

Full wwPDB X-ray Structure Validation Report (i)

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 Title : Crystal structure of the multidrug efflux transporter BpeB from Burkholderia pseudomallei Authors : Kato, T.; Hung, LW.; Yamashita, E.; Okada, U.; Terwilliger, T.C.; Mu rakami, S. Deposited on : 2022-01-13 Resolution : 2.94 Å(reported) 	PDB ID	:	7WLS
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Resolution : $2.94 \text{ Å}(\text{reported})$	Deposited on	:	2022-01-13
	Resolution	:	2.94 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 (i)) 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	:	2.36
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)	:	2.36

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 2.94 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	1051	9%	20%	•
		1001	7%	20,0	_
1	В	1051	77%	20%	••
1	С	1051	78%	19%	••



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23250 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1 A	Δ	1010	Total	С	Ν	Ο	\mathbf{S}	0 0	0	
	1019	7703	4974	1272	1424	33	0	0	0	
1	р	1024	Total	С	Ν	Ο	S	0	0	0
1	I D	1024	7744	5002	1278	1431	33	0	0	0
1	C	1018	Total	С	Ν	Ο	S	0	0	0
	1018	7688	4961	1270	1424	33	0	0	U	

• Molecule 1 is a protein called Efflux pump membrane transporter.

Chain	Residue	Modelled	Actual	Comment	Reference
А	?	-	ALA	deletion	UNP Q63WS7
А	?	-	HIS	deletion	UNP Q63WS7
А	?	-	GLU	deletion	UNP Q63WS7
А	?	-	HIS	deletion	UNP Q63WS7
А	?	-	MET	deletion	UNP Q63WS7
А	?	-	HIS	deletion	UNP Q63WS7
А	?	-	ARG	deletion	UNP Q63WS7
А	?	-	ASP	deletion	UNP Q63WS7
А	?	-	ASP	deletion	UNP Q63WS7
А	?	-	LYS	deletion	UNP Q63WS7
А	?	-	PRO	deletion	UNP Q63WS7
А	?	-	GLU	deletion	UNP Q63WS7
А	?	-	HIS	deletion	UNP Q63WS7
А	?	-	GLY	deletion	UNP Q63WS7
А	?	-	ASP	deletion	UNP Q63WS7
А	?	-	ASP	deletion	UNP Q63WS7
А	?	-	ALA	deletion	UNP Q63WS7
А	?	-	GLY	deletion	UNP Q63WS7
А	?	-	LYS	deletion	UNP Q63WS7
А	?	-	LYS	deletion	UNP Q63WS7
A	?	-	ASP	deletion	UNP Q63WS7
A	1046	HIS	-	expression tag	UNP Q63WS7
A	1047	HIS	-	expression tag	UNP Q63WS7

There are 81 discrepancies between the modelled and reference sequences:



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Continued from previous page							
Chain	Residue	Modelled	Actual	Comment	Reference		
А	1048	HIS	-	expression tag	UNP Q63WS7		
А	1049	HIS	-	expression tag	UNP Q63WS7		
А	1050	HIS	-	expression tag	UNP Q63WS7		
А	1051	HIS	-	expression tag	UNP Q63WS7		
В	?	-	ALA	deletion	UNP Q63WS7		
В	?	-	HIS	deletion	UNP Q63WS7		
В	?	-	GLU	deletion	UNP Q63WS7		
В	?	-	HIS	deletion	UNP Q63WS7		
В	?	-	MET	deletion	UNP Q63WS7		
В	?	-	HIS	deletion	UNP Q63WS7		
В	?	-	ARG	deletion	UNP Q63WS7		
В	?	-	ASP	deletion	UNP Q63WS7		
В	?	-	ASP	deletion	UNP Q63WS7		
В	?	-	LYS	deletion	UNP Q63WS7		
В	?	-	PRO	deletion	UNP Q63WS7		
В	?	-	GLU	deletion	UNP Q63WS7		
В	?	-	HIS	deletion	UNP Q63WS7		
В	?	-	GLY	deletion	UNP Q63WS7		
В	?	-	ASP	deletion	UNP Q63WS7		
В	?	-	ASP	deletion	UNP Q63WS7		
В	?	-	ALA	deletion	UNP Q63WS7		
В	?	-	GLY	deletion	UNP Q63WS7		
В	?	-	LYS	deletion	UNP Q63WS7		
В	?	-	LYS	deletion	UNP Q63WS7		
В	?	-	ASP	deletion	UNP Q63WS7		
В	1046	HIS	-	expression tag	UNP Q63WS7		
В	1047	HIS	-	expression tag	UNP Q63WS7		
В	1048	HIS	-	expression tag	UNP Q63WS7		
В	1049	HIS	-	expression tag	UNP Q63WS7		
В	1050	HIS	-	expression tag	UNP Q63WS7		
В	1051	HIS	-	expression tag	UNP Q63WS7		
С	?	-	ALA	deletion	UNP Q63WS7		
С	?	-	HIS	deletion	UNP Q63WS7		
С	?	-	GLU	deletion	UNP Q63WS7		
С	?	_	HIS	deletion	UNP Q63WS7		
С	?	_	MET	deletion	UNP Q63WS7		
С	?	-	HIS	deletion	UNP Q63WS7		
С	?	-	ARG	deletion	UNP Q63WS7		
С	?	-	ASP	deletion	UNP Q63WS7		
С	?	_	ASP	deletion	UNP Q63WS7		
C	?	-	LYS	deletion	UNP Q63WS7		
С	?	-	PRO	deletion	UNP Q63WS7		

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7	W	LS
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Chain	Residue	Modelled	Actual	Comment	Reference
С	?	-	GLU	deletion	UNP Q63WS7
С	?	-	HIS	deletion	UNP Q63WS7
С	?	-	GLY	deletion	UNP Q63WS7
С	?	-	ASP	deletion	UNP Q63WS7
С	?	-	ASP	deletion	UNP Q63WS7
С	?	-	ALA	deletion	UNP Q63WS7
С	?	-	GLY	deletion	UNP Q63WS7
С	?	-	LYS	deletion	UNP Q63WS7
С	?	-	LYS	deletion	UNP Q63WS7
С	?	-	ASP	deletion	UNP Q63WS7
С	1046	HIS	-	expression tag	UNP Q63WS7
С	1047	HIS	-	expression tag	UNP Q63WS7
С	1048	HIS	-	expression tag	UNP Q63WS7
C	1049	HIS	-	expression tag	UNP Q63WS7
С	1050	HIS	-	expression tag	UNP Q63WS7
C	1051	HIS	-	expression tag	UNP Q63WS7

