



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:19 AM GMT

PDB ID : 2WOG
Title : INTERMEDIATE AND FINAL STATES OF HUMAN KINESIN EG5 IN
COMPLEX WITH S-TRITYL-L-CYSTEINE
Authors : Kaan, H.Y.K.; Ulaganathan, V.; Hackney, D.D.; Kozielski, F.
Deposited on : 2009-07-23
Resolution : 2.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

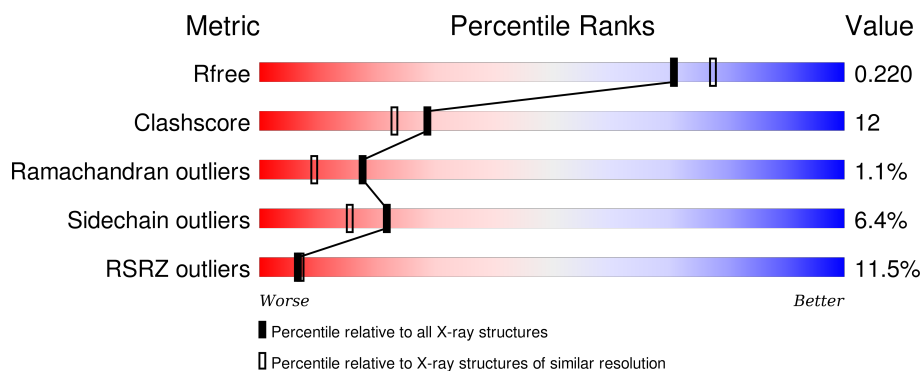
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 $\leq 5\%$. 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	368	<div> <div>9%</div> <div>77%</div> <div>12%</div> <div>10%</div> </div>
1	B	368	<div> <div>9%</div> <div>72%</div> <div>13%</div> <div>11%</div> </div>
1	C	368	<div> <div>13%</div> <div>66%</div> <div>21%</div> <div>10%</div> </div>

2 Entry composition [i](#)

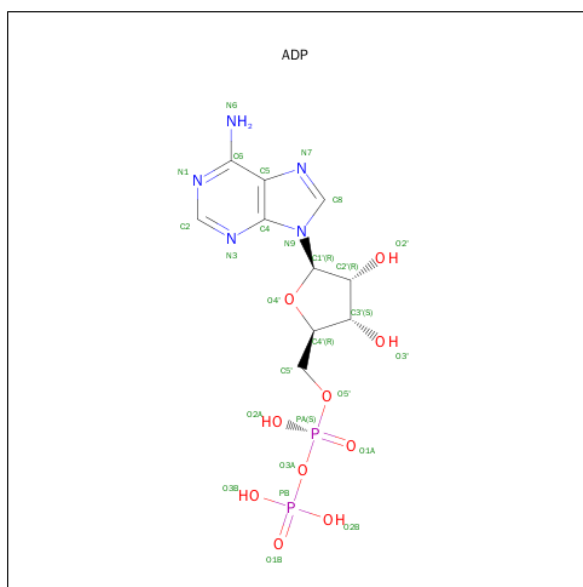
There are 5 unique types of molecules in this entry. The entry contains 9044 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	333	Total	C	N	O	S	0	15	0
			2701	1697	468	524	12			
1	B	328	Total	C	N	O	S	0	23	0
			2706	1712	465	518	11			
1	C	330	Total	C	N	O	S	0	9	0
			2637	1656	457	514	10			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

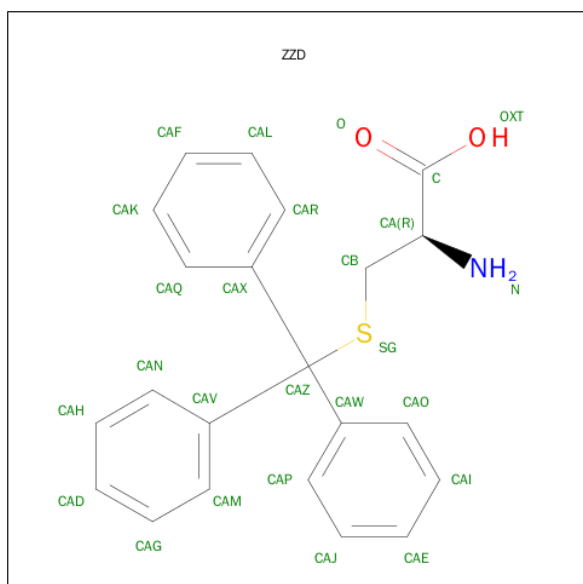


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

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

- Molecule 4 is S-TRITYL-L-CYSTEINE (three-letter code: ZSD) (formula: C₂₂H₂₁NO₂S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 26 22 1 2 1	0	0
4	B	1	Total C N O S 26 22 1 2 1	0	0
4	C	1	Total C N O S 26 22 1 2 1	0	0

