOH:O	2.16	0.61
1:A:38:HIS:CD2	1:A:38:HIS:H	2.18	0.61
1:A:351:GLU:CG	8:A:718:HOH:O	2.48	0.60
1:A:216:LYS:NZ	8:A:685:HOH:O	2.31	0.60
1:A:210:VAL:O	1:A:214:LEU:HG	2.01	0.60
1:B:327:ARG:O	1:B:363:PRO:HA	2.00	0.60
1:A:30:LEU:HD13	1:A:33[A]:ARG:HH21	1.66	0.60
1:B:172:LEU:O	1:B:174:PRO:HD3	2.02	0.59
1:A:107:THR:CB	1:A:270:GLU:OE2	2.51	0.59
1:A:249:THR:CB	1:A:253[A]:GLU:HG3	2.32	0.59
1:A:17:LYS:HD3	8:A:652:HOH:O	2.02	0.58
1:B:181:ARG:NH1	1:B:181:ARG:HG3	2.17	0.58
1:A:113:PHE:CE1	1:A:118:GLU:HG3	2.39	0.58
1:A:249:THR:HB	1:A:253[A]:GLU:CG	2.33	0.58
1:B:57:LEU:HD23	1:B:58:ALA:H	1.68	0.58
1:A:103:ALA:HB2	1:A:115:MET:HE3	1.86	0.58
1:A:74:ALA:O	7:A:606:PG4:C1	2.53	0.57
1:A:184:MET:HG3	1:A:196:ILE:HD13	1.85	0.57
1:B:143:ILE:HD13	1:B:243:ILE:HD11	1.87	0.57
1:B:244:HIS:CD2	8:B:665:HOH:O	2.58	0.57
1:A:162:GLU:HG2	1:A:237:SER:HA	1.87	0.56
1:A:162:GLU:CD	8:A:714:HOH:O	2.47	0.56
1:A:40:ILE:CD1	1:A:343:LEU:HD13	2.36	0.56
1:B:113:PHE:HD1	1:B:118:GLU:OE2	1.87	0.56
1:A:78:GLN:N	7:A:606:PG4:H52	2.18	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:HB3	1:A:154:PHE:CE2	2.41	0.55
1:A:106:GLN:HG3	1:A:270:GLU:HG2	1.88	0.55
1:B:192:ARG:HD3	1:B:321:GLN:HE21	1.72	0.55
1:A:113:PHE:HE1	1:A:118:GLU:HG3	1.71	0.55
1:A:77:LYS:HB3	7:A:606:PG4:H52	1.88	0.55
1:B:92:GLU:HG3	1:B:329:ARG:NH1	2.22	0.55
1:A:77:LYS:CB	7:A:606:PG4:H81	2.34	0.55
1:A:184:MET:HE3	1:A:318:ARG:CZ	2.37	0.55
1:A:178:VAL:HG12	1:A:220:LYS:HE2	1.88	0.55
1:B:173:ASN:ND2	1:B:200:GLU:HG2	2.20	0.55
1:B:271:ASN:O	1:B:292:LEU:CD1	2.55	0.54
1:B:40:ILE:HD12	1:B:340:SER:CB	2.37	0.54
1:B:49:GLU:CG	1:B:67:THR:HG22	2.30	0.54
1:B:205:HIS:HB2	1:B:209:GLU:OE2	2.07	0.54
1:B:327:ARG:HG3	1:B:327:ARG:NH1	2.23	0.54
1:A:219:ALA:O	1:A:222:THR:HG23	2.06	0.54
1:A:157:LYS:HE3	1:A:201:GLU:OE1	2.07	0.54
5:B:603:ADP:H3'	8:B:702:HOH:O	2.07	0.53
1:A:170:ASP:HB2	1:A:182:LEU:HD21	1.89	0.53
1:B:57:LEU:HD22	1:B:58:ALA:H	1.70	0.53
1:B:244:HIS:HD2	8:B:665:HOH:O	1.92	0.53
1:A:150:ASN:HB3	8:A:682:HOH:O	2.07	0.53
1:A:54:THR:HG21	1:A:64:LYS:CG	2.38	0.52
1:A:53:ARG:NH1	1:A:58:ALA:HB2	2.24	0.52
1:A:131:PRO:HB2	7:A:606:PG4:H72	1.91	0.52
1:A:303:VAL:HG11	1:A:355:ARG:O	2.09	0.52
1:A:260:LYS:HE2	1:A:262:ASN:HD21	1.73	0.52
1:A:42:GLU:HG3	1:A:63:ARG:NH2	2.24	0.52
1:B:154:PHE:HA	1:B:244:HIS:O	2.09	0.52
1:B:187:ASP:OD1	1:B:189:ARG:N	2.41	0.52
