

Full wwPDB X-ray Structure Validation Report (i)

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:	8SSN
:	Abl kinase in complex with SKI and asciminib
:	Ludewig, H.; Kim, C.; Kern, D.
:	2023-05-08
:	2.86 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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	:	2.35
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)	:	2.35

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 2.86 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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							
			26%							
1	А	448		62%		29%		• 6%		
			29%							
1	В	448		62%		22%	•	14%		

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
3	SKI	В	602	-	-	-	Х
5	SO4	В	603	-	-	-	Х



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6667 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 Tyrosine-protein kinase ABL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	420	Total 3367	C 2147	N 568	O 635	S 17	0	0	0
1	В	386	Total 3099	C 1977	N 526	O 582	S 14	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	82	GLY	-	expression tag	UNP P00519
В	82	GLY	-	expression tag	UNP P00519

• Molecule 2 is asciminib (three-letter code: AY7) (formula: $C_{20}H_{18}ClF_2N_5O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	А	1	Total 31	C 20	Cl 1	F 2	N 5	O 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	В	1	Total 31	C 20	Cl 1	F 2	N 5	O 3	0	0

• Molecule 3 is 6,7-dimethoxy-N-(4-phenoxyphenyl)quinazolin-4-amine (three-letter code: SKI) (formula: $C_{22}H_{19}N_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	A	ton	ıs		ZeroOcc	AltConf
3	А	1	Total 28	C 22	N 3	O 3	0	0
3	В	1	Total 28	C 22	N 3	O 3	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: $\rm C_2H_6OS).$



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
6	А	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	0 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	А	1	Total 4	${ m C} 2$	0 1	S 1	0	0
6	А	1	Total 4	C 2	0 1	S 1	0	0
6	В	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	0 1	S 1	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	23	TotalO2323	0	0
7	В	28	TotalO2828	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: Tyrosine-protein kinase ABL1

 \bullet Molecule 1: Tyrosine-protein kinase ABL1







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	92.48Å 103.21Å 107.96Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	47.83 - 2.86	Depositor
Resolution (A)	47.83 - 2.86	EDS
% Data completeness	98.3 (47.83-2.86)	Depositor
(in resolution range)	81.1 (47.83-2.86)	EDS
R _{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.21 (at 2.86 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
D D.	0.298 , 0.348	Depositor
Π, Π_{free}	0.297 , 0.350	DCC
R_{free} test set	1189 reflections (4.87%)	wwPDB-VP
Wilson B-factor $(Å^2)$	59.5	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.35, 94.0	EDS
L-test for $twinning^2$	$< L >=0.46, < L^2>=0.29$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6667	wwPDB-VP
Average B, all atoms $(Å^2)$	93.0	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 56.63 % 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 2.6637e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: AY7, CL, SKI, DMS, SO4

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	Chain	Bond lengths		Bond angles	
1VIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.32	0/3448	0.55	1/4669~(0.0%)
1	В	0.34	0/3171	0.51	0/4289
All	All	0.33	0/6619	0.53	1/8958~(0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	381	ARG	CB-CA-C	-5.10	100.19	110.40

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 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	А	3367	0	3282	102	0
1	В	3099	0	3010	62	0
2	А	31	0	0	0	0
2	В	31	0	0	1	0
3	А	28	0	0	0	0
3	В	28	0	0	1	0
4	А	1	0	0	0	0
5	А	10	0	0	0	0