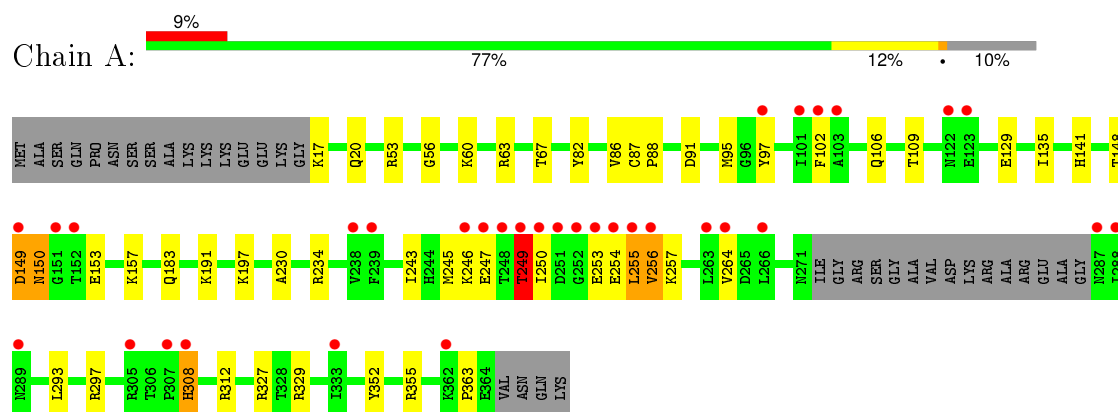
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	309	Total O 309 309	0	0
5	B	318	Total O 318 318	0	0
5	C	211	Total O 211 211	0	0

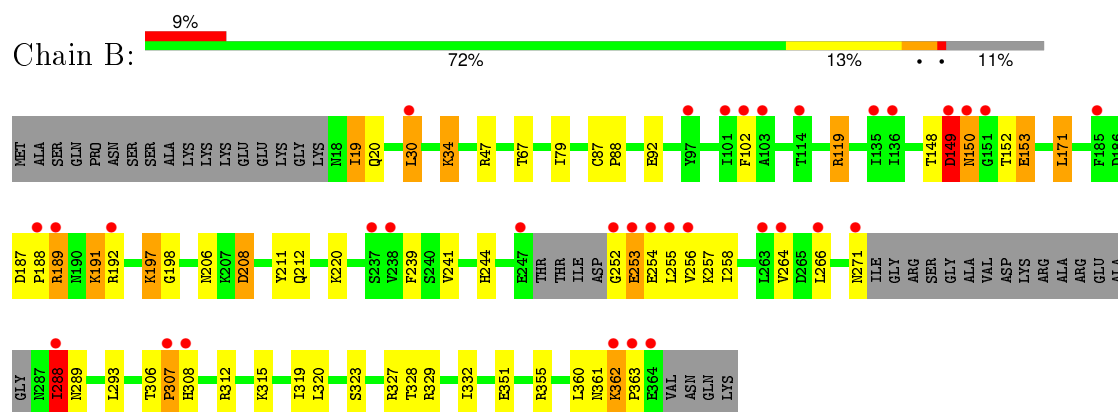
3 Residue-property plots [i](#)

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.

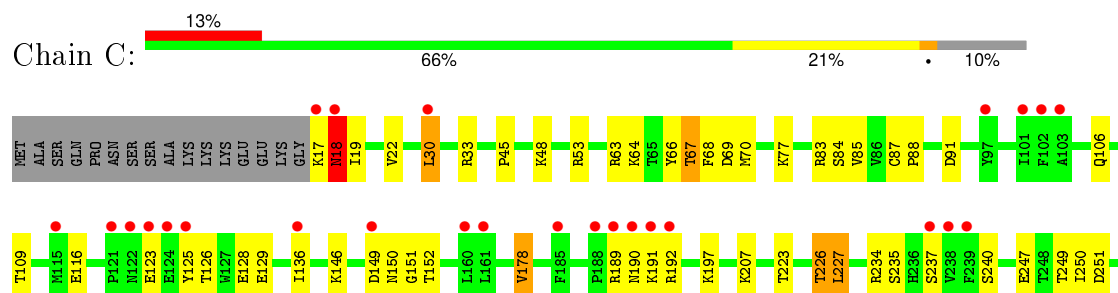
• Molecule 1: KINESIN-LIKE PROTEIN KIF11