• Molecule 2 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total C O 34 23 11	0	0
2	В	1	Total C O 34 23 11	0	0
2	В	1	Total C O 34 23 11	0	0



• Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total C O 13 8 5	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: Efflux pump membrane transporter

 \bullet Molecule 1: Efflux pump membrane transporter

Chain B:

77%















4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	207.88Å 135.98Å 157.82Å	Depositor
a, b, c, α , β , γ	90.00° 98.21° 90.00°	Depositor
Bosolution(A)	48.80 - 2.94	Depositor
Resolution (A)	48.80 - 2.94	EDS
% Data completeness	99.3 (48.80-2.94)	Depositor
(in resolution range)	99.5(48.80-2.94)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.20 (at 2.96 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20rc1_4387	Depositor
P. P.	0.230 , 0.284	Depositor
n, n_{free}	0.229 , 0.281	DCC
R_{free} test set	4615 reflections (5.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	97.7	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29 , 78.8	EDS
L-test for $twinning^2$	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23250	wwPDB-VP
Average B, all atoms $(Å^2)$	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.44% 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: UMQ, PG4

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		Bo	nd lengths	Bond angles		
Moi Chain	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	А	0.51	0/7857	0.77	$7/10701 \ (0.1\%)$	
1	В	0.55	1/7900~(0.0%)	0.79	5/10760~(0.0%)	
1	С	0.48	0/7839	0.73	6/10674~(0.1%)	
All	All	0.51	1/23596~(0.0%)	0.76	18/32135~(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	А	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	236	GLU	CB-CG	-5.09	1.42	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	236	GLU	CB-CA-C	-6.80	96.81	110.40
1	В	236	GLU	CA-CB-CG	6.55	127.81	113.40
1	А	988	LEU	CA-CB-CG	6.36	129.92	115.30
1	С	127	LEU	CB-CG-CD2	-5.75	101.22	111.00
1	А	625	LEU	CA-CB-CG	5.60	128.18	115.30
1	А	221	GLY	C-N-CA	-5.55	107.81	121.70
1	В	395	MET	CG-SD-CE	5.55	109.08	100.20
1	В	76	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	С	472	LEU	CA-CB-CG	-5.42	102.84	115.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	797	MET	CB-CG-SD	5.34	128.42	112.40
1	С	370	ILE	CG1-CB-CG2	-5.33	99.67	111.40
1	А	76	LEU	CB-CG-CD1	-5.32	101.96	111.00
1	А	745	ASP	CB-CG-OD2	-5.27	113.55	118.30
1	С	673	LEU	CA-CB-CG	5.22	127.31	115.30
1	С	164	ASP	CB-CG-OD1	5.09	122.88	118.30
1	А	189	ASP	CB-CG-OD1	5.09	122.88	118.30
1	В	408	ASP	CB-CG-OD2	5.06	122.86	118.30
1	А	164	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	236	GLU	Mainchain

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	7703	0	7890	143	0
1	В	7744	0	7930	158	0
1	С	7688	0	7878	138	0
2	В	102	0	132	5	0
3	В	13	0	18	1	0
All	All	23250	0	23848	415	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 9.

All (415) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:THR:HG22	1:C:213:GLN:HE21	1.13	1.10
1:A:702:LEU:HD11	1:A:716:PRO:HB3	1.37	1.02