$j \cdots j \cdots$								
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
5	В	5	0	0	0	0		
6	А	12	0	18	0	0		
6	В	4	0	6	0	0		
7	А	23	0	0	1	0		
7	В	28	0	0	0	0		
All	All	6667	0	6316	164	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 13.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 9	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:264:LYS:HD2	1:A:279:VAL:HG23	1.44	0.96
1:A:379:ILE:HD11	1:A:381:ARG:HH21	1.39	0.88
1:A:453:THR:HB	1:A:456:MET:HG3	1.68	0.76
1:B:159:LEU:HD21	1:B:239:ARG:HB3	1.68	0.75
1:A:96:ASP:OD1	1:A:97:ASN:N	2.20	0.75
1:A:297:MET:SD	1:A:297:MET:N	2.61	0.73
1:A:324:CYS:HB3	1:A:331:TYR:HB2	1.67	0.73
1:B:313:LYS:N	1:B:372:TYR:HH	1.86	0.72
1:A:261:ILE:HG22	1:A:262:THR:H	1.52	0.72
1:B:427:PRO:HB2	1:B:497:TRP:CH2	2.28	0.69
1:A:140:SER:HB2	1:A:142:GLU:OE1	1.93	0.69
1:B:453:THR:HB	1:B:456:MET:HG3	1.76	0.68
1:A:223:THR:HG22	1:A:224:VAL:HG13	1.77	0.66
1:A:172:GLU:HG3	1:A:180:ARG:HE	1.60	0.66
1:B:122:GLN:HB2	1:B:127:GLN:HG2	1.79	0.65
1:A:141:LEU:HD11	1:A:214:LEU:HB3	1.79	0.64
1:A:428:GLU:HG3	1:A:434:LYS:HD2	1.80	0.64
1:B:459:TYR:H	1:B:477:MET:HE2	1.63	0.63
1:A:360:LEU:HD12	1:A:521:ILE:HD12	1.79	0.63
1:B:277:GLU:HG3	1:B:336:PHE:HE2	1.64	0.63
1:B:180:ARG:HB3	1:B:195:ILE:HD12	1.80	0.63
1:B:354:VAL:HG13	1:B:358:VAL:HG11	1.83	0.61
1:A:264:LYS:HB2	1:A:277:GLU:HG3	1.82	0.61
1:A:317:LEU:HD11	1:A:373:LEU:HG	1.82	0.61
1:B:239:ARG:HD3	1:B:239:ARG:H	1.65	0.61
1:A:487:VAL:O	1:A:491:MET:HG2	2.01	0.60
1:B:117:GLU:OE2	1:B:245:TYR:HD2	1.82	0.60
1:A:358:VAL:O	1:A:362:MET:HG3	2.01	0.60