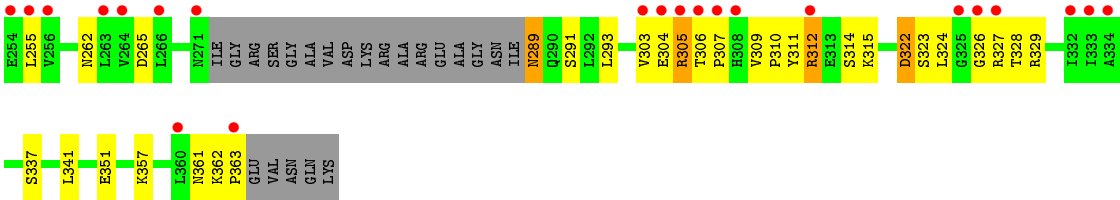


• Molecule 1: KINESIN-LIKE PROTEIN KIF11



• Molecule 1: KINESIN-LIKE PROTEIN KIF11





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	96.50Å 96.50Å 124.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.16 – 2.00 29.16 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.16-2.00) 99.9 (29.16-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0090	Depositor
R, R_{free}	0.155 , 0.218 0.158 , 0.220	Depositor DCC
R_{free} test set	4351 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.0	EDS
Estimated twinning fraction	0.008 for -h,-k,l 0.029 for h,-h-k,-l 0.019 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 87455 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9044	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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, 0.375 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: MG, ZSD, ADP

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	0.61	0/2786	0.72	0/3763
1	B	0.62	0/2815	0.81	9/3800 (0.2%)
1	C	0.59	0/2703	0.73	2/3652 (0.1%)
All	All	0.61	0/8304	0.75	11/11215 (0.1%)

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	B	1	0

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257[A]	LYS	N-CA-CB	-7.95	96.28	110.60
1	B	257[B]	LYS	N-CA-CB	-7.95	96.28	110.60
1	C	178	VAL	CB-CA-C	-7.17	97.77	111.40
1	B	119	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	B	256	VAL	N-CA-C	-6.55	93.31	111.00
1	B	257[A]	LYS	N-CA-C	-6.40	93.72	111.00
1	B	257[B]	LYS	N-CA-C	-6.40	93.72	111.00
1	B	119	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	B	256	VAL	CB-CA-C	-6.04	99.92	111.40
1	B	171	LEU	CB-CG-CD1	5.43	120.23	111.00
1	C	178	VAL	CG1-CB-CG2	5.21	119.24	110.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	150[B]	ASN	CA

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	2701	0	2765	51	0
1	B	2706	0	2796	75	0
1	C	2637	0	2688	67	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	26	0	20	1	0
4	B	26	0	20	0	0
4	C	26	0	20	0	0
5	A	309	0	0	17	0
5	B	318	0	0	17	0
5	C	211	0	0	10	0
All	All	9044	0	8345	191	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 12.

