

Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2021 – 07:52 PM EDT

PDB ID	:	3EA5
Title	:	Kap95p Binding Induces the Switch Loops of RanGDP to adopt the GTP-
		bound Conformation: Implications for Nuclear Import Complex Assembly
		Dynamics
Authors	:	Forwood, J.K.; Lonhienne, J.K.; Guncar, G.; Stewart, M.; Marfori, M.; Kobe,
		В.
Deposited on	:	2008-08-24
Resolution	:	2.50 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 (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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.50 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	$\begin{array}{c} {\rm Whole \ archive} \\ (\#{\rm Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	А	216	7% 65% 13%	• 19%	-
1	С	216	16% 69% 9%	22%	_
2	В	861	83%	15%	•
2	D	861	16%	12%	•••

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
4	MG	А	222	-	-	Х	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16428 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 GTP-binding nuclear protein Ran.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	1 A	174	Total	С	Ν	0	\mathbf{S}	0	0	0
			1415	918	248	244	5	0		0
1	C	160	Total	С	Ν	0	S	0	0	0
	U	109	1377	895	242	236	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	181	CYS	ALA	engineered mutation	UNP P62826
С	181	CYS	ALA	engineered mutation	UNP P62826

• Molecule 2 is a protein called Importin subunit beta-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	859	Total 6642	C 4197	N 1099	O 1310	S 36	0	0	0
2	D	849	Total 6570	C 4157	N 1086	O 1291	S 36	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	254	LYS	LEU	engineered mutation	UNP Q06142
D	254	LYS	LEU	engineered mutation	UNP Q06142

• Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
2	3 A	٨	1	Total	С	Ν	Ο	Р	0	0
0		1	28	10	5	11	2	0	0	
2	C	1	Total	С	Ν	Ο	Р	0	0	
J	U	1	28	10	5	11	2	0	0	

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	2	Total Mg 2 2	0	0
4	С	2	Total Mg 2 2	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	68	Total O 68 68	0	0
5	В	178	Total O 178 178	0	0
5	С	34	$\begin{array}{cc} \text{Total} & \text{O} \\ 34 & 34 \end{array}$	0	0
5	D	84	Total O 84 84	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: GTP-binding nuclear protein Ran

I663 1510 A664 1510 A644 M224 A644 M224 A644 M224 A644 M224 A644 M224 A644 M224 A644 W224 A644 W224 A644 W224 A644 W235 A644 W235 A644 W235 A644 W236 A644 W236 A644 W236 A644 W356 A644 W366 A741 W564 M336 W564 M336 W564 M43 M664 M38 W564 M38 W564 M38 W564 M38 W564 M38 M364 M38 M364 M38 W564 M39 M660 M39</td

• Molecule 2: Importin subunit beta-1

16% Chain D: • • 85% 12% 0141 1142 A61 A62 L5 N6 T143 C163 E164 S165 ASP ASP ASP ASR ALA LEU LEU LEU SER SER SER 4242 4243 I 182 A 183 A244 E338 D339 P340 E341 D343 D343 D343 N346 N346 V347 S587 P588 //383 8384 1639 2640 1664 E853 Q854 Q855 K856 K856 L861



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	110.85Å 127.81Å 171.79Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	20.00 - 2.50	Depositor
Resolution (A)	19.99 - 2.50	EDS
% Data completeness	100.0 (20.00-2.50)	Depositor
(in resolution range)	$100.0 \ (19.99-2.50)$	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.78 (at 2.50 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
D D .	0.189 , 0.232	Depositor
n, n_{free}	0.193 , 0.233	DCC
R_{free} test set	4240 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	50.5	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.29, 54.9	EDS
L-test for $twinning^2$	$ < L >=0.51, < L^2>=0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16428	wwPDB-VP
Average B, all atoms $(Å^2)$	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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).

Mal	Mal Chain		Bond lengths		ond angles
1VIOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.72	0/1450	0.84	2/1958~(0.1%)
1	С	0.56	0/1411	0.72	2/1905~(0.1%)
2	В	0.61	1/6755~(0.0%)	0.67	1/9179~(0.0%)
2	D	0.52	0/6682	0.63	2/9079~(0.0%)
All	All	0.58	1/16298~(0.0%)	0.68	7/22121~(0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	247	CYS	CB-SG	-5.86	1.72	1.81

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	29	ARG	NE-CZ-NH2	-11.25	114.67	120.30
1	А	29	ARG	NE-CZ-NH1	10.12	125.36	120.30
2	D	577	LEU	CA-CB-CG	-6.73	99.81	115.30
2	В	577	LEU	CA-CB-CG	-6.28	100.87	115.30
1	С	29	ARG	NE-CZ-NH2	-5.98	117.31	120.30
2	D	800	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	С	29	ARG	NE-CZ-NH1	5.18	122.89	120.30

All (7) bond angle outliers are listed below:

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1415	0	1435	32	0
1	С	1377	0	1400	19	0
2	В	6642	0	6592	116	0
2	D	6570	0	6530	85	0
3	А	28	0	12	0	0
3	С	28	0	12	1	0
4	А	2	0	0	2	0
4	С	2	0	0	1	0
5	А	68	0	0	4	0
5	В	178	0	0	15	0
5	С	34	0	0	2	0
5	D	84	0	0	15	0
All	All	16428	0	15981	231	0

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.