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:305:GLU:O	1:B:309:MET:HG2	2.00	0.60
1:A:492:ARG:NH1	1:A:493:ALA:HB2	2.18	0.58
1:A:391:GLY:N	1:A:395:LEU:O	2.35	0.58
1:A:362:MET:HB3	1:A:396:VAL:HG21	1.85	0.58
1:B:436:SER:O	1:B:439:SER:OG	2.23	0.57
1:A:423:LYS:HB3	1:A:459:TYR:HD2	1.70	0.57
1:A:403:LEU:HD11	1:A:406:LEU:HD23	1.86	0.56
1:A:159:LEU:HD21	1:A:239:ARG:HB3	1.87	0.56
1:A:289:VAL:HG22	1:A:333:ILE:HD12	1.88	0.55
1:A:424:TRP:NE1	1:A:450:GLU:OE2	2.40	0.55
1:B:349:CYS:HB2	1:B:354:VAL:HG21	1.88	0.55
1:A:362:MET:HA	1:A:365:GLN:HE21	1.71	0.55
1:A:380:HIS:O	1:A:381:ARG:HB2	2.06	0.55
1:A:449:TRP:HB2	1:A:491:MET:HE3	1.87	0.55
1:B:336:PHE:HD1	1:B:337:MET:N	2.05	0.55
1:A:387:ASN:HB3	1:A:400:ASP:HB2	1.88	0.54
1:B:498:ASN:HB2	1:B:501:ASP:OD2	2.08	0.54
1:B:141:LEU:HD23	1:B:147:TYR:CE2	2.43	0.54
1:B:277:GLU:HG3	1:B:336:PHE:CE2	2.42	0.53
1:B:459:TYR:O	1:B:462:ILE:N	2.41	0.53
1:A:172:GLU:HG3	1:A:180:ARG:NE	2.23	0.53
1:A:280:TRP:O	1:A:284:SER:N	2.41	0.53
1:A:462:ILE:HG23	1:A:470:LEU:HD13	1.89	0.53
1:A:280:TRP:HB3	1:A:285:LEU:HD23	1.91	0.53
1:A:292:LEU:HD11	1:A:330:PHE:HB2	1.90	0.53
1:B:261:ILE:HG21	1:B:289:VAL:HG21	1.91	0.53
1:A:266:LYS:HA	1:A:276:TYR:HA	1.90	0.52
1:A:203:LEU:HD12	1:A:203:LEU:H	1.75	0.52
1:A:380:HIS:CD2	1:A:401:PHE:HB3	2.46	0.51
1:A:248:SER:HB2	1:A:283:TYR:CE2	2.45	0.51
1:B:497:TRP:O	1:B:499:PRO:HD3	2.10	0.51
1:A:423:LYS:HB3	1:A:459:TYR:CD2	2.45	0.51
1:B:343:LEU:HD23	1:B:386:ARG:HE	1.75	0.51
1:B:442:TRP:O	1:B:446:VAL:HG23	2.11	0.51
1:A:131:PRO:HB3	1:A:244:VAL:HG11	1.92	0.50
1:A:154:ASN:CG	1:A:360:LEU:HD22	2.31	0.50
1:A:280:TRP:O	1:A:284:SER:HA	2.12	0.50
1:B:358:VAL:HG13	1:B:394:HIS:CD2	2.47	0.50
1:B:497:TRP:O	1:B:497:TRP:HE3	1.94	0.50
1:A:490:LEU:HD21	1:A:508:ILE:HG23	1.94	0.49
1:B:101:ILE:HG21	1:B:107:LEU:HD21	1.93	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:280:TRP:O	1:B:284:SER:N	2.45	0.49
1:A:292:LEU:HD13	1:A:297:MET:HG2	1.94	0.49
1:A:370:MET:HB3	1:A:505:PHE:CG	2.47	0.49
1:A:373:LEU:HD22	1:A:378:PHE:HB3	1.93	0.49
1:B:459:TYR:N	1:B:477:MET:HE2	2.28	0.48
1:B:427:PRO:HB2	1:B:497:TRP:CZ3	2.47	0.48
1:B:384:ALA:HA	1:B:447:LEU:HD11	1.96	0.48
1:B:516:PHE:CE1	1:B:524:GLU:HG3	2.49	0.48
1:A:318:VAL:HG11	1:A:399:ALA:HB2	1.96	0.48
1:A:379:ILE:CD1	1:A:381:ARG:HE	2.27	0.47
1:B:466:GLN:O	1:B:470:LEU:HG	2.14	0.47
1:B:488:TYR:HA	1:B:491:MET:HE3	1.95	0.47
1:A:262:THR:OG1	1:A:281:LYS:HE3	2.13	0.47
1:A:479:ARG:HD3	1:A:488:TYR:CD2	2.49	0.47
1:A:280:TRP:O	1:A:284:SER:CA	2.62	0.47
1:A:380:HIS:N	1:A:440:ASP:OD2	2.45	0.47
1:B:337:MET:HG3	1:B:389:LEU:HB2	1.97	0.47
1:A:88:LEU:HD11	1:A:136:THR:HB	1.97	0.47
1:A:239:ARG:HG2	1:A:240:ASN:N	2.30	0.47
1:A:196:ASN:ND2	7:A:701:HOH:O	2.33	0.47
1:A:477:MET:O	1:A:488:TYR:OH	2.23	0.47
1:A:224:VAL:HG23	1:A:226:ASP:HB2	1.95	0.46
1:B:83:ASN:OD1	1:B:83:ASN:N	2.43	0.46
1:A:380:HIS:O	1:A:381:ARG:CB	2.63	0.46
1:B:498:ASN:O	1:B:499:PRO:C	2.55	0.46
1:B:429:SER:OG	1:B:434:LYS:O	2.24	0.46
1:A:442:TRP:CE3	1:A:495:TRP:HA	2.52	0.45
1:A:292:LEU:HB3	1:A:406:LEU:CD2	2.47	0.45
1:B:342:LEU:HB3	1:B:385:ALA:O	2.16	0.45
1:A:310:LYS:HG2	1:A:311:GLU:OE2	2.16	0.45