All (191) 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:B:220[A]:LYS:CE	5:B:2160:HOH:O	1.73	1.32
1:B:102[B]:PHE:CZ	1:B:320[B]:LEU:HD12	1.64	1.31
1:C:30:LEU:HD23	1:C:33:ARG:HH21	1.06	1.12
1:B:327:ARG:O	1:B:363:PRO:HA	1.50	1.12
1:B:208:ASP:HB3	5:B:2200:HOH:O	1.54	1.05
1:A:246:LYS:HA	5:A:2227:HOH:O	1.58	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LEU:CD2	1:C:33:ARG:HH21	1.71	1.03
1:B:92:GLU:HG2	5:B:2095:HOH:O	1.60	1.02
1:B:102[B]:PHE:CZ	1:B:320[B]:LEU:CD1	2.45	1.00
1:B:197[A]:LYS:HD3	1:B:198:GLY:N	1.77	0.99
1:B:92:GLU:OE2	1:B:329:ARG:HD2	1.63	0.99
1:C:48[B]:LYS:HE2	1:C:68:PHE:O	1.62	0.99
1:C:17:LYS:O	1:C:19:ILE:HG22	1.64	0.98
1:B:102[B]:PHE:HZ	1:B:320[B]:LEU:HD12	1.21	0.98
1:B:312:ARG:HG2	5:B:2267:HOH:O	1.61	0.97
1:B:220[A]:LYS:HE2	5:B:2160:HOH:O	1.41	0.97
1:C:30:LEU:HD23	1:C:33:ARG:NH2	1.83	0.94
1:C:249[B]:THR:HG22	1:C:251[B]:ASP:H	1.33	0.93
1:B:254[B]:GLU:HA	1:B:254[B]:GLU:OE1	1.68	0.92
1:A:88:PRO:HG3	1:C:249[B]:THR:HG21	1.52	0.92
1:C:66:TYR:OH	1:C:351:GLU:OE1	1.89	0.90
1:A:88:PRO:HG3	1:C:249[B]:THR:CG2	2.01	0.89
1:C:289:ASN:O	1:C:293:LEU:HD13	1.69	0.89
1:B:220[A]:LYS:HE3	5:B:2160:HOH:O	1.48	0.89
1:C:17:LYS:HE2	5:C:2178:HOH:O	1.72	0.88
1:C:123[B]:GLU:HA	1:C:123[B]:GLU:OE2	1.73	0.87
1:B:191:LYS:H	1:B:191:LYS:HE3	1.40	0.86
1:B:319:ILE:HG22	1:B:320[B]:LEU:CD2	2.06	0.85
1:B:206[B]:ASN:HD21	1:B:208:ASP:CG	1.79	0.84
1:B:191:LYS:H	1:B:191:LYS:CE	1.93	0.82
1:C:123[B]:GLU:CA	1:C:123[B]:GLU:OE2	2.27	0.82
1:B:47[B]:ARG:NH1	5:B:2042:HOH:O	2.11	0.81
1:A:247:GLU:HG2	5:A:2226:HOH:O	1.81	0.80
1:B:319:ILE:HG22	1:B:320[B]:LEU:HD22	1.63	0.80
1:C:251[B]:ASP:OD1	5:C:2161:HOH:O	1.99	0.80
1:B:47[B]:ARG:NE	5:B:2041:HOH:O	2.14	0.80
1:B:92:GLU:OE2	1:B:329:ARG:CD	2.30	0.79
1:C:323:SER:O	1:C:328:THR:HG21	1.85	0.77
1:C:192[B]:ARG:NH2	1:C:324:LEU:O	2.17	0.76
1:C:362:LYS:HB2	1:C:363:PRO:HD2	1.66	0.76
1:B:361:ASN:CG	5:B:2271:HOH:O	2.24	0.75
1:C:226:THR:HG22	1:C:227:LEU:HD13	1.70	0.73
1:B:361:ASN:HB3	5:B:2271:HOH:O	1.90	0.72
1:A:308:HIS:HB2	5:A:2253:HOH:O	1.90	0.72
1:A:247:GLU:CG	5:A:2226:HOH:O	2.39	0.70
1:B:206[B]:ASN:OD1	1:B:208:ASP:OD1	2.11	0.69
1:C:17:LYS:O	1:C:18:ASN:ND2	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:LYS:N	1:B:362:LYS:HD2	2.10	0.66
1:C:329:ARG:NH2	5:C:2181:HOH:O	2.28	0.65
1:B:244:HIS:CD2	1:B:258:ILE:HG12	2.32	0.65
1:B:220[B]:LYS:HE2	5:B:2160:HOH:O	1.96	0.65
1:A:355:ARG:NH2	5:A:2291:HOH:O	2.28	0.65
1:C:48[B]:LYS:CE	1:C:68:PHE:O	2.42	0.65
1:C:304:GLU:O	1:C:306:THR:N	2.30	0.64
1:B:361:ASN:CB	5:B:2271:HOH:O	2.44	0.64
1:B:197[A]:LYS:HD3	1:B:198:GLY:H	1.62	0.64
1:A:256:VAL:HA	5:A:2227:HOH:O	1.98	0.64
1:A:141:HIS:ND1	5:A:2129:HOH:O	2.30	0.64
1:B:67[A]:THR:HG22	5:B:2296:HOH:O	1.97	0.63
1:C:289:ASN:O	1:C:293:LEU:CD1	2.44	0.63
1:C:149:ASP:O	1:C:150:ASN:C	2.37	0.63