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 7.

All (231) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:D:594:VAL:HG23	5:D:885:HOH:O	1.39	1.18
2:D:226:MET:HE1	2:D:251:ILE:HG21	1.19	1.14
2:B:226:MET:HE1	2:B:251:ILE:HG21	1.14	1.14
2:B:169:GLN:HE21	2:B:174:VAL:HG21	1.23	1.04
2:D:226:MET:CE	2:D:251:ILE:HG21	1.90	1.00
2:B:167:ASP:O	2:B:169:GLN:N	2.03	0.92
1:C:154:ASN:HD21	2:D:567:GLN:HE21	1.18	0.87
1:C:142:LYS:HE2	2:D:281:LYS:HZ3	1.40	0.86
2:D:371:LEU:O	5:D:926:HOH:O	1.93	0.85
1:C:29:ARG:HH11	2:D:567:GLN:HE22	1.21	0.85
2:B:257:THR:HG22	5:D:865:HOH:O	1.76	0.84
2:B:169:GLN:NE2	2:B:174:VAL:HG21	1.93	0.82
2:B:620:TYR:HE2	2:B:658:THR:HG21	1.46	0.81
2:B:639:THR:HG22	5:B:878:HOH:O	1.80	0.80
2:B:169:GLN:HE21	2:B:174:VAL:CG2	1.93	0.80
2:B:411:GLN:HG2	5:B:1000:HOH:O	1.82	0.79
2:D:742:GLU:HG2	5:D:921:HOH:O	1.83	0.79
2:B:140:VAL:HG21	2:B:178:ASN:HB3	1.64	0.79
4:A:222:MG:MG	5:A:224:HOH:O	1.27	0.78



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:169:GLN:NE2	2:B:174:VAL:HG11	1.99	0.78
5:B:863:HOH:O	2:D:838:GLN:HG3	1.84	0.77
1:C:141:LYS:HB2	1:C:144:LEU:HD12	1.66	0.76
2:B:169:GLN:HA	5:B:935:HOH:O	1.86	0.76
2:B:226:MET:CE	2:B:251:ILE:HG21	2.07	0.75
2:B:113:ASN:HD21	2:B:153:ARG:HH12	1.35	0.75
4:C:222:MG:MG	5:C:223:HOH:O	1.30	0.74
2:D:226:MET:HE1	2:D:251:ILE:HD13	1.69	0.74
2:D:374:VAL:HB	5:D:926:HOH:O	1.90	0.72
2:B:609:LYS:HD3	5:B:933:HOH:O	1.89	0.71
2:B:261:PRO:O	2:B:265:GLN:HG2	1.92	0.70
1:A:149:ILE:HD11	1:A:160:PRO:HG3	1.74	0.69
2:D:338:GLU:HG2	2:D:384:ARG:HH21	1.57	0.68
1:C:29:ARG:HH11	2:D:567:GLN:NE2	1.92	0.68
2:D:604:ARG:HD2	5:D:869:HOH:O	1.93	0.68
1:A:82:GLN:NE2	2:B:110:ARG:HH22	1.92	0.68
2:B:674:PHE:HB3	2:B:713:ILE:HD11	1.76	0.68
2:B:680:ALA:O	2:B:684:VAL:HG23	1.94	0.67
2:D:374:VAL:N	5:D:926:HOH:O	2.27	0.67
2:D:338:GLU:HG2	2:D:384:ARG:NH2	2.09	0.67
2:B:169:GLN:HG2	2:B:174:VAL:HG21	1.77	0.66
2:B:608:LYS:O	5:B:961:HOH:O	2.14	0.66
2:D:226:MET:HE1	2:D:251:ILE:CG2	2.11	0.66
2:D:508:ASN:OD1	2:D:549:LYS:NZ	2.28	0.65
2:D:691:ASN:HD22	2:D:693:ASN:H	1.44	0.65
4:A:222:MG:MG	5:A:223:HOH:O	1.40	0.64
2:B:169:GLN:HE21	2:B:174:VAL:HG11	1.62	0.64
2:D:113:ASN:HD21	2:D:153:ARG:HH12	1.45	0.64
2:B:577:LEU:HD13	2:B:614:ILE:HD11	1.78	0.64
1:A:154:ASN:HD21	2:B:567:GLN:HE21	1.44	0.64
2:B:729:VAL:HG22	2:B:778:THR:HG21	1.78	0.64
1:A:149:ILE:HD11	1:A:160:PRO:CG	2.28	0.64
1:C:154:ASN:HD21	2:D:567:GLN:NE2	1.94	0.64
3:C:220:GDP:O1B	5:C:223:HOH:O	2.15	0.63
2:D:371:LEU:C	5:D:926:HOH:O	2.35	0.63
2:D:588:PRO:C	2:D:590:SER:H	1.99	0.63
1:A:159:LYS:NZ	5:A:281:HOH:O	2.31	0.62
2:B:108:GLU:HG3	5:B:905:HOH:O	1.99	0.61
2:D:658:THR:HG22	5:D:890:HOH:O	2.00	0.61
2:D:66:LYS:HE3	2:D:67:ASN:OD1	2.00	0.61
2:D:1:MET:N	5:D:872:HOH:O	2.34	0.60