1:A:467:VAL:HA	1:A:470:LEU:HD12	1.99	0.45
1:B:88:LEU:HD21	1:B:136:THR:HG22	1.98	0.45
1:B:184:LEU:HD13	1:B:232:LEU:HD23	1.99	0.45
1:A:379:ILE:HD11	1:A:381:ARG:NH2	2.20	0.45
1:B:99:LEU:HB2	1:B:128:GLY:HA3	1.99	0.45
1:A:444:PHE:CE1	1:A:508:ILE:HG21	2.52	0.45
1:B:218:VAL:O	1:B:222:SER:N	2.50	0.45
1:A:468:TYR:HE1	1:A:497:TRP:HH2	1.65	0.45
1:A:476:ARG:NH2	1:A:495:TRP:O	2.49	0.44
1:B:310:LYS:HD3	1:B:310:LYS:C	2.37	0.44
1:A:306:ALA:HA	1:A:309:MET:HB2	1.99	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:334:THR:HG21	3:B:602:SKI:C26	2.46	0.44
1:A:463:ASP:HB3	1:A:466:GLN:HG2	2.00	0.44
1:B:449:TRP:CH2	1:B:456:MET:HB2	2.53	0.44
1:A:496:GLN:O	1:A:502:ARG:NH2	2.44	0.44
1:A:428:GLU:CG	1:A:434:LYS:HD2	2.48	0.44
1:A:429:SER:HA	1:A:434:LYS:H	1.83	0.44
1:B:141:LEU:HD21	1:B:214:LEU:HD23	2.00	0.44
1:B:355:ASN:O	1:B:359:LEU:HG	2.18	0.44
1:A:184:LEU:HD21	1:A:230:THR:HG22	2.00	0.43
1:A:341:ASN:HD21	1:A:343:LEU:HB3	1.81	0.43
1:A:486:LYS:HE2	1:A:486:LYS:HB2	1.75	0.43
1:A:434:LYS:HG3	1:A:435:PHE:N	2.34	0.43
1:B:198:ALA:HB2	1:B:204:TYR:HE1	1.83	0.43
1:A:189:ARG:HA	1:A:189:ARG:HD3	1.90	0.43
1:B:159:LEU:HD11	1:B:239:ARG:HD2	2.00	0.43
1:B:370:MET:HB3	1:B:505:PHE:CG	2.54	0.43
1:A:476:ARG:HE	1:A:495:TRP:HB2	1.84	0.43
1:A:463:ASP:OD2	2:B:601:AY7:O23	2.35	0.43
1:A:469:GLU:C	1:A:471:LEU:N	2.71	0.43
1:A:341:ASN:OD1	1:A:386:ARG:HA	2.19	0.42
1:A:146:TRP:CZ3	1:A:218:VAL:HG21	2.53	0.42
1:A:437:ILE:O	1:A:441:VAL:HG23	2.19	0.42
1:B:341:ASN:HB3	1:B:344:ASP:HB2	2.01	0.42
1:B:464:LEU:HD23	1:B:464:LEU:HA	1.79	0.42
1:A:375:LYS:HE3	1:A:375:LYS:HB3	1.90	0.42
1:B:358:VAL:CG1	1:B:394:HIS:CD2	3.02	0.42
1:B:189:ARG:NH1	1:B:520:SER:OG	2.53	0.41
1:B:448:LEU:HD21	1:B:487:VAL:CG2	2.50	0.41
1:A:87:ALA:HA	1:A:135:ILE:HG22	2.02	0.41
1:B:153:ARG:HB3	1:B:513:GLU:OE2	2.20	0.41
1:A:220:HIS:NE2	1:A:226:ASP:OD2	2.36	0.41
1:A:405:ARG:HD3	1:A:405:ARG:HA	1.87	0.41
1:A:468:TYR:HB3	1:A:469:GLU:OE1	2.21	0.41
1:A:195:ILE:HG22	1:A:203:LEU:HB3	2.02	0.41
1:A:316:ASN:HB2	1:A:369:ALA:HB2	2.03	0.41
1:A:321:LEU:N	1:A:333:ILE:O	2.53	0.41
1:A:434:LYS:CG	1:A:435:PHE:N	2.84	0.41
1:A:479:ARG:HD3	1:A:488:TYR:HD2	1.85	0.41
1:B:196:ASN:ND2	1:B:204:TYR:CZ	2.89	0.41
1:A:186:TYR:HB3	1:A:191:TYR:HE1	1.86	0.41
1:A:289:VAL:HG22	1:A:333:ILE:CD1	2.50	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:VAL:O	1:A:143:LYS:HD3	2.21	0.40
1:B:453:THR:CB	1:B:456:MET:HG3	2.47	0.40
1:A:328:PRO:HB2	1:A:329:PRO:HD3	2.03	0.40
1:A:354:VAL:O	1:A:454:TYR:OH	2.37	0.40
1:A:468:TYR:CE1	1:A:497:TRP:HH2	2.39	0.40
1:A:341:ASN:OD1	1:A:342:LEU:N	2.54	0.40
1:A:490:LEU:HD12	1:A:490:LEU:HA	1.93	0.40
1:B:437:ILE:HD13	1:B:437:ILE:HA	1.89	0.40
1:A:266:LYS:HG2	1:A:267:LEU:N	2.37	0.40
1:A:434:LYS:NZ	1:A:499:PRO:HG3	2.36	0.40
1:B:204:TYR:HB3	1:B:210:ARG:HA	2.04	0.40
1:B:353:GLU:HG3	1:B:354:VAL:HG23	2.02	0.40
1:B:469:GLU:OE1	1:B:469:GLU:N	2.55	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	ntiles
1	А	408/448 (91%)	385~(94%)	22~(5%)	1 (0%)	47	75
1	В	366/448~(82%)	356~(97%)	10 (3%)	0	100	100
All	All	774/896~(86%)	741 (96%)	32~(4%)	1 (0%)	51	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	404	SER