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:640:ASP:O	1:C:649:ARG:NH1	1.92	1.01
1:C:678:GLY:HA3	1:C:828:GLY:O	1.70	0.90
1:A:717:ASN:ND2	1:A:816:GLU:OE2	2.10	0.85
1:B:32:ILE:HG12	1:B:298:ASN:HB2	1.60	0.81
1:B:254:ASN:ND2	1:B:256:ASP:OD2	2.13	0.81
1:A:56:THR:HG22	1:C:213:GLN:NE2	1.93	0.80
1:A:637:GLN:OE1	1:A:992:ASN:ND2	2.15	0.79
1:B:197:GLY:O	1:B:791:ARG:NH2	2.16	0.79
1:B:164:ASP:OD1	1:B:168:ARG:NH1	2.16	0.79
1:C:403:GLY:HA3	1:C:981:PHE:HA	1.65	0.78
1:C:463:VAL:HG21	1:C:868:SER:HB2	1.66	0.78
1:B:36:PRO:HG3	1:B:469:GLN:HG3	1.66	0.76
1:C:307:ARG:NH1	1:C:328:ASP:OD2	2.18	0.75
1:C:13:TRP:HH2	1:C:370:ILE:HD11	1.51	0.75
1:B:281:TYR:O	1:B:283:GLY:N	2.21	0.74
1:B:978:SER:OG	1:B:1014:THR:HG21	1.89	0.72
1:A:884:PHE:HB2	1:A:901:ILE:HD11	1.70	0.72
1:A:356:TYR:HA	1:A:365:THR:HG21	1.72	0.71
1:B:327:TYR:HB2	2:B:1101:UMQ:HI2	1.72	0.71
1:C:663:ILE:HD12	1:C:715:ARG:HD3	1.73	0.70
1:A:133:SER:O	1:A:292:GLN:NE2	2.24	0.70
1:B:408:ASP:OD1	1:B:939:LYS:NZ	2.18	0.69
1:A:704:MET:HB3	1:A:846:LEU:HD22	1.74	0.69
1:B:467:TYR:OH	1:B:927:GLN:OE1	2.13	0.66
1:B:590:LEU:CD1	1:B:612:ASN:HB3	2.27	0.65
1:C:734:ALA:HB1	1:C:739:VAL:HG23	1.79	0.65
1:C:404:LEU:HD11	1:C:936:LEU:HD21	1.77	0.65
1:A:101:ASP:OD1	1:A:131:LYS:NZ	2.30	0.64
1:B:590:LEU:HD12	1:B:612:ASN:HB3	1.80	0.63
1:A:307:ARG:NH2	1:A:328:ASP:OD2	2.32	0.63
1:A:404:LEU:HD13	1:A:449:LEU:HD11	1.81	0.63
1:A:972:ARG:HB3	1:A:973:PRO:HD3	1.82	0.62
1:B:959:PRO:HG3	2:B:1102:UMQ:HK1	1.81	0.62
1:B:47:ALA:HB3	1:B:88:ALA:HB3	1.82	0.62
1:A:715:ARG:NH2	1:A:827:GLN:OE1	2.32	0.62
1:B:32:ILE:H	1:B:298:ASN:HA	1.64	0.61
1:B:236:GLU:O	1:C:726:LYS:NZ	2.23	0.61
1:B:236:GLU:OE2	1:C:748:PHE:HB3	1.99	0.61
1:B:253:VAL:HG22	1:B:259:GLN:HG2	1.82	0.61
1:C:13:TRP:CH2	1:C:370:ILE:HD11	2.35	0.61
1:C:30:LEU:HD21	1:C:384:SER:HB2	1.82	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:466:ILE:HG21	1:C:924:VAL:HG11	1.82	0.61
1:B:340:VAL:HG11	1:B:395:MET:SD	2.40	0.60
1:C:597:LEU:HD13	1:C:628:VAL:HG11	1.83	0.60
1:A:577:THR:HG21	1:A:586:THR:HA	1.83	0.60
1:B:250:LEU:HD13	1:C:735:ASN:HB2	1.83	0.60
1:A:108:GLN:HE21	1:B:109:ASN:HB3	1.67	0.60
1:A:453:PHE:HZ	1:A:932:THR:HG22	1.67	0.59
1:B:990:ILE:O	1:B:990:ILE:HG13	2.03	0.59
1:A:1012:THR:HB	1:A:1016:LEU:HD12	1.85	0.59
1:B:188:LEU:HD13	1:B:193:LEU:HD11	1.85	0.58
1:C:277:PHE:HA	1:C:612:ASN:O	2.03	0.58
1:B:32:ILE:CD1	1:B:390:ILE:HB	2.34	0.58
1:A:636:ARG:HB2	1:A:641:GLN:HB3	1.85	0.58
1:B:153:ASP:OD1	1:B:182:TYR:OH	2.11	0.58
1:B:426:PRO:HG2	1:B:429:GLU:OE1	2.04	0.58
1:A:456:VAL:HG12	1:A:875:LEU:HD13	1.86	0.57
1:C:642:LYS:O	1:C:646:LEU:N	2.35	0.57
1:A:43:ILE:HD13	1:A:131:LYS:HB3	1.86	0.57
1:A:56:THR:CG2	1:C:213:GLN:HE21	2.04	0.57
1:A:558:LEU:HD23	1:A:922:ASN:HB2	1.85	0.57
1:C:188:LEU:HD21	1:C:203:VAL:HG11	1.85	0.57
1:C:379:THR:HG21	1:C:398:LEU:HD21	1.86	0.57
1:A:992:ASN:N	1:A:992:ASN:OD1	2.36	0.57
1:B:168:ARG:NH2	1:C:66:GLU:HB3	2.19	0.57
1:B:348:ILE:HD13	1:B:373:PRO:HG3	1.87	0.57
1:C:279:THR:HG22	1:C:611:VAL:HG12	1.87	0.57
1:B:585:THR:HA	1:B:588:ARG:HH21	1.69	0.57
1:B:1032:PHE:O	1:B:1033:SER:OG	2.20	0.56
1:C:3:LYS:NZ	1:C:436:GLY:HA2	2.20	0.56
1:A:451:ALA:HB1	1:A:882:VAL:HG12	1.88	0.56
1:A:213:GLN:HE21	1:A:239:LEU:H	1.53	0.56
1:C:756:TYR:HB2	1:C:771:TYR:CE1	2.40	0.55
1:A:10:ILE:HD12	1:B:894:TRP:NE1	2.21	0.55
1:B:456:VAL:HG12	1:B:467:TYR:HB3	1.89	0.55
1:A:698:ARG:HH22	1:A:720:ASN:HB3	1.70	0.55
1:A:782:PRO:O	1:A:785:MET:HG2	2.06	0.55
1:B:925:PHE:HB3	1:B:1002:ILE:HG22	1.88	0.55
1:A:929:GLY:O	1:A:933:THR:HG23	2.07	0.55
1:B:348:ILE:CD1	1:B:373:PRO:HG3	2.37	0.55
1:B:762:ASP:HB3	1:B:764:ASP:OD1	2.07	0.55
1:B:164:ASP:HB3	1:B:165:PRO:HD3	1.89	0.55



	• • • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:973:PRO:HA	1:A:976:MET:HB3	1.89	0.55
1:C:399:VAL:HG11	1:C:988:LEU:HD13	1.89	0.55
1:C:929:GLY:O	1:C:933:THR:HG23	2.06	0.55
1:B:32:ILE:CG1	1:B:298:ASN:HB2	2.35	0.54
1:C:725:TYR:OH	1:C:806:GLY:HA3	2.07	0.54
1:A:93:THR:OG1	1:A:673:LEU:HD11	2.07	0.54
1:B:363:ARG:HD3	1:B:496:ILE:O	2.08	0.54
1:A:133:SER:HB2	1:A:672:GLU:HA	1.89	0.54
1:C:399:VAL:HG11	1:C:988:LEU:CD1	2.37	0.54
1:C:752:TRP:O	1:C:773:GLN:NE2	2.39	0.54
1:A:418:ARG:NH2	1:A:437:GLN:OE1	2.40	0.54
1:B:840:MET:O	1:B:844:GLU:HG3	2.08	0.54
1:C:450:SER:HB2	1:C:475:VAL:HG13	1.89	0.53
1:B:361:ASN:O	1:B:365:THR:HG23	2.08	0.53
1:B:450:SER:O	1:B:454:VAL:HG13	2.08	0.53
1:B:400:LEU:HB3	1:B:932:THR:HG21	1.90	0.53
1:C:637:GLN:HB2	1:C:642:LYS:NZ	2.24	0.53
1:C:1003:GLY:O	1:C:1007:ILE:HG12	2.09	0.53
1:B:145:GLU:OE2	1:B:322:VAL:HG11	2.08	0.53
1:A:399:VAL:O	1:A:402:ILE:HG12	2.09	0.53
1:B:691:HIS:CE1	1:B:812:SER:HB2	2.44	0.53
1:B:637:GLN:O	1:B:641:GLN:NE2	2.42	0.53
1:C:188:LEU:HD23	1:C:266:ALA:HB2	1.90	0.53
1:B:356:TYR:O	1:B:360:GLN:N	2.37	0.53
1:C:895:SER:HB3	1:C:1032:PHE:CD2	2.44	0.53
1:B:31:PRO:O	1:B:32:ILE:HD13	2.09	0.52
1:B:526:TYR:CD2	1:B:971:LEU:HD22	2.44	0.52
1:A:884:PHE:CD1	1:A:901:ILE:HD11	2.44	0.52
1:B:173:GLY:O	1:C:70:SER:OG	2.17	0.52
1:A:756:TYR:HB2	1:A:771:TYR:CE2	2.44	0.52
1:B:35:TYR:CD1	1:B:670:ILE:HD11	2.44	0.52
1:B:573:VAL:HB	1:B:626:VAL:HB	1.91	0.52
1:B:577:THR:HG21	1:B:586:THR:HG22	1.91	0.52
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.91	0.52
1:C:519:PHE:HZ	1:C:972:ARG:HG3	1.75	0.52
1:A:724:GLN:HB2	1:C:233:THR:O	2.10	0.52
1:C:558:LEU:HD23	1:C:922:ASN:HB2	1.92	0.52
1:C:695:MET:SD	1:C:698:ARG:NH2	2.83	0.52
1:A:150:ASN:OD1	1:A:152:TYR:N	2.43	0.52
1:A:573:VAL:HB	1:A:626:VAL:HB	1.92	0.52
1:A:756:TYR:CE1	1:A:769:LYS:HD3	2.44	0.52