A is a set of the set	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:281:LYS:O	2:B:285:MET:HG3	2.02	0.60
2:B:738:ASN:HD22	2:B:739:GLY:N	2.00	0.60
2:D:691:ASN:ND2	2:D:693:ASN:H	2.00	0.59
1:A:29:ARG:HH11	2:B:567:GLN:HE22	1.49	0.59
2:B:420:MET:HG3	2:B:458:ALA:HB1	1.83	0.59
2:B:729:VAL:HG22	2:B:778:THR:CG2	2.33	0.59
2:B:226:MET:CE	2:B:251:ILE:HD13	2.33	0.59
2:B:346:ASN:ND2	2:B:348:SER:OG	2.35	0.59
2:B:786:VAL:O	2:B:793:TYR:HB3	2.03	0.59
2:D:281:LYS:O	2:D:285:MET:HG3	2.03	0.58
2:B:66:LYS:HE3	2:B:67:ASN:OD1	2.02	0.58
2:D:261:PRO:O	2:D:265:GLN:HG2	2.04	0.58
2:D:738:ASN:HD22	2:D:739:GLY:N	2.00	0.57
2:D:346:ASN:ND2	2:D:348:SER:OG	2.37	0.57
1:A:136:ILE:HD13	1:A:146:TYR:CZ	2.39	0.57
2:B:609:LYS:O	2:B:610:ASP:HB2	2.03	0.57
2:B:691:ASN:ND2	2:B:693:ASN:H	2.02	0.57
2:D:226:MET:CE	2:D:251:ILE:HD13	2.35	0.57
1:A:91:ASP:OD1	1:A:93:THR:HB	2.06	0.56
2:B:275:MET:HA	2:B:286:THR:HG21	1.88	0.56
1:C:142:LYS:HE2	2:D:281:LYS:NZ	2.18	0.56
2:D:275:MET:HA	2:D:286:THR:HG21	1.88	0.56
2:B:283:ALA:O	2:B:286:THR:HG22	2.05	0.55
2:D:577:LEU:HD13	2:D:614:ILE:HD11	1.88	0.55
2:D:609:LYS:O	2:D:610:ASP:HB2	2.06	0.55
2:B:169:GLN:CG	2:B:174:VAL:HG21	2.36	0.55
2:D:786:VAL:O	2:D:793:TYR:HB3	2.06	0.55
2:B:169:GLN:HE21	2:B:174:VAL:CG1	2.20	0.55
2:B:691:ASN:C	2:B:691:ASN:HD22	2.10	0.55
1:C:53:HIS:O	1:C:176:PHE:O	2.25	0.54
2:D:382:ASN:HD22	2:D:383:TRP:N	2.05	0.54
2:D:163:CYS:SG	2:D:180:ILE:HG21	2.48	0.54
2:D:803:VAL:HG12	2:D:847:THR:HG22	1.89	0.53
2:B:169:GLN:HE21	2:B:174:VAL:CB	2.21	0.53
1:A:77:ASP:OD2	2:B:66:LYS:NZ	2.41	0.53
2:B:382:ASN:HD22	2:B:383:TRP:N	2.06	0.53
2:D:234:GLN:NE2	2:D:270:LEU:HD13	2.23	0.53
1:A:142:LYS:CE	2:B:281:LYS:HD3	2.39	0.53
2:B:729:VAL:CG2	2:B:778:THR:HG21	2.39	0.53
1:A:56:ARG:NH1	1:A:171:ASP:OD2	2.42	0.53
2:B:554:MET:CE	2:B:601:LEU:HD22	2.38	0.53