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	368/390~(94%)	350~(95%)	18 (5%)	25 54		
1	В	338/390~(87%)	315~(93%)	23~(7%)	16 38		
All	All	706/780~(90%)	665 (94%)	41 (6%)	20 46		

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	141	LEU
1	А	185	ARG
1	А	189	ARG
1	А	194	ARG
1	А	239	ARG
1	А	263	MET
1	А	295	ASP
1	А	297	MET
1	А	375	LYS
1	А	405	ARG
1	А	407	MET
1	А	435	PHE
1	А	468	TYR
1	А	469	GLU
1	А	473	LYS
1	А	476	ARG
1	А	479	ARG
1	А	512	PHE
1	В	139	ASN
1	В	147	TYR
1	В	176	SER
1	В	203	LEU
1	В	207	SER
1	В	208	GLU
1	В	239	ARG
1	В	263	MET
1	В	301	GLU



Mol	Chain	Res	Type
1	В	323	VAL
1	В	336	PHE
1	В	346	LEU
1	В	381	ARG
1	В	386	ARG
1	В	395	LEU
1	В	429	SER
1	В	435	PHE
1	В	468	TYR
1	В	474	ASP
1	В	486	LYS
1	В	497	TRP
1	В	512	PHE
1	В	518	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	387	ASN
1	В	196	ASN
1	В	393	ASN
1	В	394	HIS
1	В	466	GLN
1	В	496	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 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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).

Mal	Turne	Chain	Dec	Tink	B	ond lengths		В	ond ang	gles
WIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
5	SO4	А	605	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0
5	SO4	В	603	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0
6	DMS	В	604	-	3,3,3	0.66	0	3,3,3	0.51	0
2	AY7	В	601	-	34,34,34	0.76	2 (5%)	40,49,49	1.12	2 (5%)
6	DMS	А	608	-	3,3,3	0.65	0	3,3,3	0.49	0
2	AY7	А	601	-	34,34,34	0.75	0	40,49,49	1.15	2(5%)
6	DMS	А	606	-	3,3,3	0.66	0	3,3,3	0.52	0
6	DMS	А	607	-	3,3,3	0.66	0	3,3,3	0.51	0
3	SKI	В	602	-	31,31,31	2.84	11 (35%)	42,42,42	2.05	14 (33%)
5	SO4	А	604	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0
3	SKI	A	602	-	$31,\!31,\!31$	2.85	11 (35%)	42,42,42	2.12	16 (38%)

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	SKI	А	602	-	-	3/12/12/12	0/4/4/4
3	SKI	В	602	-	-	2/12/12/12	0/4/4/4
2	AY7	А	601	-	-	6/19/30/30	0/4/4/4
2	AY7	В	601	-	-	6/19/30/30	0/4/4/4

All	(24)	bond	length	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	В	602	SKI	O27-C04	8.15	1.50	1.37
3	А	602	SKI	O27-C04	8.13	1.50	1.37
3	А	602	SKI	C09-N13	6.61	1.46	1.36



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
3	В	602	SKI	C09-N13	6.52	1.46	1.36
3	А	602	SKI	C15-C14	4.95	1.47	1.39
3	В	602	SKI	C15-C14	4.88	1.47	1.39
3	А	602	SKI	C11-N12	4.88	1.40	1.32
3	В	602	SKI	C11-N12	4.76	1.39	1.32
3	В	602	SKI	C18-C17	3.97	1.46	1.38
3	А	602	SKI	C18-C17	3.93	1.46	1.38
3	А	602	SKI	C25-C26	3.51	1.46	1.38
3	В	602	SKI	C25-C26	3.49	1.46	1.38
3	В	602	SKI	C04-C03	3.48	1.48	1.40
3	А	602	SKI	C04-C03	3.39	1.48	1.40
3	А	602	SKI	O20-C17	-2.76	1.33	1.39
3	А	602	SKI	C09-N10	2.72	1.37	1.34
3	В	602	SKI	C09-N10	2.70	1.37	1.34
3	В	602	SKI	O20-C17	-2.59	1.34	1.39
3	А	602	SKI	C22-C21	2.30	1.43	1.38
3	В	602	SKI	C22-C21	2.29	1.43	1.38
3	В	602	SKI	C19-C18	2.13	1.42	1.38
3	А	602	SKI	C19-C18	2.06	1.42	1.38
2	В	601	AY7	N25-N24	-2.05	1.33	1.37
2	В	601	AY7	C27-C26	2.05	1.40	1.38