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:716:PRO:O	1:A:718:GLY:N	2.42	0.52	
1:B:816:GLU:OE1	1:B:824:MET:HA	2.09	0.52	
1:A:236:GLU:HB2	1:B:748:PHE:CE2	2.45	0.51	
1:C:955:GLU:O	1:C:957:MET:HG3	2.10	0.51	
1:C:698:ARG:NH1	1:C:716:PRO:HG3	2.24	0.51	
1:C:464:GLY:HA2	1:C:467:TYR:HB2	1.92	0.51	
1:A:416:VAL:HG22	1:A:431:THR:HA	1.93	0.51	
1:A:907:GLY:O	1:A:1009:GLY:HA2	2.11	0.51	
1:C:40:PRO:HD2	1:C:673:LEU:HD13	1.92	0.51	
1:B:348:ILE:O	1:B:351:VAL:HG12	2.10	0.51	
1:C:463:VAL:HG22	1:C:562:PHE:CE1	2.45	0.51	
1:C:463:VAL:HG22	1:C:562:PHE:HE1	1.75	0.51	
1:A:560:LYS:HG2	1:A:922:ASN:HB3	1.93	0.51	
1:B:526:TYR:O	1:B:530:VAL:HG23	2.11	0.51	
1:B:985:VAL:HG21	1:B:1006:VAL:CG2	2.41	0.51	
1:B:38:ILE:HG22	1:B:462:SER:HB3	1.92	0.51	
1:A:184:MET:HB3	1:A:770:VAL:HG22	1.92	0.51	
1:C:463:VAL:HG21	1:C:868:SER:CB	2.39	0.51	
1:A:223:PRO:HD3	1:B:275:TYR:CD2	2.45	0.51	
1:A:4:PHE:O	1:A:8:ARG:HD2	2.10	0.50	
1:C:638:SER:H	1:C:642:LYS:HE2	1.76	0.50	
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.94	0.50	
1:A:903:VAL:HB	1:A:1021:ILE:HD11	1.93	0.50	
1:B:68:GLN:HG3	1:B:114:ALA:CB	2.41	0.50	
1:C:891:TYR:OH	1:C:942:ILE:HD11	2.11	0.50	
1:A:73:ASP:OD2	1:C:131:LYS:NZ	2.28	0.50	
1:C:218:GLN:CB	1:C:233:THR:HA	2.42	0.50	
1:A:705:ALA:HB1	1:A:714:VAL:HG21	1.93	0.50	
1:C:26:ALA:HB1	1:C:384:SER:HB2	1.94	0.50	
1:C:636:ARG:NH1	1:C:643:VAL:HG23	2.27	0.50	
1:A:816:GLU:OE1	1:A:824:MET:HA	2.12	0.50	
1:A:253:VAL:HG22	1:A:259:GLN:HG2	1.93	0.49	
1:A:17:ILE:O	1:A:21:LEU:HB2	2.12	0.49	
1:A:404:LEU:HD21	1:A:936:LEU:CD2	2.42	0.49	
1:C:36:PRO:O	1:C:38:ILE:HG23	2.12	0.49	
1:A:729:ILE:HD11	1:A:731:ARG:HE	1.76	0.49	
1:B:13:TRP:HD1	1:B:488:LEU:HD11	1.77	0.49	
1:B:534:ILE:HG23	1:B:1026:VAL:HG21	1.95	0.49	
1:B:168:ARG:CZ	1:C:820:GLY:HA3	2.42	0.49	
1:B:267:GLN:C	1:B:268:ILE:HD13	2.32	0.49	
1:B:704:MET:HB3	1:B:846:LEU:HD22	1.93	0.49	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:C:543:ILE:O	1:C:547:VAL:HG23	2.13	0.49	
1:B:32:ILE:HD12	1:B:390:ILE:HB	1.95	0.49	
1:C:776:ALA:O	1:C:780:MET:HG2	2.12	0.49	
1:A:52:ALA:HB1	1:A:56:THR:OG1	2.12	0.49	
1:B:577:THR:HB	1:B:578:PRO:HD2	1.95	0.49	
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.95	0.49	
1:C:897:PRO:O	1:C:901:ILE:HG12	2.13	0.49	
1:C:53:SER:O	1:C:57:VAL:HG23	2.13	0.48	
1:A:762:ASP:OD1	1:A:763:THR:N	2.45	0.48	
1:C:577:THR:HG22	1:C:660:ALA:HB2	1.95	0.48	
1:C:840:MET:HG2	1:C:858:TRP:CZ3	2.48	0.48	
1:C:604:ILE:HG22	1:C:636:ARG:HG2	1.95	0.48	
1:A:213:GLN:CG	1:A:239:LEU:HG	2.43	0.48	
1:B:161:HIS:O	1:B:313:MET:HE1	2.14	0.48	
1:A:108:GLN:NE2	1:B:109:ASN:HB3	2.29	0.48	
1:C:457:ALA:O	1:C:468:ARG:NH1	2.39	0.48	
1:A:14:VAL:HG13	1:B:885:LEU:HB3	1.95	0.48	
1:A:33:ALA:O	1:A:391:ASN:HA	2.14	0.48	
1:A:527:HIS:CE1	1:A:964:LEU:HB3	2.49	0.48	
1:B:13:TRP:CD1	1:B:488:LEU:HD11	2.49	0.48	
1:B:186:ILE:HG23	1:B:268:ILE:HD12	1.95	0.48	
1:A:400:LEU:HD23	1:A:932:THR:HG21	1.95	0.47	
1:B:413:VAL:HG22	1:B:493:CYS:SG	2.54	0.47	
1:A:4:PHE:CE1	1:A:8:ARG:CZ	2.97	0.47	
1:A:617:ALA:HB1	1:A:718:GLY:HA2	1.96	0.47	
1:C:307:ARG:HG2	1:C:325:TYR:CE2	2.50	0.47	
1:A:836:THR:O	1:A:840:MET:HG3	2.14	0.47	
1:A:932:THR:O	1:A:936:LEU:HG	2.14	0.47	
1:C:419:VAL:HG13	1:C:430:ALA:HB1	1.95	0.47	
1:B:34:GLN:HG2	1:B:35:TYR:CE2	2.49	0.47	
1:C:638:SER:O	1:C:642:LYS:HE2	2.14	0.47	
1:A:544:TYR:CD1	1:A:1024:PHE:HZ	2.33	0.47	
1:B:451:ALA:HB1	1:B:882:VAL:HG23	1.96	0.47	
1:B:900:VAL:O	1:B:903:VAL:HG12	2.15	0.47	
1:B:985:VAL:HG21	1:B:1006:VAL:HG23	1.96	0.47	
1:B:45:ILE:HG13	1:B:129:VAL:HG22	1.97	0.47	
1:C:470:PHE:CD2	1:C:928:VAL:HG11	2.49	0.47	
1:A:658:LYS:O	1:A:659:ASP:HB2	2.15	0.47	
1:B:193:LEU:HD23	1:B:265:VAL:HG21	1.97	0.47	
1:B:683:LEU:O	1:B:823:ALA:HA	2.15	0.47	
1:C:491:ALA:O	1:C:495:THR:HG22	2.15	0.47	