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:664:ALA:HB2	2:B:705:VAL:HG23	1.91	0.53
1:C:142:LYS:CE	2:D:281:LYS:HZ3	2.17	0.53
2:B:620:TYR:CE2	2:B:658:THR:HG21	2.35	0.52
2:D:632:GLY:N	5:D:877:HOH:O	2.42	0.52
2:B:738:ASN:ND2	2:B:740:THR:OG1	2.42	0.52
1:A:71:LYS:HB3	1:A:71:LYS:HZ3	1.75	0.52
2:B:837:GLY:N	5:B:996:HOH:O	2.39	0.52
2:B:78:GLN:NE2	5:B:1013:HOH:O	2.18	0.52
1:A:142:LYS:HE2	2:B:281:LYS:HD3	1.92	0.52
1:A:71:LYS:CB	1:A:71:LYS:NZ	2.73	0.51
2:B:288:GLU:OE1	5:B:906:HOH:O	2.19	0.51
2:B:546:VAL:HB	2:B:576:ILE:HG23	1.92	0.51
2:D:680:ALA:O	2:D:684:VAL:HG23	2.10	0.51
2:D:420:MET:HG3	2:D:458:ALA:HB1	1.93	0.51
1:A:133:ALA:HA	1:A:136:ILE:HD12	1.93	0.51
1:A:12:LYS:HE3	1:A:64:TRP:CE2	2.47	0.50
1:A:82:GLN:NE2	2:B:110:ARG:NH2	2.58	0.50
2:B:531:ALA:O	2:B:586:LYS:HE2	2.11	0.50
2:B:691:ASN:HD22	2:B:693:ASN:H	1.58	0.50
2:D:691:ASN:HD22	2:D:691:ASN:C	2.15	0.50
2:B:382:ASN:ND2	2:B:384:ARG:H	2.09	0.50
2:D:664:ALA:HB2	2:D:705:VAL:HG23	1.94	0.50
2:B:171:GLN:O	2:B:174:VAL:N	2.45	0.49
2:B:803:VAL:HG11	2:B:848:ALA:HA	1.94	0.49
2:D:48:LEU:HD13	2:D:62:ALA:HB2	1.94	0.49
2:B:205:LEU:HD11	2:B:225:LEU:HD11	1.93	0.49
2:B:549:LYS:O	2:B:553:THR:HG23	2.12	0.49
1:A:154:ASN:HD21	2:B:567:GLN:NE2	2.10	0.49
2:B:303:GLU:OE2	2:D:303:GLU:OE2	2.30	0.49
1:C:12:LYS:HE3	1:C:64:TRP:CE2	2.48	0.48
2:D:283:ALA:O	2:D:286:THR:HG22	2.13	0.48
2:B:161:TYR:O	2:B:165:SER:HB2	2.13	0.48
1:A:71:LYS:HB3	1:A:71:LYS:NZ	2.28	0.48
2:B:411:GLN:CG	5:B:1000:HOH:O	2.49	0.48
2:D:346:ASN:HD22	2:D:348:SER:H	1.59	0.48
1:A:26:PHE:CE1	1:A:30:HIS:HE1	2.31	0.48
2:D:738:ASN:ND2	2:D:740:THR:OG1	2.45	0.48
2:B:226:MET:HE1	2:B:251:ILE:HD13	1.96	0.48
1:A:112:CYS:O	1:A:113:GLU:C	2.51	0.48
2:B:108:GLU:HB3	2:B:111:ILE:HD12	1.96	0.48
2:B:679:ASP:HB3	5:B:899:HOH:O	2.14	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:176:PHE:O	1:C:177:VAL:C	2.51	0.47
1:C:118:VAL:HG23	1:C:164:LEU:HD21	1.96	0.47
1:A:120:CYS:SG	1:A:149:ILE:HD13	2.54	0.47
1:A:141:LYS:HB2	1:A:144:LEU:HD12	1.96	0.47
2:B:592:GLU:N	2:B:593:PRO:HD2	2.28	0.47
1:A:120:CYS:SG	1:A:149:ILE:CD1	3.02	0.47
2:D:658:THR:CG2	5:D:890:HOH:O	2.62	0.47
2:B:346:ASN:HD22	2:B:348:SER:H	1.61	0.47
2:B:275:MET:CA	2:B:286:THR:HG21	2.45	0.47
2:B:656:SER:OG	2:B:698:LEU:HD21	2.15	0.47
2:D:592:GLU:N	2:D:593:PRO:HD2	2.29	0.47
2:D:159:LEU:HD22	2:D:180:ILE:HG23	1.98	0.46
2:D:729:VAL:HG22	2:D:778:THR:HG21	1.97	0.46
2:B:226:MET:HE2	2:B:251:ILE:HD13	1.97	0.46
2:B:382:ASN:HD22	2:B:382:ASN:C	2.19	0.46
2:D:674:PHE:HB3	2:D:713:ILE:HD11	1.96	0.46
1:C:141:LYS:HB2	1:C:144:LEU:CD1	2.40	0.46
2:D:274:THR:HG23	2:D:282:VAL:CG1	2.45	0.46
1:C:142:LYS:HZ1	2:D:281:LYS:HD3	1.80	0.46
1:A:92:VAL:HG13	1:A:129:ARG:HB3	1.97	0.46
1:C:142:LYS:NZ	2:D:281:LYS:NZ	2.64	0.46
1:C:14:VAL:HG11	1:C:80:TYR:HA	1.98	0.45
2:B:837:GLY:CA	5:B:996:HOH:O	2.63	0.45
2:D:374:VAL:CA	5:D:926:HOH:O	2.64	0.45
2:D:126:GLU:OE1	2:D:132:TRP:HB2	2.17	0.45
1:A:82:GLN:HE21	2:B:110:ARG:HH12	1.65	0.44
2:D:606:LEU:HB3	2:D:643:TYR:CZ	2.52	0.44
2:B:180:ILE:HD12	5:B:980:HOH:O	2.15	0.44
2:B:363:GLY:O	2:B:366:ILE:HG22	2.17	0.44