1:B:46:VAL:HG23	1:B:47:ARG:N	2.25	0.52
1:B:52:VAL:HG11	1:B:347:LEU:HD13	1.88	0.52
1:B:111:LYS:HZ3	1:B:268:GLY:HA2	1.75	0.51
1:B:92:GLU:CG	1:B:329:ARG:NH1	2.74	0.51
1:B:211:TYR:O	1:B:215:GLU:HG3	2.10	0.51
1:B:365:VAL:CG1	1:B:366:ASN:N	2.74	0.51
1:A:19:ILE:HD12	1:A:330:THR:HB	1.93	0.50
1:B:83:ARG:HG2	1:B:83:ARG:HH11	1.76	0.50
1:B:166:GLU:OE1	1:B:315:LYS:HG2	2.12	0.50
1:B:111:LYS:HE3	5:B:603:ADP:O2B	2.11	0.50
1:B:220:LYS:O	1:B:223:THR:N	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:HIS:HB2	1:A:209:GLU:OE2	2.11	0.49
1:B:212:GLN:HG2	1:B:216:LYS:NZ	2.28	0.49
1:A:178:VAL:CG1	1:A:220:LYS:HE2	2.42	0.49
1:A:124:GLU:HG2	1:A:125:TYR:CD1	2.47	0.49
1:A:322:ASP:OD1	1:A:327:ARG:N	2.34	0.49
1:B:44:ASP:OD2	1:B:47:ARG:HG3	2.12	0.49
1:A:160:LEU:HD13	1:A:239:PHE:HD2	1.76	0.49
1:A:255:LEU:HD23	1:A:255:LEU:N	2.28	0.49
1:A:363:PRO:O	1:A:364:GLU:HG3	2.13	0.49
1:B:92:GLU:OE1	1:B:92:GLU:HA	2.11	0.49
1:B:173:ASN:ND2	1:B:200:GLU:CG	2.75	0.49
1:A:22:VAL:CG2	1:A:333:ILE:HG23	2.42	0.48
1:B:299:ILE:HG23	1:B:359:ILE:HD11	1.95	0.48
1:A:127:TRP:HB2	6:A:602:MOY:H27	1.95	0.48
1:B:143:ILE:CD1	1:B:243:ILE:HD11	2.43	0.48
1:A:176:SER:HB3	1:A:180:GLU:OE1	2.12	0.48
1:B:177:ASP:C	1:B:179:SER:N	2.65	0.48
1:B:206:ASN:OD1	1:B:208:ASP:HB2	2.14	0.48
1:A:177:ASP:O	1:A:180:GLU:HG2	2.14	0.48
1:B:111:LYS:NZ	1:B:268:GLY:HA2	2.28	0.48
1:A:207:LYS:HG2	1:A:208:ASP:N	2.29	0.48
1:B:41:VAL:HG22	1:B:52:VAL:HG23	1.96	0.48
1:B:43:CYS:HB3	1:B:71:VAL:HG12	1.96	0.48
1:A:77:LYS:HD2	7:A:606:PG4:H61	1.96	0.48
1:A:94:ILE:O	1:A:257:LYS:HE2	2.14	0.48
1:A:124:GLU:HB3	1:A:125:TYR:HD1	1.79	0.48
1:A:19:ILE:CG1	1:A:359:ILE:HB	2.44	0.47
1:B:181:ARG:HG3	1:B:181:ARG:HH11	1.78	0.47
1:A:322:ASP:O	1:A:326:GLY:HA3	2.14	0.47
1:A:312:ARG:HA	1:A:318:ARG:CG	2.43	0.47
1:A:223:THR:O	1:A:223:THR:HG22	2.14	0.47
1:B:111:LYS:HZ3	1:B:268:GLY:CA	2.26	0.47
1:B:187:ASP:OD1	1:B:187:ASP:C	2.54	0.47
1:A:29:ASN:OD1	1:A:32:GLU:HG3	2.14	0.47
1:B:19:ILE:HD12	1:B:359:ILE:HB	1.97	0.47
1:A:78:GLN:HG2	7:A:606:PG4:H51	1.96	0.47
1:B:176:SER:CB	8:B:704:HOH:O	2.62	0.47
1:B:365:VAL:HG12	1:B:366:ASN:N	2.29	0.47
1:A:97:TYR:CE2	1:A:364:GLU:HA	2.40	0.47
1:B:219:ALA:O	1:B:222:THR:HB	2.14	0.46
1:A:248:THR:HA	1:A:253[B]:GLU:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:GLU:OE1	1:B:65:THR:HG21	2.15	0.46