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:840:MET:HE1	1:C:866:ILE:HD11	1.96	0.47
1:B:375:VAL:HG22	1:B:484:VAL:HG21	1.96	0.46
1:A:273:GLU:OE2	1:A:769:LYS:HG3	2.15	0.46
1:A:289:LEU:HD12	1:A:289:LEU:HA	1.80	0.46
1:B:13:TRP:HE1	1:B:492:LEU:HD21	1.79	0.46
1:A:739:VAL:HG11	1:A:790:VAL:CG2	2.44	0.46
1:C:76:LEU:HD11	1:C:863:PHE:HE2	1.79	0.46
1:C:251:LEU:HD21	1:C:265:VAL:HG11	1.98	0.46
1:B:186:ILE:HG23	1:B:268:ILE:CD1	2.45	0.46
1:B:637:GLN:O	1:B:641:GLN:HB2	2.15	0.46
1:C:12:ALA:HB1	1:C:488:LEU:HA	1.98	0.46
1:A:559:PRO:HB2	1:A:835:SER:HB3	1.98	0.46
1:A:748:PHE:HZ	1:C:234:ILE:HG21	1.80	0.46
1:C:530:VAL:HG11	1:C:1022:PRO:HG2	1.97	0.46
1:B:45:ILE:HA	1:B:128:SER:O	2.16	0.46
1:B:68:GLN:HG3	1:B:114:ALA:HB2	1.98	0.46
1:B:536:ARG:NH2	1:B:539:ARG:HG2	2.31	0.46
1:C:37:THR:HG21	1:C:296:ASN:HA	1.98	0.46
1:A:363:ARG:HB3	1:A:496:ILE:HG22	1.98	0.46
1:A:895:SER:HB3	1:A:1032:PHE:CD2	2.51	0.46
1:C:647:ILE:HG23	1:C:664:PRO:HG2	1.97	0.46
1:C:38:ILE:HD11	1:C:670:ILE:CD1	2.45	0.45
1:A:139:VAL:O	1:A:326:PRO:HD2	2.16	0.45
1:A:186:ILE:HG12	1:A:268:ILE:HD12	1.97	0.45
1:C:218:GLN:HB2	1:C:233:THR:HA	1.97	0.45
1:C:577:THR:CG2	1:C:586:THR:HG22	2.47	0.45
1:A:701:LEU:HB2	1:A:850:LEU:HD11	1.99	0.45
1:C:355:MET:SD	1:C:368:PRO:HB2	2.56	0.45
1:C:603:ASP:OD1	1:C:603:ASP:N	2.49	0.45
1:A:3:LYS:HA	1:A:6:ILE:HD12	1.97	0.45
1:B:382:ILE:HD12	1:B:480:LEU:HD12	1.97	0.45
1:C:298:ASN:OD1	1:C:301:ALA:HB3	2.17	0.45
1:A:885:LEU:HB3	1:C:14:VAL:HG13	1.98	0.45
1:B:615:SER:HB3	1:B:623:SER:OG	2.17	0.45
1:C:46:THR:OG1	1:C:128:SER:OG	2.34	0.45
1:A:678:GLY:HA3	1:A:828:GLY:O	2.16	0.45
1:A:708:ASP:OD2	1:A:842:ALA:HB1	2.17	0.45
1:A:729:ILE:O	1:A:729:ILE:HG13	2.17	0.45
1:B:448:VAL:O	1:B:452:VAL:HG23	2.15	0.45
1:C:530:VAL:CG1	1:C:1022:PRO:HG2	2.46	0.45
1:C:526:TYR:CD2	1:C:971:LEU:HD22	2.52	0.45