2:B:674:PHE:HB3	2:B:713:ILE:CD1	2.46	0.44
1:A:29:ARG:HH11	2:B:567:GLN:NE2	2.14	0.44
1:A:136:ILE:HD13	1:A:146:TYR:CE2	2.52	0.44
2:B:803:VAL:CG1	2:B:848:ALA:HA	2.46	0.44
1:A:140:ARG:HG2	2:B:345:TRP:NE1	2.33	0.44
2:B:260:LYS:HB3	2:B:261:PRO:HD3	1.99	0.44
2:B:510:ILE:HG22	2:B:510:ILE:O	2.16	0.44
2:D:275:MET:CA	2:D:286:THR:HG21	2.48	0.44
2:D:762:VAL:HG21	2:D:805:LEU:HD22	2.00	0.44
2:B:274:THR:HG23	2:B:282:VAL:HG12	1.99	0.44
2:B:48:LEU:HD13	2:B:62:ALA:HB2	2.00	0.43
2:B:800:ARG:HD3	2:B:844:THR:HA	1.99	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:142:LYS:CE	2:D:281:LYS:NZ	2.78	0.43
2:D:382:ASN:HD22	2:D:382:ASN:C	2.21	0.43
2:D:117:GLN:NE2	5:D:912:HOH:O	2.49	0.43
2:B:462:GLY:HA3	2:B:473:CYS:SG	2.58	0.43
2:D:606:LEU:HB3	2:D:643:TYR:CE1	2.54	0.43
2:B:169:GLN:O	2:B:170:SER:CB	2.66	0.43
2:B:170:SER:HA	5:B:1023:HOH:O	2.19	0.43
2:D:729:VAL:HG22	2:D:778:THR:CG2	2.49	0.43
2:B:181:LEU:HD23	2:B:181:LEU:C	2.39	0.42
1:A:139:HIS:HB2	1:A:145:GLN:HA	2.01	0.42
2:B:167:ASP:O	2:B:169:GLN:CA	2.65	0.42
2:B:346:ASN:HD22	2:B:348:SER:N	2.17	0.42
2:D:346:ASN:HD22	2:D:348:SER:N	2.16	0.42
1:A:82:GLN:HE22	2:B:110:ARG:NH2	2.17	0.42
2:B:835:ARG:NH1	2:B:849:ARG:HG3	2.33	0.42
2:D:10:LEU:HD13	2:D:61:ALA:HB2	2.00	0.42
1:C:122:ASN:OD1	1:C:149:ILE:HG22	2.19	0.42
2:D:577:LEU:HD13	2:D:614:ILE:CD1	2.49	0.42
2:B:209:LEU:O	2:B:255:TYR:OH	2.30	0.42
2:B:738:ASN:ND2	2:B:743:ALA:CB	2.82	0.42
2:B:592:GLU:HG3	2:B:593:PRO:CD	2.50	0.42
2:D:588:PRO:C	2:D:590:SER:N	2.69	0.42
2:D:374:VAL:CB	5:D:926:HOH:O	2.60	0.42
2:D:549:LYS:O	2:D:553:THR:HG23	2.20	0.42
1:A:142:LYS:NZ	2:B:281:LYS:HD3	2.35	0.42
2:B:10:LEU:HD13	2:B:61:ALA:HB2	2.01	0.42
2:B:274:THR:HG23	2:B:282:VAL:CG1	2.50	0.42
2:D:592:GLU:HG3	2:D:593:PRO:CD	2.50	0.42
2:D:748:ILE:HD13	2:D:791:GLN:HG2	2.02	0.41
2:B:97:LYS:CE	2:B:126:GLU:OE1	2.69	0.41
2:B:181:LEU:HD12	2:B:212:ILE:HD12	2.01	0.41
2:B:695:ARG:HG2	2:B:698:LEU:HD23	2.02	0.41
2:D:242:ALA:HA	2:D:285:MET:SD	2.60	0.41
2:D:750:VAL:O	2:D:754:VAL:HG23	2.21	0.41
2:D:810:ALA:HB2	2:D:822:TYR:CZ	2.55	0.41
2:B:592:GLU:HG3	2:B:593:PRO:HD3	2.02	0.41
2:B:691:ASN:HD22	2:B:692:PRO:N	2.19	0.41
2:D:709:ILE:O	2:D:713:ILE:HB	2.21	0.41
5:A:254:HOH:O	2:B:563:LEU:HD22	2.20	0.41
2:B:554:MET:CE	2:B:601:LEU:CD2	2.99	0.41
2:D:525:THR:HG23	2:D:582:ALA:HB2	2.01	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:679:ASP:CG	2:B:720:TYR:HH	2.24	0.40
2:B:699:LYS:HB3	2:B:700:PRO:CD	2.51	0.40
2:D:66:LYS:HE2	2:D:66:LYS:HB3	1.94	0.40
2:B:158:ALA:O	2:B:162:MET:HB2	2.21	0.40
2:B:322:ILE:O	2:B:323:LYS:C	2.60	0.40
2:B:698:LEU:HA	2:B:698:LEU:HD13	1.88	0.40
1:C:142:LYS:NZ	2:D:281:LYS:HZ2	2.20	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	Perce	entiles
1	А	172/216~(80%)	166 (96%)	6 (4%)	0	100	100
1	С	167/216~(77%)	160 (96%)	7 (4%)	0	100	100
2	В	855/861~(99%)	827~(97%)	25~(3%)	3~(0%)	34	54
2	D	845/861~(98%)	821 (97%)	22 (3%)	2(0%)	47	68
All	All	2039/2154~(95%)	1974 (97%)	60 (3%)	5 (0%)	47	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	168	PRO
2	В	169	GLN
2	В	170	SER
2	D	266	ALA
2	D	589	SER