1:A:86:VAL:HG21	1:A:135:ILE:HG12	1.81	0.62
1:C:306:THR:HG23	1:C:307:PRO:HD2	1.82	0.61
1:B:254[B]:GLU:CA	1:B:254[B]:GLU:OE1	2.44	0.61
1:C:249[B]:THR:HG22	1:C:250:ILE:N	2.17	0.60
1:C:312:ARG:HH11	1:C:312:ARG:HB3	1.66	0.60
1:B:102[B]:PHE:CE1	1:B:320[B]:LEU:CD1	2.84	0.60
1:C:17:LYS:C	1:C:19:ILE:H	2.05	0.60
1:C:235:SER:O	5:C:2152:HOH:O	2.16	0.60
1:B:239:PHE:HE1	1:B:241[A]:VAL:CG2	2.15	0.59
1:A:88:PRO:HG3	1:C:249[B]:THR:HG23	1.82	0.59
1:B:327:ARG:HA	1:B:362:LYS:O	2.02	0.59
1:A:352:TYR:O	1:A:355:ARG:HG2	2.02	0.59
1:C:249[B]:THR:CG2	1:C:250:ILE:N	2.66	0.58
1:B:252:GLY:O	1:B:253:GLU:HG3	2.04	0.58
1:B:323:SER:HA	1:B:328:THR:HB	1.86	0.58
1:B:47[B]:ARG:NH1	5:B:2038:HOH:O	2.36	0.57
1:C:70:MET:HE3	1:C:85:VAL:HG22	1.86	0.57
1:B:206[B]:ASN:ND2	1:B:208:ASP:OD2	2.36	0.57
1:B:288:ILE:O	1:B:289:ASN:ND2	2.35	0.57
1:B:149:ASP:OD1	1:B:149:ASP:N	2.34	0.56
1:A:183[A]:GLN:HG3	5:A:2159:HOH:O	2.05	0.56
1:A:293:LEU:HD21	1:A:297[A]:ARG:NH2	2.21	0.56
1:C:106:GLN:HG2	1:C:109:THR:HG23	1.87	0.55
1:A:87[B]:CYS:HB3	1:A:88:PRO:HD3	1.89	0.54
1:C:223:THR:O	1:C:226:THR:HB	2.07	0.54
1:A:148:THR:CG2	1:A:149:ASP:N	2.71	0.53
1:B:361:ASN:HB2	5:B:2303:HOH:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:THR:O	1:A:150[B]:ASN:ND2	2.41	0.53
1:C:234:ARG:NH1	5:C:2150:HOH:O	2.34	0.53
1:C:240:SER:OG	1:C:262:ASN:ND2	2.41	0.53
1:A:312:ARG:HG3	5:A:2114:HOH:O	2.07	0.53
1:B:87[A]:CYS:HB2	1:B:88:PRO:HD3	1.90	0.53
1:B:252:GLY:O	1:B:253:GLU:CB	2.57	0.52
1:B:239:PHE:HE1	1:B:241[A]:VAL:HG22	1.75	0.52
1:B:191:LYS:CD	1:B:191:LYS:N	2.72	0.52
1:C:67:THR:HG22	1:C:361:ASN:OD1	2.09	0.52
1:B:306:THR:HB	1:B:307:PRO:HD2	1.91	0.52
1:B:319:ILE:HG22	1:B:320[B]:LEU:HD23	1.89	0.52
1:C:67:THR:CG2	1:C:361:ASN:OD1	2.58	0.52
1:C:17:LYS:O	1:C:19:ILE:N	2.43	0.51
1:B:148:THR:O	1:B:149:ASP:O	2.26	0.51
1:B:351:GLU:O	1:B:355:ARG:HG3	2.10	0.51
1:B:87[B]:CYS:HB3	1:B:88:PRO:HD3	1.91	0.51
1:A:254[B]:GLU:OE2	1:A:256:VAL:HG23	2.09	0.51
1:C:315:LYS:HE3	5:C:2096:HOH:O	2.10	0.50
1:B:197[A]:LYS:CD	1:B:198:GLY:N	2.64	0.50
1:C:67:THR:HG21	1:C:361:ASN:HA	1.92	0.50
1:A:67[B]:THR:HG23	5:A:2288:HOH:O	2.10	0.50
1:A:56:GLY:O	1:A:60:LYS:HE3	2.12	0.50
1:C:48[A]:LYS:HD3	1:C:69:ASP:O	2.11	0.50
1:B:191:LYS:CD	1:B:191:LYS:H	2.25	0.50
1:B:30:LEU:O	1:B:34:LYS:HE2	2.12	0.50
1:C:237:SER:HB3	1:C:265:ASP:HB3	1.94	0.49
1:C:45:PRO:HB3	5:C:2045:HOH:O	2.11	0.49
1:B:206[B]:ASN:ND2	1:B:208:ASP:CG	2.59	0.49
1:A:257:LYS:NZ	5:A:2228:HOH:O	2.43	0.49
1:A:148:THR:HG22	1:A:149:ASP:N	2.28	0.48
1:A:106:GLN:HG2	1:A:109:THR:HG23	1.96	0.48
1:B:191:LYS:HD3	1:B:191:LYS:N	2.29	0.48
1:B:252:GLY:O	1:B:253:GLU:CG	2.62	0.48
1:A:148:THR:O	1:A:149:ASP:C	2.51	0.48
1:C:128:GLU:OE2	1:C:207:LYS:HE2	2.13	0.48
1:A:20:GLN:HE22	1:A:329:ARG:HH21	1.60	0.47
1:C:17:LYS:C	1:C:19:ILE:N	2.67	0.47