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
3	В	602	SKI	C11-N10-C09	4.42	120.38	116.59
3	В	602	SKI	O02-C03-C08	-4.33	119.64	125.24
3	А	602	SKI	O02-C03-C08	-4.28	119.71	125.24
3	А	602	SKI	C11-N10-C09	4.27	120.25	116.59
3	А	602	SKI	C09-C07-C06	4.21	118.53	115.88
3	В	602	SKI	O27-C04-C05	-4.01	120.05	125.24
3	В	602	SKI	N12-C11-N10	-3.89	122.59	128.68
2	А	601	AY7	C27-C12-N24	-3.88	105.50	110.42
3	А	602	SKI	O27-C04-C05	-3.82	120.30	125.24
3	А	602	SKI	C08-C07-C09	-3.80	121.45	124.88
3	А	602	SKI	N12-C11-N10	-3.80	122.74	128.68
3	В	602	SKI	C09-C07-C06	3.66	118.18	115.88
2	В	601	AY7	C27-C12-N24	-3.65	105.80	110.42
3	В	602	SKI	O27-C04-C03	3.58	120.39	115.41
3	В	602	SKI	C11-N12-C06	3.51	120.23	115.40
3	A	602	SKI	C07-C06-N12	-3.49	119.12	122.83
3	А	602	SKI	C11-N12-C06	3.46	120.17	115.40



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	В	602	SKI	O02-C03-C04	3.38	120.12	115.41
3	А	602	SKI	O27-C04-C03	3.35	120.08	115.41
3	В	602	SKI	C07-C06-N12	-3.30	119.32	122.83
3	А	602	SKI	O02-C03-C04	3.25	119.94	115.41
3	В	602	SKI	C08-C07-C09	-3.24	121.95	124.88
3	А	602	SKI	C21-O20-C17	-3.12	111.51	118.80
2	А	601	AY7	C27-C12-C11	2.98	131.56	128.77
3	А	602	SKI	C07-C09-N10	-2.62	119.19	121.35
3	А	602	SKI	C05-C06-N12	2.61	120.95	117.97
2	В	601	AY7	C27-C12-C11	2.57	131.17	128.77
3	В	602	SKI	C07-C09-N10	-2.51	119.28	121.35
3	В	602	SKI	C05-C06-N12	2.42	120.73	117.97
3	В	602	SKI	C14-N13-C09	-2.33	122.20	128.26
3	А	602	SKI	C14-N13-C09	-2.21	122.49	128.26
3	А	602	SKI	C01-O02-C03	-2.20	114.21	117.53
3	A	602	SKI	C28-O27-C04	-2.11	114.35	117.53
3	B	602	SKI	C01-O02-C03	-2.08	114.38	117.53

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
2	А	601	AY7	C11-C1-N2-C3
2	А	601	AY7	C11-C1-N2-C6
2	А	601	AY7	N7-C1-N2-C3
2	А	601	AY7	N7-C1-N2-C6
2	А	601	AY7	C10-C11-C12-C27
2	А	601	AY7	C10-C11-C12-N24
2	В	601	AY7	C11-C1-N2-C3
2	В	601	AY7	C11-C1-N2-C6
2	В	601	AY7	N7-C1-N2-C3
2	В	601	AY7	N7-C1-N2-C6
2	В	601	AY7	C10-C11-C12-C27
2	В	601	AY7	C10-C11-C12-N24
3	В	602	SKI	C08-C03-O02-C01
3	А	602	SKI	N10-C09-N13-C14
3	В	602	SKI	C04-C03-O02-C01
3	А	602	SKI	C07-C09-N13-C14
3	А	602	SKI	C04-C03-O02-C01

All (17) torsion outliers are listed below:

There are no ring outliers.

2 monomers are involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	601	AY7	1	0
3	В	602	SKI	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 sufficient 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	$\mathbf{OWAB}(\mathbf{A}^2)$	Q < 0.9
1	А	420/448~(93%)	1.56	118 (28%) 0 0	53, 87, 132, 157	0
1	В	386/448~(86%)	1.74	130 (33%) 0 0	55, 90, 137, 155	0
All	All	806/896~(89%)	1.64	248 (30%) 0 0	53, 88, 134, 157	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	519	SER	9.9
1	В	260	ASP	8.4
1	А	381	ARG	8.2
1	В	280	TRP	8.2
1	А	264	LYS	8.0
1	А	435	PHE	7.8
1	В	261	ILE	7.5
1	В	196	ASN	7.4
1	А	517	GLN	7.1
1	В	517	GLN	6.8
1	В	483	CYS	6.8
1	В	284	SER	6.5
1	В	401	PHE	6.4
1	В	179	GLN	6.2
1	А	279	VAL	6.1
1	В	304	LYS	6.1
1	А	494	CYS	6.0
1	В	164	ILE	5.9
1	А	282	LYS	5.8
1	А	401	PHE	5.7
1	A	280	TRP	5.6
1	A	498	ASN	5.6
1	В	302	PHE	5.6
1	В	309	MET	5.4