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	153/186~(82%)	144 (94%)	9~(6%)	19	37	
1	С	149/186~(80%)	142 (95%)	7 (5%)	26	49	
2	В	725/726~(100%)	680 (94%)	45~(6%)	18	35	
2	D	715/726~(98%)	668~(93%)	47 (7%)	16	32	
All	All	1742/1824~(96%)	1634 (94%)	108 (6%)	18	35	

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	29	ARG
1	А	43	LEU
1	А	71	LYS
1	А	92	VAL
1	А	93	THR
1	А	95	ARG
1	А	114	ASN
1	А	134	LYS
1	А	149	ILE
2	В	19	GLN
2	В	32	LEU
2	В	34	ASN
2	В	55	LEU
2	В	66	LYS
2	В	70	VAL
2	В	132	TRP
2	В	164	GLU
2	В	165	SER
2	В	178	ASN
2	В	227	GLN
2	В	238	ILE
2	В	254	LYS
2	В	270	LEU
2	В	295	GLU



Mol	Chain	Res	Type
2	В	319	LEU
2	В	346	ASN
2	В	382	ASN
2	В	390	VAL
2	В	415	SER
2	В	442	VAL
2	В	488	THR
2	В	496	TYR
2	В	501	ASP
2	В	560	GLN
2	В	564	GLU
2	В	568	SER
2	В	577	LEU
2	В	592	GLU
2	В	598	LEU
2	В	609	LYS
2	В	610	ASP
2	В	639	THR
2	В	658	THR
2	В	683	ASN
2	В	691	ASN
2	В	705	VAL
2	В	713	ILE
2	В	738	ASN
2	В	740	THR
2	В	755	LEU
2	В	791	GLN
2	В	835	ARG
2	В	836	SER
2	В	838	GLN
1	С	29	ARG
1	С	43	LEU
1	С	71	LYS
1	С	92	VAL
1	С	96	VAL
1	С	149	ILE
1	С	159	LYS
2	D	19	GLN
2	D	32	LEU
2	D	34	ASN
2	D	55	LEU
2	D	66	LYS



N/L - 1		D	T
WIOI	Chain	Res	Type
2	D	70	VAL
2	D	132	TRP
2	D	164	GLU
2	D	165	SER
2	D	190	SER
2	D	227	GLN
2	D	238	ILE
2	D	254	LYS
2	D	270	LEU
2	D	294	CYS
2	D	295	GLU
2	D	319	LEU
2	D	346	ASN
2	D	382	ASN
2	D	390	VAL
2	D	415	SER
2	D	442	VAL
2	D	488	THR
2	D	496	TYR
2	D	501	ASP
2	D	560	GLN
2	D	568	SER
2	D	577	LEU
2	D	589	SER
2	D	592	GLU
2	D	594	VAL
2	D	598	LEU
2	D	609	LYS
2	D	610	ASP
2	D	639	THR
2	D	658	THR
2	D	683	ASN
2	D	691	ASN
2	D	705	VAL
2	D	711	SER
2	D	713	ILE
2	D	738	ASN
2	D	740	THR
2	D	791	GLN
2	D	836	SER
2	D	850	TRP
2	D	855	GLN
	1	-	1

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	69	GLN
1	А	82	GLN
1	А	100	ASN
1	А	114	ASN
2	В	79	GLN
2	В	113	ASN
2	В	169	GLN
2	В	215	ASN
2	В	306	GLN
2	В	346	ASN
2	В	376	GLN
2	В	382	ASN
2	В	385	ASN
2	В	423	GLN
2	В	567	GLN
2	В	649	ASN
2	В	691	ASN
2	В	712	ASN
2	В	738	ASN
2	В	785	GLN
2	В	838	GLN
1	С	82	GLN
1	С	100	ASN
2	D	79	GLN
2	D	113	ASN
2	D	215	ASN
2	D	234	GLN
2	D	346	ASN
2	D	376	GLN
2	D	382	ASN
2	D	385	ASN
2	D	423	GLN
2	D	567	GLN
2	D	649	ASN
2	D	691	ASN
2	D	712	ASN
2	D	738	ASN
2	D	785	GLN
2	D	838	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	Turne	Chain Bos		Tink	Bond lengths				Bond angles		
WIOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	GDP	С	220	4	24,30,30	1.16	2 (8%)	31,47,47	2.00	7 (22%)	
3	GDP	А	220	4	24,30,30	0.98	2 (8%)	31,47,47	1.88	8 (25%)	

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
3	GDP	С	220	4	-	6/12/32/32	0/3/3/3
3	GDP	А	220	4	-	4/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
3	С	220	GDP	C6-C5	3.50	1.47	1.41



001000	Continued from prettods page								
Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$		
3	А	220	GDP	C6-C5	2.54	1.45	1.41		
3	С	220	GDP	C5-C4	2.30	1.47	1.40		
3	A	220	GDP	C5-C4	2.09	1.46	1.40		

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	С	220	GDP	C5-C6-N1	-5.88	115.39	123.43
3	А	220	GDP	C5-C6-N1	-5.48	115.94	123.43
3	С	220	GDP	C6-N1-C2	5.01	123.89	115.93
3	А	220	GDP	C6-N1-C2	4.52	123.12	115.93
3	С	220	GDP	PA-O3A-PB	-3.69	120.16	132.83
3	А	220	GDP	C6-C5-C4	-3.19	117.75	120.80
3	С	220	GDP	C6-C5-C4	-3.16	117.78	120.80
3	А	220	GDP	PA-O3A-PB	-2.95	122.71	132.83
3	С	220	GDP	N3-C2-N1	-2.73	123.59	127.22
3	С	220	GDP	C4-C5-N7	-2.64	106.65	109.40
3	С	220	GDP	C2-N3-C4	2.57	118.29	115.36
3	А	220	GDP	O2B-PB-O3A	2.48	112.96	104.64
3	А	220	GDP	N2-C2-N1	2.32	120.87	117.25
3	А	220	GDP	C2-N3-C4	2.29	117.97	115.36
3	А	220	GDP	N2-C2-N3	-2.06	114.44	117.79