1:B:102[A]:PHE:HB3	1:B:264:VAL:HB	1.96	0.47
1:A:293:LEU:HD21	1:A:297[A]:ARG:CZ	2.45	0.47
1:B:119:ARG:HD2	1:B:211:TYR:HE2	1.81	0.46
1:A:246:LYS:HZ2	1:A:254[B]:GLU:CD	2.18	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:THR:OG1	1:A:255:LEU:HD21	2.16	0.46
1:B:152:THR:HG22	1:B:153:GLU:O	2.15	0.46
1:A:327:ARG:O	1:A:363:PRO:HA	2.16	0.46
1:C:87:CYS:HB2	1:C:88:PRO:HD3	1.96	0.46
1:A:246:LYS:NZ	1:A:254[B]:GLU:CD	2.69	0.46
1:A:91:ASP:O	1:A:95[B]:MET:HG3	2.16	0.46
1:A:230:ALA:HB3	1:A:234:ARG:HD2	1.98	0.45
1:A:257:LYS:HE2	5:A:2229:HOH:O	2.16	0.45
1:B:212[B]:GLN:HG3	5:B:2205:HOH:O	2.16	0.45
1:C:67:THR:HG21	5:C:2028:HOH:O	2.16	0.45
1:C:91:ASP:OD1	1:C:146:LYS:NZ	2.47	0.45
1:A:87[B]:CYS:HB3	1:A:88:PRO:CD	2.47	0.45
1:C:116:GLU:HG2	1:C:136:ILE:HD12	1.99	0.45
1:B:187:ASP:OD1	1:B:188:PRO:HD2	2.16	0.45
1:C:126:THR:OG1	1:C:129:GLU:HG2	2.17	0.45
1:C:149:ASP:O	1:C:151:GLY:N	2.49	0.45
1:A:88:PRO:CG	1:C:249[B]:THR:HG23	2.47	0.44
1:C:303:VAL:C	1:C:305:ARG:H	2.21	0.44
1:A:106:GLN:HG2	1:A:109:THR:CG2	2.47	0.44
1:B:119:ARG:HD2	1:B:211:TYR:CE2	2.52	0.44
1:C:309:VAL:CG1	1:C:311:TYR:CE2	3.01	0.44
1:B:191:LYS:CE	1:B:191:LYS:N	2.73	0.44
1:C:106:GLN:HG2	1:C:109:THR:CG2	2.48	0.44
1:A:82:TYR:CE1	1:A:87[A]:CYS:SG	3.10	0.44
1:C:309:VAL:HG12	1:C:311:TYR:CE2	2.53	0.44
1:B:102[A]:PHE:CD1	1:B:266:LEU:HD11	2.53	0.44
4:A:1365:ZZD:CAO	4:A:1365:ZZD:HB1C	2.47	0.44
1:C:53:ARG:HA	1:C:63:ARG:HD3	2.01	0.43
1:A:88:PRO:CG	1:C:249[B]:THR:CG2	2.86	0.43
1:B:315:LYS:HE3	5:B:2154:HOH:O	2.18	0.43
1:B:19[A]:ILE:HD12	1:B:20:GLN:O	2.19	0.43
1:B:19[A]:ILE:CD1	1:B:332:ILE:HG13	2.49	0.43
1:A:102:PHE:HB3	1:A:264:VAL:HB	2.00	0.43
1:B:189[B]:ARG:CG	1:B:189[B]:ARG:HH11	2.32	0.42
1:A:243:ILE:HG22	1:A:245:MET:HG3	2.00	0.42
1:A:293:LEU:HD11	5:A:2252:HOH:O	2.20	0.42
1:A:293:LEU:O	1:A:297[A]:ARG:HG3	2.19	0.42
1:A:53:ARG:HA	1:A:63:ARG:HD3	2.01	0.42
1:A:97:TYR:CZ	5:A:2296:HOH:O	2.67	0.42
1:B:288:ILE:C	1:B:289:ASN:HD22	2.22	0.42
1:A:56:GLY:O	1:A:60:LYS:CE	2.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:THR:CG2	1:A:149:ASP:H	2.32	0.41
1:C:18:ASN:OD1	1:C:326:GLY:O	2.38	0.41
1:C:291:SER:HA	1:C:314:SER:HB2	2.01	0.41
1:B:362:LYS:N	1:B:362:LYS:CD	2.82	0.41
1:B:252:GLY:O	1:B:253:GLU:HB2	2.20	0.41
1:C:309:VAL:HA	1:C:310:PRO:HD3	1.47	0.41
1:C:322:ASP:HB3	5:C:2115:HOH:O	2.21	0.41
1:A:255:LEU:C	5:A:2227:HOH:O	2.59	0.41
1:A:355:ARG:NH1	5:A:2292:HOH:O	2.42	0.41
1:C:309:VAL:HG11	1:C:311:TYR:CZ	2.56	0.41
1:C:22:VAL:CG1	1:C:70:MET:HB2	2.51	0.40
1:B:119:ARG:HD3	1:B:211:TYR:OH	2.21	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	344/368 (94%)	337 (98%)	4 (1%)	3 (1%)	21	13
1	B	344/368 (94%)	336 (98%)	2 (1%)	6 (2%)	11	4
1	C	335/368 (91%)	320 (96%)	12 (4%)	3 (1%)	21	13
All	All	1023/1104 (93%)	993 (97%)	18 (2%)	12 (1%)	17	8