	• • • • • • •	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:451:ALA:CB	1:B:882:VAL:HG23	2.46	0.45	
1:B:456:VAL:CG1	1:B:467:TYR:HB3	2.46	0.45	
1:B:888:ALA:O	1:B:892:GLU:N	2.50	0.45	
1:B:952:GLN:HG3	1:B:957:MET:O	2.16	0.45	
1:A:900:VAL:O	1:A:903:VAL:HG12	2.16	0.45	
1:A:197:GLY:HA2	1:A:797:MET:SD	2.57	0.44	
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.16	0.44	
1:C:367:ILE:O	1:C:370:ILE:HG22	2.16	0.44	
1:A:943:LEU:O	1:A:970:ARG:HD2	2.17	0.44	
1:B:466:ILE:HG21	1:B:924:VAL:HG21	1.99	0.44	
1:B:540:TRP:HA	1:B:543:ILE:HB	2.00	0.44	
1:B:809:THR:OG1	1:B:810:TYR:N	2.50	0.44	
1:B:140:LEU:HD21	1:B:310:ILE:HG13	1.99	0.44	
1:C:468:ARG:HA	1:C:471:SER:HB3	1.99	0.44	
1:A:307:ARG:HG3	1:A:325:TYR:OH	2.18	0.44	
1:A:698:ARG:HD2	1:A:702:LEU:HG	1.99	0.44	
1:B:75:PHE:CE1	1:B:92:ILE:HG23	2.53	0.44	
1:B:244:GLU:O	1:B:248:ASN:ND2	2.36	0.44	
1:B:666:ASN:OD1	1:B:667:PRO:HD2	2.18	0.44	
1:B:988:LEU:HD13	1:B:1002:ILE:HD11	2.00	0.44	
1:A:453:PHE:CZ	1:A:932:THR:HG22	2.49	0.44	
1:B:186:ILE:HG13	1:B:772:VAL:HG12	2.00	0.44	
1:C:587:ALA:HB2	1:C:612:ASN:ND2	2.33	0.44	
1:A:457:ALA:HB2	1:A:472:LEU:HD21	2.00	0.44	
1:B:211:ASN:OD1	1:B:240:LEU:N	2.46	0.44	
1:B:250:LEU:HD13	1:C:735:ASN:CB	2.48	0.44	
1:B:1002:ILE:HG13	1:B:1003:GLY:N	2.33	0.43	
1:C:666:ASN:HB3	1:C:677:ALA:HB2	2.00	0.43	
1:B:8:ARG:HB2	1:C:892:GLU:OE2	2.19	0.43	
1:C:393:LEU:HD13	1:C:466:ILE:HG23	2.00	0.43	
1:C:541:LEU:HA	1:C:541:LEU:HD23	1.76	0.43	
1:C:982:ILE:HG13	1:C:1010:MET:HG2	2.00	0.43	
1:A:167:SER:O	1:B:70:SER:HB2	2.18	0.43	
1:A:489:THR:OG1	1:A:490:PRO:HD3	2.18	0.43	
1:A:539:ARG:O	1:A:542:ILE:HB	2.19	0.43	
1:A:791:ARG:HB3	1:A:797:MET:SD	2.58	0.43	
1:B:45:ILE:HD11	1:B:107:VAL:CG1	2.49	0.43	
1:B:156:ASN:OD1	1:B:768:LYS:NZ	2.51	0.43	
1:B:393:LEU:HD23	1:B:393:LEU:HA	1.79	0.43	
1:B:767:ILE:HG12	1:C:60:THR:HG21	2.00	0.43	
1:A:163:LYS:HG3	1:A:175:VAL:HG11	2.01	0.43	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:407:ASP:O	1:A:411:VAL:HG23	2.18	0.43
1:A:722:THR:HG22	1:A:813:PRO:HD3	1.99	0.43
1:A:1007:ILE:O	1:A:1011:ILE:HG12	2.19	0.43
1:B:925:PHE:HB3	1:B:1002:ILE:CG2	2.49	0.43
1:B:328:ASP:OD1	1:B:330:THR:OG1	2.31	0.43
1:B:428:LYS:HB3	1:B:432:ARG:NH2	2.33	0.43
1:C:332:PHE:HB2	1:C:633:TYR:OH	2.19	0.43
1:A:717:ASN:CG	1:A:718:GLY:N	2.71	0.43
1:B:502:GLN:N	1:B:502:GLN:OE1	2.51	0.43
1:C:134:SER:O	1:C:136:PHE:N	2.51	0.43
1:C:939:LYS:O	1:C:942:ILE:HG22	2.19	0.43
1:A:2:ALA:O	1:A:6:ILE:HG13	2.18	0.43
1:A:615:SER:HA	1:A:625:LEU:HG	2.01	0.43
1:B:651:PHE:CE1	1:B:664:PRO:HD2	2.54	0.43
1:C:196:TYR:HB2	1:C:198:LEU:HD23	2.01	0.43
1:A:76:LEU:HD12	1:A:76:LEU:HA	1.83	0.43
1:B:23:GLY:O	1:B:27:ILE:HG12	2.19	0.43
1:B:638:SER:O	1:B:642:LYS:HE2	2.18	0.43
1:B:4:PHE:CE2	1:B:8:ARG:HD2	2.54	0.43
1:C:136:PHE:HD1	1:C:136:PHE:HA	1.67	0.43
1:C:791:ARG:HB3	1:C:797:MET:SD	2.59	0.43
1:A:470:PHE:CE2	1:A:928:VAL:HB	2.54	0.42
1:A:485:ALA:HA	1:A:489:THR:OG1	2.19	0.42
1:A:776:ALA:O	1:A:780:MET:HG2	2.19	0.42
1:A:973:PRO:O	1:A:976:MET:HB3	2.19	0.42
1:B:734:ALA:HB1	1:B:744:ILE:HD11	2.01	0.42
1:A:58:GLU:HA	1:A:62:THR:HB	2.01	0.42
1:A:227:GLY:O	1:A:229:VAL:HG13	2.18	0.42
1:B:467:TYR:CE1	1:B:924:VAL:HG23	2.54	0.42
1:B:577:THR:OG1	1:B:586:THR:HG22	2.19	0.42
1:B:698:ARG:HD2	1:B:716:PRO:HB3	2.01	0.42
1:C:399:VAL:HG11	1:C:988:LEU:CD2	2.49	0.42
1:A:683:LEU:HG	1:A:854:ILE:CG2	2.49	0.42
1:A:1012:THR:O	1:A:1016:LEU:HB2	2.19	0.42
1:C:141:ALA:HB1	1:C:286:THR:HG21	2.01	0.42
1:C:419:VAL:CG1	1:C:430:ALA:HB1	2.50	0.42
1:A:3:LYS:HE2	1:A:432:ARG:HD3	2.00	0.42
1:A:300:LEU:N	1:A:300:LEU:HD12	2.35	0.42
1:A:687:ALA:HB2	1:C:316:TYR:CD1	2.54	0.42
1:B:762:ASP:HB2	1:B:768:LYS:HE3	2.01	0.42
1:B:960:ILE:HD12	2:B:1102:UMQ:HD1	2.02	0.42