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	220	GDP	PA-O3A-PB-O2B
3	С	220	GDP	PA-O3A-PB-O3B
3	С	220	GDP	C5'-O5'-PA-O1A
3	А	220	GDP	O4'-C4'-C5'-O5'
3	С	220	GDP	O4'-C4'-C5'-O5'
3	С	220	GDP	C5'-O5'-PA-O3A
3	С	220	GDP	C3'-C4'-C5'-O5'
3	А	220	GDP	PA-O3A-PB-O1B
3	С	220	GDP	PA-O3A-PB-O2B
3	А	220	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	220	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 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	А	174/216~(80%)	0.55	15 (8%) 10 10	52, 62, 88, 121	0
1	С	169/216~(78%)	1.08	34 (20%) 1 0	55, 65, 93, 111	0
2	В	859/861~(99%)	0.61	57 (6%) 18 19	51, 65, 83, 110	0
2	D	849/861 (98%)	0.98	134 (15%) 2 1	53, 67, 82, 99	0
All	All	2051/2154~(95%)	0.80	240 (11%) 4 4	51, 66, 84, 121	0

All (240) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	С	142	LYS	10.0
1	С	138	PHE	8.0
2	В	861	LEU	7.6
1	С	127	LYS	7.0
2	В	488	THR	6.7
2	D	128	PRO	6.1
1	С	143	ASN	5.8
2	D	861	LEU	5.7
2	В	692	PRO	5.7
2	D	639	THR	5.6
1	А	179	MET	5.4
2	D	166	ALA	5.4
2	D	591	VAL	5.4
1	С	141	LYS	5.3
2	D	839	LEU	5.3
2	D	559	ASN	5.2
2	D	587	SER	5.0
2	В	836	SER	4.9
2	D	741	LEU	4.8
1	С	139	HIS	4.7
2	D	340	PRO	4.5

3EA5

Mol	Chain	Res	Type	RSRZ
2	D	663	ILE	4.5
2	D	560	GLN	4.5
2	D	156	LEU	4.5
2	D	140	VAL	4.5
2	D	149	GLU	4.4
2	D	449	GLN	4.4
2	D	737	GLU	4.3
2	D	107	ILE	4.3
2	В	302	TYR	4.2
1	С	134	LYS	4.2
2	D	441	SER	4.2
2	D	825	ASP	4.2
1	A	142	LYS	4.1
2	D	137	LYS	4.0
2	D	488	THR	4.0
2	D	191	THR	4.0
2	D	236	GLU	3.9
2	D	320	SER	3.9
2	В	477	ILE	3.9
2	В	167	ASP	3.9
2	В	489	PRO	3.8
2	D	341	GLU	3.8
2	В	168	PRO	3.8
2	D	237	ASP	3.8
2	D	94	ASN	3.8
2	D	338	GLU	3.7
2	D	767	ASP	3.7
2	В	4	ALA	3.7
1	С	144	LEU	3.6
1	С	89	MET	3.6
1	С	72	PHE	3.6
2	В	535	VAL	3.6
2	B	837	GLY	3.6
2	D	210	ILE	3.6
1	C	87	ILE	3.5
2	D	75	VAL	3.5
2	D	489	PRO	3.5
2	D	662	PHE	3.4
2	D	634	GLU	3.4
2	D	514	PHE	3.4
2	D	713	ILE	3.4
2	D	61	ALA	3.4

Mol	Chain	Res	Type	RSRZ
1	А	89	MET	3.3
2	D	184	ILE	3.3
2	D	330	LEU	3.3
2	D	768	LYS	3.3
2	В	783	ILE	3.3
2	D	486	GLU	3.3
2	В	737	GLU	3.3
1	С	90	PHE	3.3
2	В	802	ALA	3.2
2	D	806	ILE	3.2
1	С	120	CYS	3.2
1	С	9	VAL	3.2
1	С	131	VAL	3.2
2	В	527	MET	3.2
2	D	79	GLN	3.2
1	С	114	ASN	3.2
2	В	838	GLN	3.2
2	D	20	ASN	3.2
2	D	822	TYR	3.1
2	D	745	ASP	3.1
2	D	74	SER	3.1
2	D	766	HIS	3.1
1	С	136	ILE	3.1
1	А	173	ASN	3.1
2	В	449	GLN	3.1
2	D	592	GLU	3.1
2	D	696	ARG	3.1
2	D	305	ALA	3.1
2	D	638	GLU	3.0
2	D	676	ARG	3.0
1	А	164	LEU	3.0
2	D	165	SER	3.0
2	В	663	ILE	3.0
2	D	666	ILE	3.0
1	С	164	LEU	3.0
2	D	143	THR	3.0
1	С	16	VAL	2.9
1	A	90	PHE	2.9
2	D	205	LEU	2.9
2	D	19	GLN	2.9
2	D	610	ASP	2.9
2	D	632	GLY	2.9