Mol	Chain	Res	Type	RSRZ
1	В	516	PHE	5.2
1	А	470	LEU	5.1
1	А	283	TYR	5.1
1	А	456	MET	5.1
1	В	524	GLU	5.1
1	В	503	PRO	5.0
1	В	390	VAL	5.0
1	В	382	ASP	4.9
1	А	262	THR	4.9
1	В	303	LEU	4.8
1	В	96	ASP	4.8
1	А	298	GLU	4.7
1	А	328	PRO	4.6
1	В	323	VAL	4.6
1	В	495	TRP	4.6
1	В	186	TYR	4.6
1	А	338	THR	4.6
1	А	519	SER	4.6
1	А	497	TRP	4.5
1	А	261	ILE	4.5
1	А	483	CYS	4.4
1	А	377	ASN	4.4
1	А	465	SER	4.4
1	А	462	ILE	4.4
1	А	265	HIS	4.4
1	В	435	PHE	4.3
1	В	488	TYR	4.3
1	В	512	PHE	4.3
1	А	309	MET	4.2
1	В	386	ARG	4.2
1	В	486	LYS	4.2
1	В	84	LEU	4.2
1	В	498	ASN	4.2
1	B	391	GLY	4.2
1	В	426	ALA	4.1
1	В	515	MET	4.0
1	A	457	SER	4.0
1	A	486	LYS	4.0
1	В	205	VAL	3.9
1	A	434	LYS	3.9
1	В	283	TYR	3.9
1	В	345	TYR	3.8



Mol	Chain	Res	Type	RSRZ
1	А	424	TRP	3.8
1	А	490	LEU	3.8
1	В	301	GLU	3.8
1	В	338	THR	3.8
1	А	392	GLU	3.8
1	А	382	ASP	3.8
1	В	520	SER	3.7
1	А	276	TYR	3.7
1	А	301	GLU	3.7
1	В	126	GLY	3.7
1	В	250	ASN	3.7
1	В	199	SER	3.7
1	В	108	ARG	3.6
1	A	370	MET	3.6
1	A	331	TYR	3.6
1	В	229	ILE	3.6
1	А	399	ALA	3.6
1	В	154	ASN	3.6
1	В	499	PRO	3.6
1	А	495	TRP	3.5
1	В	388	CYS	3.5
1	В	118	TRP	3.5
1	А	174	GLU	3.5
1	В	453	THR	3.5
1	А	207	SER	3.5
1	В	265	HIS	3.5
1	В	264	LYS	3.4
1	А	275	VAL	3.4
1	А	487	VAL	3.3
1	А	442	TRP	3.3
1	В	470	LEU	3.3
1	A	308	VAL	3.3
1	В	320	LEU	3.3
1	A	164	ILE	3.2
1	В	259	THR	3.2
1	В	430	LEU	3.2
1	В	378	PHE	3.1
1	В	101	ILE	3.1
1	A	464	LEU	3.1
1	A	290	LYS	3.1
1	A	324	CYS	3.0
1	В	501	ASP	3.0



Mol	Chain	Res	Type	RSRZ
1	А	339	TYR	3.0
1	В	502	ARG	3.0
1	А	196	ASN	3.0
1	В	228	LEU	2.9
1	В	375	LYS	2.9
1	В	467	VAL	2.9
1	А	320	LEU	2.9
1	А	407	MET	2.9
1	А	267	LEU	2.9
1	А	321	LEU	2.9
1	А	296	THR	2.9
1	А	292	LEU	2.9
1	А	297	MET	2.9
1	В	244	VAL	2.9
1	В	514	THR	2.9
1	В	216	GLU	2.9
1	В	279	VAL	2.9
1	В	136	THR	2.9
1	А	488	TYR	2.9
1	А	323	VAL	2.8
1	А	402	GLY	2.8
1	В	175	SER	2.8
1	В	500	SER	2.8
1	В	480	PRO	2.8
1	В	206	SER	2.8
1	А	98	THR	2.8
1	В	392	GLU	2.8
1	А	287	VAL	2.8
1	А	395	LEU	2.8
1	В	377	ASN	2.8
1	В	457	SER	2.7
1	В	322	GLY	2.7
1	В	277	GLU	2.7
1	В	434	LYS	2.7
1	В	281	LYS	2.7
1	А	449	TRP	2.7
1	В	335	GLU	2.7
1	А	162	SER	2.7
1	В	193	TYR	2.7
1	А	277	GLU	2.7
1	В	336	PHE	2.6
1	А	284	SER	2.6