1:A:186:ASP:OD2	1:A:312:ARG:NH2	2.49	0.46
1:A:312:ARG:HG2	1:A:312:ARG:NH1	2.31	0.46
1:B:176:SER:HB3	8:B:704:HOH:O	2.14	0.46
1:A:108:GLY:H	5:A:600:ADP:PB	2.38	0.46
1:A:162:GLU:CD	1:A:171:LEU:HD13	2.40	0.46
1:B:162:GLU:CD	1:B:171:LEU:CD1	2.89	0.46
1:A:312:ARG:HG2	1:A:312:ARG:HH11	1.81	0.45
1:B:128:GLU:OE1	1:B:207:LYS:NZ	2.49	0.45
1:B:191:LYS:HB2	1:B:191:LYS:HE2	1.81	0.45
1:A:90:LEU:HD13	1:A:139:THR:HG23	1.97	0.45
1:A:161:LEU:HD23	1:A:199:LEU:HD13	1.98	0.45
1:B:119:ARG:HD2	6:B:605:MOY:C26	2.46	0.45
1:B:162:GLU:CD	1:B:171:LEU:HD11	2.41	0.45
1:B:299:ILE:O	1:B:303:VAL:HG23	2.17	0.45
1:A:248:THR:HA	1:A:253[A]:GLU:O	2.16	0.45
1:A:248:THR:O	1:A:248:THR:HG23	2.16	0.45
1:B:79:ILE:HG22	8:B:628:HOH:O	2.16	0.45
1:A:22:VAL:HG22	1:A:333:ILE:HA	1.98	0.45
1:B:205:HIS:ND1	1:B:209:GLU:OE2	2.45	0.45
1:A:187:ASP:HA	1:A:195:ILE:CD1	2.47	0.45
1:A:294:THR:OG1	1:A:314:SER:HB3	2.17	0.45
1:B:192:ARG:HB3	1:B:321:GLN:NE2	2.31	0.45
1:A:82:TYR:OH	1:A:142:GLN:HG3	2.18	0.44
1:A:171:LEU:HD22	1:A:221:ARG:HD3	1.99	0.44
1:B:86:VAL:O	1:B:87:CYS:C	2.59	0.44
1:B:181:ARG:HH11	1:B:181:ARG:CG	2.31	0.44
1:B:190:ASN:HB3	1:B:191:LYS:H	1.68	0.44
1:A:77:LYS:HZ3	7:A:606:PG4:C1	2.30	0.44
1:A:82:TYR:CD2	1:A:86:VAL:HB	2.53	0.44
1:A:184:MET:HG3	1:A:196:ILE:CD1	2.48	0.44
1:A:40:ILE:HG21	1:A:340:SER:CA	2.46	0.43
1:A:249:THR:CG2	1:A:250:ILE:N	2.80	0.43
1:A:154:PHE:HA	1:A:244:HIS:O	2.19	0.43
1:A:22:VAL:HG22	1:A:333:ILE:HG12	2.00	0.43
1:A:144:PHE:CZ	1:A:156:VAL:HG21	2.54	0.43
1:B:148:THR:HG23	1:B:149:ASP:N	2.33	0.43
1:A:98:ASN:O	1:A:328:THR:HG23	2.19	0.43
1:A:19:ILE:HG13	1:A:359:ILE:HB	2.00	0.43
1:A:249:THR:CG2	1:A:250:ILE:H	2.30	0.43
1:B:40:ILE:HD13	8:B:620:HOH:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LYS:CG	1:B:192:ARG:N	2.82	0.43
1:A:21:VAL:HG11	1:A:353:ALA:HB1	2.01	0.42
1:A:311:TYR:O	1:A:317:THR:OG1	2.30	0.42
1:B:46:VAL:CG2	1:B:47:ARG:N	2.81	0.42
1:B:343:LEU:HD22	1:B:343:LEU:C	2.43	0.42
1:B:37:ALA:HA	1:B:38:HIS:ND1	2.34	0.42
1:B:209:GLU:O	1:B:213:ILE:HG13	2.20	0.42
1:A:19:ILE:HG12	1:A:359:ILE:O	2.19	0.42
1:A:171:LEU:CD2	1:A:221:ARG:HD3	2.50	0.42
1:A:26:ARG:HG3	1:A:26:ARG:HH11	1.84	0.42
1:A:77:LYS:CD	7:A:606:PG4:H41	2.34	0.42
1:B:148:THR:HG23	1:B:149:ASP:OD1	2.20	0.42
1:A:101:ILE:HG22	1:A:102:PHE:N	2.33	0.42
1:B:116:GLU:O	1:B:134:GLY:N	2.52	0.41