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:149:MET:HB3	1:B:153:ASP:HB2	2.02	0.42	
1:B:571:MET:HB3	1:B:628:VAL:HG13	2.01	0.42	
1:C:816:GLU:HB2	1:C:823:ALA:O	2.19	0.42	
1:A:644:GLN:OE1	1:A:644:GLN:N	2.52	0.42	
1:B:903:VAL:HG11	1:B:938:ALA:HA	2.01	0.42	
1:C:388:PHE:HE2	1:C:469:GLN:HA	1.84	0.42	
1:C:891:TYR:CD2	1:C:896:ILE:HG21	2.54	0.42	
1:A:492:LEU:HD23	1:A:492:LEU:HA	1.91	0.42	
1:A:766:ARG:HB3	1:A:768:LYS:HE3	2.01	0.42	
1:B:293:LEU:HD12	1:B:293:LEU:HA	1.77	0.42	
1:B:526:TYR:OH	1:B:967:ALA:HB1	2.20	0.42	
1:B:872:ALA:N	1:B:873:PRO:HD2	2.34	0.42	
1:C:34:GLN:HB2	1:C:333:VAL:HG13	2.01	0.42	
1:A:278:ASP:HB3	1:A:612:ASN:HB3	2.02	0.42	
1:B:684:THR:HG22	1:B:823:ALA:HB2	2.02	0.42	
1:C:949:ARG:NH2	1:C:952:GLN:OE1	2.52	0.42	
1:C:960:ILE:O	1:C:964:LEU:HG	2.19	0.42	
1:A:185:ARG:HB2	1:A:269:GLY:O	2.19	0.42	
1:A:454:VAL:N	1:A:455:PRO:CD	2.83	0.42	
1:A:840:MET:HE2	1:A:866:ILE:HD11	2.02	0.42	
1:B:127:LEU:HD23	1:B:127:LEU:HA	1.71	0.42	
1:B:187:TRP:HA	1:B:773:GLN:O	2.20	0.41	
1:B:787:ILE:HD13	1:B:787:ILE:HG21	1.87	0.41	
2:B:1102:UMQ:H2'1	2:B:1102:UMQ:HB2	2.02	0.41	
1:C:193:LEU:HD23	1:C:265:VAL:HG21	2.02	0.41	
1:C:358:PHE:CD2	1:C:976:MET:HG2	2.55	0.41	
1:A:372:VAL:HB	1:A:373:PRO:HD3	2.01	0.41	
1:B:854:ILE:HG23	1:B:854:ILE:HD12	1.79	0.41	
1:B:1029:ARG:O	1:B:1033:SER:HB2	2.20	0.41	
1:B:186:ILE:CG1	1:B:772:VAL:HG12	2.50	0.41	
1:C:137:LEU:HD11	1:C:299:ALA:HB1	2.02	0.41	
1:C:679:PHE:CE2	1:C:828:GLY:HA3	2.56	0.41	
1:C:911:ALA:HB2	1:C:933:THR:HG21	2.03	0.41	
1:A:463:VAL:HG21	1:A:871:GLN:HG3	2.02	0.41	
1:B:94:PHE:CE1	1:B:103:ALA:HB1	2.55	0.41	
1:B:760:PHE:CE1	1:B:768:LYS:HB2	2.56	0.41	
1:C:637:GLN:HA	1:C:642:LYS:HD3	2.03	0.41	
1:B:178:PHE:HB2	1:B:288:ALA:HB3	2.03	0.41	
1:B:512:PHE:O	1:B:515:PHE:N	2.53	0.41	
1:C:470:PHE:CE1	1:C:1002:ILE:HD11	2.56	0.41	
1:C:572:PHE:HB2	1:C:665:PHE:CE2	2.56	0.41	



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:213:GLN:HG3	1:A:239:LEU:HG	2.02	0.41
1:A:452:VAL:HG22	1:A:883:VAL:HG11	2.01	0.41
1:B:17:ILE:HA	1:B:20:MET:HE3	2.02	0.41
1:B:808:TRP:HB3	3:B:1104:PG4:H31	2.02	0.41
1:A:38:ILE:HD13	1:A:466:ILE:HD11	2.02	0.41
1:A:186:ILE:HD13	1:A:262:LEU:HD21	2.02	0.41
1:B:337:ILE:O	1:B:340:VAL:HG12	2.21	0.41
1:A:402:ILE:HG13	1:A:403:GLY:N	2.36	0.41
1:B:151:LYS:HE2	1:B:152:TYR:CZ	2.56	0.41
1:C:414:GLU:HG2	1:C:972:ARG:HH21	1.85	0.41
1:B:553:LEU:HD23	1:B:553:LEU:HA	1.79	0.41
1:B:605:VAL:HG13	1:B:628:VAL:HG23	2.02	0.41
1:B:1033:SER:O	2:B:1102:UMQ:HL2	2.21	0.41
1:C:202:ASP:OD2	1:C:791:ARG:NH1	2.54	0.41
1:C:286:THR:HG22	1:C:287:ALA:N	2.36	0.41
1:C:597:LEU:HD21	1:C:650:MET:SD	2.61	0.41
1:C:638:SER:N	1:C:642:LYS:HE2	2.35	0.41
1:A:10:ILE:HD12	1:B:894:TRP:CE2	2.56	0.41
1:A:604:ILE:HD11	1:A:641:GLN:O	2.20	0.41
1:C:399:VAL:O	1:C:402:ILE:HG12	2.20	0.41
1:A:562:PHE:CE2	1:A:563:LEU:HD23	2.56	0.40
1:B:38:ILE:CG2	1:B:462:SER:HB3	2.52	0.40
1:A:434:ALA:O	1:A:438:ILE:HG12	2.21	0.40
1:A:739:VAL:HG11	1:A:790:VAL:HG23	2.02	0.40
1:B:186:ILE:HB	1:B:772:VAL:HG12	2.03	0.40
1:B:840:MET:HG2	1:B:858:TRP:CH2	2.56	0.40
1:C:3:LYS:HE2	1:C:439:THR:HG21	2.04	0.40
1:A:3:LYS:CE	1:A:432:ARG:HD3	2.52	0.40
1:A:58:GLU:OE2	1:A:817:ARG:HD3	2.20	0.40
1:A:534:ILE:O	1:A:537:SER:HB2	2.21	0.40
1:A:585:THR:HG22	1:A:588:ARG:NH1	2.36	0.40
1:A:880:ILE:HA	1:A:883:VAL:HG22	2.04	0.40
1:C:135:SER:O	1:C:137:LEU:N	2.55	0.40
1:A:4:PHE:HE1	1:A:8:ARG:CZ	2.35	0.40
1:A:193:LEU:HA	1:A:193:LEU:HD23	1.74	0.40
1:B:776:ALA:O	1:B:780:MET:HG2	2.21	0.40
1:C:58:GLU:HA	1:C:62:THR:HB	2.03	0.40
1:C:762:ASP:HB3	1:C:764:ASP:OD1	2.22	0.40
1:C:1027:LYS:HD3	1:C:1027:LYS:HA	1.92	0.40
1:B:132:SER:H	1:B:132:SER:HG	1.66	0.40
1:B:472:LEU:HD23	1:B:472:LEU:HA	1.85	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:LYS:HZ3	1:C:436:GLY:HA2	1.87	0.40
1:C:663:ILE:HD12	1:C:715:ARG:HB3	2.02	0.40
1:C:704:MET:HE3	1:C:849:LYS:HB2	2.04	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	1015/1051~(97%)	973 (96%)	40 (4%)	2 (0%)	47	76
1	В	1020/1051~(97%)	1000 (98%)	19 (2%)	1 (0%)	51	80
1	С	1014/1051~(96%)	989 (98%)	25 (2%)	0	100	100
All	All	3049/3153~(97%)	2962 (97%)	84 (3%)	3 (0%)	51	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	282	ASN
1	А	717	ASN
1	А	2	ALA