Mol	Chain	Res	Type	RSRZ
1	В	245	TYR	2.6
1	А	491	MET	2.6
1	А	508	ILE	2.6
1	В	381	ARG	2.6
1	А	289	VAL	2.6
1	В	474	ASP	2.6
1	В	123	THR	2.6
1	А	391	GLY	2.6
1	В	370	MET	2.6
1	В	289	VAL	2.6
1	В	134	TYR	2.6
1	А	344	ASP	2.5
1	А	333	ILE	2.5
1	А	386	ARG	2.5
1	В	197	THR	2.5
1	А	500	SER	2.5
1	А	453	THR	2.5
1	В	161	SER	2.5
1	А	250	ASN	2.5
1	В	133	ASN	2.5
1	А	325	THR	2.4
1	В	339	TYR	2.4
1	А	467	VAL	2.4
1	В	494	CYS	2.4
1	В	471	LEU	2.4
1	А	406	LEU	2.4
1	А	302	PHE	2.4
1	А	327	GLU	2.4
1	В	508	ILE	2.4
1	A	111	GLY	2.4
1	А	398	VAL	2.4
1	А	127	GLN	2.4
1	А	197	THR	2.4
1	A	186	TYR	2.3
1	В	427	PRO	2.3
1	В	248	SER	2.3
1	A	518	GLU	2.3
1	В	239	ARG	2.3
1	A	330	PHE	2.3
1	В	484	PRO	2.3
1	A	198	ALA	2.3
1	А	208	GLU	2.3



Mol	Chain	Res	Type	RSRZ
1	А	249	PRO	2.3
1	А	305	GLU	2.3
1	А	385	ALA	2.3
1	А	171	ARG	2.3
1	В	163	GLY	2.3
1	В	479	ARG	2.3
1	А	380	HIS	2.3
1	В	141	LEU	2.3
1	А	291	THR	2.3
1	А	520	SER	2.3
1	В	469	GLU	2.3
1	В	449	TRP	2.3
1	A	123	THR	2.2
1	В	448	LEU	2.2
1	В	485	GLU	2.2
1	В	523	ASP	2.2
1	В	300	GLU	2.2
1	В	463	ASP	2.2
1	А	156	ALA	2.2
1	В	115	ASN	2.2
1	А	82	GLY	2.2
1	А	408	THR	2.2
1	А	285	LEU	2.2
1	В	518	GLU	2.2
1	А	133	ASN	2.2
1	В	433	ASN	2.2
1	А	229	ILE	2.2
1	В	384	ALA	2.2
1	В	473	LYS	2.2
1	А	364	THR	2.2
1	A	193	TYR	2.2
1	В	376	LYS	2.1
1	В	429	SER	2.1
1	А	499	PRO	2.1
1	А	502	ARG	2.1
1	A	121	ALA	2.1
1	В	441	VAL	2.1
1	А	163	GLY	2.1
1	В	431	ALA	2.1
1	A	430	LEU	2.1
1	В	504	SER	2.1
1	A	474	ASP	2.1



Mol	Chain	Res	Type	RSRZ
1	В	249	PRO	2.1
1	В	282	LYS	2.1
1	В	173	SER	2.0
1	В	198	ALA	2.0
1	А	124	LYS	2.0
1	В	200	ASP	2.0
1	В	178	GLY	2.0
1	А	375	LYS	2.0
1	А	516	PHE	2.0
1	В	456	MET	2.0
1	В	119	CYS	2.0
1	В	472	GLU	2.0
1	В	493	ALA	2.0
1	А	84	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
6	DMS	А	606	4/4	0.36	0.31	79,84,94,133	0
5	SO4	В	603	5/5	0.62	0.60	94,105,119,128	0
6	DMS	А	608	4/4	0.62	0.33	55,76,91,142	0
3	SKI	А	602	28/28	0.70	0.33	69,97,107,117	0
6	DMS	В	604	4/4	0.70	0.31	44,82,97,124	0
3	SKI	В	602	28/28	0.73	0.40	73,108,119,122	0
2	AY7	А	601	31/31	0.77	0.34	87,101,118,129	0
5	SO4	A	604	5/5	0.80	0.20	83,88,120,131	0
5	SO4	А	605	5/5	0.83	0.34	85,94,107,123	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B}$ -factors(${f A}^2)$	Q<0.9
2	AY7	В	601	31/31	0.84	0.28	75,103,130,135	0
4	CL	А	603	1/1	0.84	0.57	90,90,90,90	0
6	DMS	А	607	4/4	0.85	0.25	$63,\!65,\!84,\!97$	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.