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	ASP
1	B	149	ASP
1	B	253	GLU
1	C	18	ASN
1	C	305	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	191	LYS
1	B	150[A]	ASN
1	B	150[B]	ASN
1	B	288	ILE
1	C	190	ASN
1	B	307	PRO
1	A	249	THR

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	311/322 (97%)	296 (95%)	15 (5%)	31	26
1	B	314/322 (98%)	290 (92%)	24 (8%)	16	10
1	C	301/322 (94%)	276 (92%)	25 (8%)	14	8
All	All	926/966 (96%)	862 (93%)	64 (7%)	22	13

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	129	GLU
1	A	150[A]	ASN
1	A	150[B]	ASN
1	A	153	GLU
1	A	157[A]	LYS
1	A	157[C]	LYS
1	A	197[A]	LYS
1	A	197[B]	LYS
1	A	249	THR
1	A	250	ILE
1	A	253	GLU
1	A	255	LEU
1	A	256	VAL
1	A	308	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	19[A]	ILE
1	B	19[B]	ILE
1	B	30	LEU
1	B	34	LYS
1	B	79	ILE
1	B	149	ASP
1	B	150[A]	ASN
1	B	150[B]	ASN
1	B	153	GLU
1	B	171	LEU
1	B	189[A]	ARG
1	B	189[B]	ARG
1	B	191	LYS
1	B	192	ARG
1	B	197[A]	LYS
1	B	197[B]	LYS
1	B	208	ASP
1	B	255	LEU
1	B	271	ASN
1	B	288	ILE
1	B	293	LEU
1	B	308	HIS
1	B	360	LEU
1	B	362	LYS
1	C	18	ASN
1	C	30	LEU
1	C	64	LYS
1	C	67	THR
1	C	77[A]	LYS
1	C	77[B]	LYS
1	C	83	ARG
1	C	84	SER
1	C	125	TYR
1	C	152	THR
1	C	178	VAL
1	C	189	ARG
1	C	191	LYS
1	C	197	LYS
1	C	226	THR
1	C	227	LEU
1	C	247	GLU
1	C	255	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	289	ASN
1	C	312	ARG
1	C	322	ASP
1	C	327	ARG
1	C	337	SER
1	C	341	LEU
1	C	357	LYS

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

Mol	Chain	Res	Type
1	A	20	GLN
1	A	262	ASN
1	A	271	ASN
1	A	321	GLN
1	B	20	GLN
1	B	122	ASN
1	B	262	ASN
1	B	271	ASN
1	B	287	ASN
1	B	289	ASN
1	B	321	GLN
1	C	165	ASN
1	C	244	HIS
1	C	262	ASN
1	C	289	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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$
4	ZZD	A	1365	-	25,28,28	0.83	1 (4%)	31,38,38	0.92	1 (3%)
2	ADP	A	600	3	22,29,29	0.94	1 (4%)	27,45,45	1.78	4 (14%)
4	ZZD	B	1365	-	25,28,28	0.77	1 (4%)	31,38,38	0.88	0
2	ADP	B	600	3	22,29,29	1.02	1 (4%)	27,45,45	1.64	3 (11%)
4	ZZD	C	1364	-	25,28,28	0.79	1 (4%)	31,38,38	0.95	1 (3%)
2	ADP	C	600	3	22,29,29	0.97	1 (4%)	27,45,45	2.15	4 (14%)

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
4	ZZD	A	1365	-	-	0/24/28/28	0/3/3/3
2	ADP	A	600	3	-	0/12/32/32	0/3/3/3
4	ZZD	B	1365	-	-	0/24/28/28	0/3/3/3
2	ADP	B	600	3	-	0/12/32/32	0/3/3/3
4	ZZD	C	1364	-	-	0/24/28/28	0/3/3/3
2	ADP	C	600	3	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1365	ZZD	CAZ-SG	-2.02	1.84	1.87
4	C	1364	ZZD	CB-SG	2.09	1.85	1.82
4	B	1365	ZZD	CB-SG	2.11	1.85	1.82
2	A	600	ADP	C5-C4	2.41	1.45	1.40
2	C	600	ADP	C5-C4	3.07	1.47	1.40
2	B	600	ADP	C5-C4	3.20	1.47	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	ADP	N3-C2-N1	-8.86	122.11	128.89
2	A	600	ADP	N3-C2-N1	-7.03	123.51	128.89
2	B	600	ADP	N3-C2-N1	-5.61	124.60	128.89
2	C	600	ADP	C4-C5-N7	-3.00	106.72	109.48
2	B	600	ADP	C4-C5-N7	-2.78	106.92	109.48
2	B	600	ADP	C2'-C1'-N9	-2.70	110.17	114.29
2	A	600	ADP	C1'-N9-C4	-2.70	122.87	126.94
2	C	600	ADP	C1'-N9-C4	-2.63	122.97	126.94
4	C	1364	ZZD	CAW-CAZ-CAV	-2.42	104.72	111.13
4	A	1365	ZZD	CAW-CAZ-CAV	-2.38	104.84	111.13
2	A	600	ADP	C4-C5-N7	-2.08	107.56	109.48
2	A	600	ADP	O3B-PB-O2B	2.12	115.47	107.38
2	C	600	ADP	C2-N1-C6	2.97	124.08	118.77

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
4	A	1365	ZZD	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