3EA	15

Mol	Chain	Res	Type	RSRZ
2	D	736	PRO	2.9
2	D	10	LEU	2.9
2	В	533	ASP	2.8
2	В	693	ASN	2.8
2	D	742	GLU	2.8
1	С	60	LYS	2.8
2	В	175	SER	2.8
2	В	803	VAL	2.8
2	D	423	GLN	2.8
1	А	134	LYS	2.8
2	D	594	VAL	2.8
1	С	126	ILE	2.8
2	В	650	GLN	2.8
2	D	609	LYS	2.8
2	D	835	ARG	2.8
2	D	640	PHE	2.7
2	D	849	ARG	2.7
1	А	133	ALA	2.7
2	В	193	THR	2.7
1	А	75	LEU	2.7
2	В	670	LEU	2.7
2	В	171	GLN	2.7
2	D	163	CYS	2.7
2	D	189	GLN	2.7
2	D	193	THR	2.7
2	D	329	LEU	2.6
2	D	17	PRO	2.6
1	С	71	LYS	2.6
2	D	179	ASN	2.6
2	В	825	ASP	2.6
2	D	649	ASN	2.6
2	В	815	ASP	2.6
2	В	652	ASP	2.6
2	D	576	ILE	2.6
2	D	78	GLN	2.6
2	D	154	ALA	2.6
2	D	23	LEU	2.5
2	D	828	ILE	2.5
1	А	6	GLU	2.5
2	D	82	GLN	2.5
2	D	141	ASP	2.5
2	D	5	GLU	2.5

3EA5

Mol	Chain	Res	Type	RSRZ
2	D	238	ILE	2.5
2	D	821	PHE	2.5
1	А	118	VAL	2.5
2	В	366	ILE	2.5
2	D	302	TYR	2.5
2	В	265	GLN	2.5
2	В	559	ASN	2.5
1	А	120	CYS	2.4
2	D	690	SER	2.4
2	D	136	MET	2.4
2	D	438	ILE	2.4
1	С	31	LEU	2.4
2	В	326	VAL	2.4
2	В	286	THR	2.4
2	В	44	SER	2.4
1	С	55	ASN	2.4
2	В	806	ILE	2.4
2	D	631	LYS	2.3
2	D	644	LEU	2.3
2	D	344	ASP	2.3
2	D	337	ASN	2.3
2	В	340	PRO	2.3
2	D	155	SER	2.3
2	D	264	GLU	2.3
2	D	343	ASP	2.3
2	D	533	ASP	2.3
2	D	791	GLN	2.3
2	D	803	VAL	2.3
1	С	88	ILE	2.3
1	С	130	LYS	2.3
1	С	70	GLU	2.3
2	D	146	GLU	2.3
2	D	738	ASN	2.3
1	C	42	THR	2.3
2	D	534	THR	2.3
2	D	734	THR	2.3
1	С	128	ASP	2.2
2	D	590	SER	2.2
2	D	853	GLU	2.2
2	D	838	GLN	2.2
1	C	109	VAL	2.2
2	В	305	ALA	2.2

Mol	Chain	Res	Type	RSRZ	
2	В	735	LYS	2.2	
2	В	338	GLU	2.2	
2	D	850	TRP	2.2	
2	D	715	ALA	2.2	
2	В	10	LEU	2.2	
2	D	195 LYS		2.2	
2	D	31	LYS	2.2	
2	D	556	VAL	2.2	
2	D	182	ILE	2.2	
2	В	330	LEU	2.2	
2	В	459	CYS	2.2	
2	D	843	ALA	2.1	
2	В	355	LEU	2.1	
2	D	73	ASP	2.1	
1	А	57	GLY	2.1	
2	В	850	TRP	2.1	
2	D	809	ILE	2.1	
2	В	156	LEU	2.1	
2	D	319	LEU	2.1	
2	D	628	SER	2.1	
2	В	169	GLN	2.1	
2	В	396	ILE	2.1	
2	В	524	LEU	2.1	
1	А	88	ILE	2.1	
2	D	561	LEU	2.1	
2	В	283	ALA	2.1	
2	В	591	VAL	2.1	
2	В	741	LEU	2.1	
2	D	817	SER	2.1	
2	D	34	ASN	2.1	
2	D	475	TRP	2.1	
2	D	54	LYS	2.1	
2	D	244	ALA	2.1	
2	D	743	ALA	2.1	
2	В	367	LEU	2.1	
2	D	211	PHE	2.1	
2	D	813	PHE	2.1	
2	D	294	CYS	2.1	
1	С	23	LYS	2.1	
2	В	177	SER	2.0	
1	С	22	GLY	2.0	
2	D	358	PHE	2.0	

Mol	Chain	Res	Type	RSRZ
2	В	528	VAL	2.0
2	В	155	SER	2.0
2	D	831	ILE	2.0
1	С	54	THR	2.0
2	D	362	CYS	2.0
1	С	177	VAL	2.0
2	D	190	SER	2.0
1	А	87	ILE	2.0
2	D	856	LYS	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 monosaccharides 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, 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	MG	С	221	1/1	0.94	0.09	$55,\!55,\!55,\!55$	0
4	MG	А	221	1/1	0.97	0.05	43,43,43,43	0
3	GDP	С	220	28/28	0.97	0.14	53,58,61,61	0
3	GDP	А	220	28/28	0.98	0.12	42,49,53,54	0
4	MG	С	222	1/1	0.98	0.05	58,58,58,58	0
4	MG	А	222	1/1	1.00	0.05	$55,\!55,\!55,\!55$	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

6.5 Other polymers (i)

There are no such residues in this entry.