1:B:184:MET:HE2	1:B:318:ARG:CZ	2.50	0.41
1:A:76:THR:O	7:A:606:PG4:H32	2.20	0.41
1:A:144:PHE:CE1	1:A:206:ASN:HA	2.55	0.41
1:B:189:ARG:HH11	1:B:189:ARG:CG	2.28	0.41
1:A:116:GLU:HG2	1:A:136:ILE:HD12	2.01	0.41
1:B:247:GLU:O	1:B:254:GLU:HA	2.20	0.41
1:A:30:LEU:HD11	1:A:33[A]:ARG:HH22	1.86	0.41
1:A:315:LYS:HB2	8:A:720:HOH:O	2.20	0.41
1:B:161:LEU:HD21	1:B:319:ILE:HD13	2.03	0.41
1:A:298:VAL:HG13	1:A:309:VAL:CG1	2.51	0.41
1:B:106:GLN:HG3	1:B:109:THR:CG2	2.50	0.41
1:A:270:GLU:H	1:A:270:GLU:HG3	1.18	0.41
1:B:19:ILE:HG12	1:B:330:THR:HB	2.03	0.41
1:A:38:HIS:CD2	1:A:38:HIS:N	2.87	0.41
1:A:142:GLN:O	1:A:143:ILE:C	2.63	0.41
1:B:92:GLU:CG	1:B:329:ARG:HH12	2.33	0.41
1:B:40:ILE:HD12	1:B:340:SER:HA	2.03	0.41
1:B:111:LYS:NZ	1:B:268:GLY:CA	2.84	0.41
1:B:347:LEU:HD12	1:B:347:LEU:HA	1.90	0.40
1:B:26:ARG:NH1	1:B:27:PRO:O	2.54	0.40
1:B:83:ARG:HG2	1:B:83:ARG:NH1	2.37	0.40
1:B:169:PHE:CD2	1:B:178:VAL:O	2.74	0.40
1:A:241:VAL:O	1:A:241:VAL:HG13	2.22	0.40
1:B:40:ILE:HD12	1:B:340:SER:HB3	2.02	0.40
1:B:119:ARG:HG2	6:B:605:MOY:S	2.61	0.40
1:B:220:LYS:O	1:B:223:THR:HB	2.21	0.40
1:B:288:ILE:HG22	1:B:288:ILE:O	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:LEU:HD13	1:B:352:TYR:OH	2.21	0.40
1:A:17:LYS:N	1:A:361:ASN:O	2.54	0.40
1:A:78:GLN:HG2	7:A:606:PG4:C5	2.52	0.40
1:A:160:LEU:HD13	1:A:239:PHE:CD2	2.56	0.40
1:A:74:ALA:O	7:A:606:PG4:H12	2.22	0.40
1:A:124:GLU:HG2	1:A:125:TYR:CE1	2.56	0.40
1:A:164:TYR:O	1:A:165:ASN:C	2.64	0.40
1:A:342:ASN:O	1:A:343:LEU:C	2.63	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	332/367 (90%)	311 (94%)	16 (5%)	5 (2%)	8	22
1	B	331/367 (90%)	313 (95%)	16 (5%)	2 (1%)	21	44
All	All	663/734 (90%)	624 (94%)	32 (5%)	7 (1%)	11	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	ASP
1	A	150	ASN
1	A	17	LYS
1	A	121	PRO
1	B	178	VAL
1	A	310	PRO
1	B	310	PRO

5.3.2 Protein sidechains ⓘ

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	298/321 (93%)	265 (89%)	33 (11%)	6	15
1	B	297/321 (92%)	272 (92%)	25 (8%)	10	26
All	All	595/642 (93%)	537 (90%)	58 (10%)	8	20

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	22	VAL
1	A	30	LEU
1	A	34	LYS
1	A	40	ILE
1	A	46	VAL
1	A	85	VAL
1	A	92	GLU
1	A	94	ILE
1	A	118	GLU
1	A	140	LEU
1	A	147	LEU
1	A	153	GLU
1	A	157	LYS
1	A	161	LEU
1	A	175	SER
1	A	177	ASP
1	A	179	SER
1	A	182	LEU
1	A	189	ARG