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	333/368 (90%)	0.33	33 (9%)  	17, 28, 62, 91	0
1	B	328/368 (89%)	0.26	33 (10%)  	17, 28, 61, 82	0
1	C	330/368 (89%)	0.52	48 (14%)  	23, 38, 65, 79	0
All	All	991/1104 (89%)	0.37	114 (11%)  	17, 31, 63, 91	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	ILE	10.6
1	A	252	GLY	9.3
1	A	248	THR	9.0
1	A	249	THR	7.7
1	B	255	LEU	7.7
1	B	363	PRO	7.5
1	B	288	ILE	6.7
1	A	288	ILE	6.2
1	A	149	ASP	5.9
1	B	149	ASP	5.8
1	C	305	ARG	5.7
1	A	251	ASP	5.6
1	B	189[A]	ARG	5.6
1	B	271	ASN	5.5
1	A	247	GLU	5.3
1	A	151	GLY	5.3
1	C	307	PRO	5.1
1	A	255	LEU	5.0
1	C	188	PRO	4.9
1	C	264	VAL	4.8
1	C	308	HIS	4.6
1	C	255	LEU	4.4
1	A	307	PRO	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	254[A]	GLU	4.4
1	A	253	GLU	4.3
1	C	238	VAL	4.3
1	B	364	GLU	4.2
1	C	360	LEU	4.2
1	A	264	VAL	4.1
1	C	123[A]	GLU	4.0
1	C	189	ARG	3.9
1	A	152	THR	3.9
1	B	307	PRO	3.8
1	C	263	LEU	3.7
1	A	287	ASN	3.7
1	C	17	LYS	3.7
1	C	271	ASN	3.7
1	C	304	GLU	3.7
1	C	103	ALA	3.7
1	B	266	LEU	3.6
1	C	30	LEU	3.6
1	B	308	HIS	3.6
1	A	305[A]	ARG	3.5
1	A	308	HIS	3.5
1	A	256	VAL	3.5
1	A	246	LYS	3.5
1	C	333	ILE	3.4
1	C	266	LEU	3.3
1	B	252	GLY	3.3
1	C	239	PHE	3.3
1	B	253	GLU	3.2
1	C	192[A]	ARG	3.1
1	A	238	VAL	3.1
1	B	102[A]	PHE	3.1
1	C	122	ASN	3.1
1	C	363	PRO	3.1
1	B	264	VAL	3.0
1	B	254[A]	GLU	3.0
1	C	18	ASN	3.0
1	C	190	ASN	3.0
1	C	185	PHE	3.0
1	B	188	PRO	3.0
1	A	289	ASN	2.9
1	C	325	GLY	2.9
1	B	256	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	122	ASN	2.8
1	B	151	GLY	2.8
1	B	362	LYS	2.7
1	C	121	PRO	2.7
1	B	247	GLU	2.7
1	B	238	VAL	2.7
1	B	97	TYR	2.7
1	A	362	LYS	2.7
1	A	263	LEU	2.7
1	C	237	SER	2.7
1	C	161	LEU	2.6
1	C	327	ARG	2.6
1	C	312	ARG	2.6
1	C	115	MET	2.6
1	A	103	ALA	2.5
1	A	97	TYR	2.5
1	A	102	PHE	2.5
1	C	191	LYS	2.5
1	C	326	GLY	2.5
1	C	125	TYR	2.5
1	B	30	LEU	2.5
1	B	136	ILE	2.5
1	C	101	ILE	2.5
1	C	124	GLU	2.4
1	C	136	ILE	2.4
1	B	263	LEU	2.4
1	C	254	GLU	2.4
1	B	237[A]	SER	2.4
1	C	149	ASP	2.3
1	C	102	PHE	2.3
1	B	150[A]	ASN	2.3
1	B	103	ALA	2.3
1	C	97	TYR	2.3
1	B	101	ILE	2.3
1	C	306	THR	2.2
1	A	333	ILE	2.2
1	C	332	ILE	2.2
1	C	303	VAL	2.1
1	B	192	ARG	2.1
1	B	135	ILE	2.1
1	A	101	ILE	2.1
1	A	123	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	239	PHE	2.1
1	B	185[A]	PHE	2.1
1	B	114	THR	2.0
1	C	256	VAL	2.0
1	A	266	LEU	2.0
1	C	160	LEU	2.0
1	C	334	ALA	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
4	ZZD	C	1364	26/26	0.85	0.15	0.48	29,43,53,57	0
4	ZZD	B	1365	26/26	0.93	0.14	0.40	20,31,44,48	0
4	ZZD	A	1365	26/26	0.93	0.11	-0.04	27,35,46,48	0
2	ADP	A	600	27/27	0.99	0.09	-0.55	15,24,28,34	0
2	ADP	B	600	27/27	0.99	0.11	-0.70	16,23,27,31	0
2	ADP	C	600	27/27	0.99	0.09	-0.87	24,32,36,37	0
3	MG	B	601	1/1	1.00	0.12	-	20,20,20,20	0
3	MG	A	601	1/1	0.92	0.14	-	21,21,21,21	0
3	MG	C	601	1/1	0.99	0.13	-	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.