1	A	207	LYS
1	A	212	GLN
1	A	216	LYS
1	A	221	ARG
1	A	222	THR
1	A	253[A]	GLU
1	A	253[B]	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	255	LEU
1	A	270	GLU
1	A	271	ASN
1	A	292	LEU
1	A	295	LEU
1	A	348	SER
1	B	38	HIS
1	B	40	ILE
1	B	42	GLU
1	B	52	VAL
1	B	57	LEU
1	B	60	LYS
1	B	75	SER
1	B	118	GLU
1	B	122	ASN
1	B	162	GLU
1	B	175	SER
1	B	177	ASP
1	B	181	ARG
1	B	191	LYS
1	B	216	LYS
1	B	241	VAL
1	B	246	LYS
1	B	292	LEU
1	B	295	LEU
1	B	329	ARG
1	B	343	LEU
1	B	347	LEU
1	B	348	SER
1	B	350	LEU
1	B	362	LYS

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

Mol	Chain	Res	Type
1	A	18	ASN
1	A	229	ASN
1	A	262	ASN
1	A	308	HIS
1	B	18	ASN
1	B	98	ASN
1	B	106	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	141	HIS
1	B	212	GLN
1	B	244	HIS
1	B	262	ASN
1	B	321	GLN
1	B	342	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	334/367 (91%)	0.30	19 (5%)	29 26	5, 21, 56, 75	5 (1%)
1	B	335/367 (91%)	0.31	23 (6%)	23 20	3, 24, 63, 84	1 (0%)
All	All	669/734 (91%)	0.30	42 (6%)	26 23	3, 23, 61, 84	6 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	178	VAL	4.6
1	B	16	GLY	4.4
1	B	366	ASN	4.2
1	A	253[A]	GLU	3.8
1	A	34	LYS	3.8
1	A	149	ASP	3.8
1	A	192	ARG	3.7
1	A	57	LEU	3.6
1	B	57	LEU	3.6
1	B	38	HIS	3.6
1	B	192	ARG	3.6
1	A	364	GLU	3.4
1	A	15	LYS	3.2
1	A	189	ARG	3.1
1	B	175	SER	3.1
1	B	58	ALA	3.0
1	B	271	ASN	3.0
1	B	55	GLY	3.0
1	B	177	ASP	2.8
1	A	252	GLY	2.8
1	A	150	ASN	2.7
1	B	36	SER	2.7
1	A	190	ASN	2.6
1	A	251	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	191	LYS	2.6
1	B	176	SER	2.6
1	B	56	GLY	2.6
1	B	306	THR	2.5
1	B	190	ASN	2.4
1	B	288	ILE	2.4
1	B	173	ASN	2.4
1	A	180	GLU	2.3
1	B	35	ALA	2.3
1	A	62	SER	2.2
1	B	59	ASP	2.2
1	A	56	GLY	2.2
1	B	31	ALA	2.2
1	A	191	LYS	2.1
1	B	34	LYS	2.1
1	A	33[A]	ARG	2.1
1	A	97	TYR	2.1
1	A	363	PRO	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(Å ²)	Q<0.9
7	PG4	A	606	13/13	0.87	0.18	35,49,54,54	0
6	MOY	B	605	24/24	0.91	0.13	14,27,38,40	0
2	MG	B	604	1/1	0.92	0.11	11,11,11,11	0
6	MOY	A	602	24/24	0.93	0.11	15,25,30,45	0
3	K	A	607	1/1	0.95	0.09	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ADP	B	603	27/27	0.96	0.09	10,21,36,44	0
4	CL	A	608	1/1	0.96	0.04	33,33,33,33	0
5	ADP	A	600	27/27	0.97	0.07	4,17,27,29	0
2	MG	A	601	1/1	0.98	0.08	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.