5.3.2 Protein sidechains (i)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	828/855~(97%)	826 (100%)	2 (0%)	93	98
1	В	833/855~(97%)	826~(99%)	7 (1%)	81	93
1	С	827/855~(97%)	820 (99%)	7 (1%)	81	93
All	All	2488/2565~(97%)	2472 (99%)	16 (1%)	86	95

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	11	PHE
1	А	49	TYR
1	В	49	TYR
1	В	470	PHE
1	В	500	ILE
1	В	512	PHE
1	В	637	GLN
1	В	717	ASN
1	В	1032	PHE
1	С	11	PHE
1	С	136	PHE
1	С	277	PHE
1	С	519	PHE
1	С	644	GLN
1	С	669	SER
1	С	829	GLN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such side chains are listed below:

Mol	Chain	Res	Type
1	А	527	HIS
1	В	827	GLN
1	В	952	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)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Turne	Chain	Dec	Tink	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	UMQ	В	1101	-	$35,\!35,\!35$	1.61	8 (22%)	46,46,46	1.74	15 (32%)
3	PG4	В	1104	-	12,12,12	0.57	0	11,11,11	0.56	0
2	UMQ	В	1103	-	35,35,35	1.65	4 (11%)	46,46,46	1.58	9 (19%)
2	UMQ	В	1102	-	35,35,35	2.42	12 (34%)	46,46,46	2.02	14 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UMQ	В	1101	-	-	8/20/60/60	0/2/2/2
3	PG4	В	1104	-	-	5/10/10/10	-
2	UMQ	В	1103	-	-	10/20/60/60	0/2/2/2
2	UMQ	В	1102	-	-	12/20/60/60	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	1102	UMQ	C3'- $C2$ '	5.62	1.66	1.52
2	В	1102	UMQ	C1'-C2'	5.04	1.67	1.52
2	В	1102	UMQ	O1'-C1'	5.04	1.48	1.40
2	В	1101	UMQ	C3-C4	4.54	1.63	1.52
2	В	1102	UMQ	C3-C4	4.53	1.63	1.52
2	В	1101	UMQ	C4-C5	4.43	1.62	1.53



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	1103	UMQ	C3'-C2'	4.24	1.63	1.52
2	В	1102	UMQ	C4'-C5'	4.13	1.63	1.52
2	В	1102	UMQ	O5-C1	3.23	1.50	1.41
2	В	1103	UMQ	O1'-C1'	3.11	1.45	1.40
2	В	1102	UMQ	C3'-C4'	2.98	1.60	1.52
2	В	1102	UMQ	CB-CA	2.92	1.63	1.51
2	В	1102	UMQ	C1-C2	2.74	1.60	1.52
2	В	1102	UMQ	O1'-CA	2.62	1.50	1.43
2	В	1101	UMQ	C1-C2	2.56	1.59	1.52
2	В	1103	UMQ	CB-CA	2.45	1.61	1.51
2	В	1101	UMQ	O1'-C1'	2.33	1.44	1.40
2	В	1103	UMQ	O5-C1	2.27	1.47	1.41
2	В	1102	UMQ	CF-CD	2.22	1.64	1.51
2	В	1101	UMQ	O1-C4'	-2.19	1.38	1.43
2	В	1101	UMQ	O2'-C2'	-2.16	1.37	1.43
2	В	1101	UMQ	CH-CG	2.14	1.63	1.51
2	В	1102	UMQ	O5'-C1'	2.12	1.47	1.41
2	В	1101	UMQ	O3'-C3'	-2.10	1.38	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	1102	UMQ	O5'-C5'-C4'	5.03	120.36	109.75
2	В	1101	UMQ	O3-C3-C2	-4.70	99.49	110.35
2	В	1102	UMQ	CA-01'-C1'	4.53	121.35	113.84
2	В	1102	UMQ	O1'-C1'-C2'	4.39	115.16	108.30
2	В	1103	UMQ	C3'-C4'-C5'	-4.22	101.25	110.93
2	В	1101	UMQ	O5'-C5'-C4'	3.72	117.60	109.75
2	В	1102	UMQ	O3-C3-C2	-3.72	101.74	110.35
2	В	1102	UMQ	O5-C1-C2	3.52	117.80	110.35
2	В	1102	UMQ	O6-C6-C5	-3.04	100.87	111.29
2	В	1103	UMQ	O5'-C5'-C4'	2.99	116.06	109.75
2	В	1103	UMQ	O5'-C1'-C2'	-2.88	104.25	110.35
2	В	1101	UMQ	O2'-C2'-C1'	-2.87	103.07	110.05
2	В	1103	UMQ	C1-O5-C5	2.77	119.13	113.69
2	В	1102	UMQ	C1-O5-C5	2.77	119.13	113.69
2	В	1101	UMQ	O3'-C3'-C4'	-2.76	102.62	109.94
2	В	1101	UMQ	C6'-C5'-C4'	-2.70	105.46	113.33
2	В	1103	UMQ	CA-01'-C1'	2.70	118.31	113.84
2	В	1102	UMQ	O6'-C6'-C5'	-2.70	102.03	111.29
2	В	1103	UMQ	O1-C4'-C3'	2.70	114.45	107.28
2	В	1101	UMQ	C3-C4-C5	2.69	115.04	110.24



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	1102	UMQ	O5-C5-C4	2.68	114.56	109.69
2	В	1101	UMQ	O2-C2-C3	-2.67	104.17	110.35
2	В	1101	UMQ	O5-C5-C4	2.57	114.36	109.69
2	В	1102	UMQ	O3'-C3'-C2'	2.54	116.22	110.35
2	В	1101	UMQ	C4-C3-C2	2.51	115.20	110.82
2	В	1102	UMQ	C1'-C2'-C3'	2.33	114.86	110.00
2	В	1103	UMQ	O5-C5-C4	2.33	113.93	109.69
2	В	1101	UMQ	O5'-C1'-O1'	-2.27	104.60	109.97
2	В	1103	UMQ	O1'-C1'-C2'	2.21	111.76	108.30
2	В	1101	UMQ	C3'-C4'-C5'	-2.20	105.89	110.93
2	В	1101	UMQ	O6-C6-C5	-2.20	103.75	111.29
2	В	1101	UMQ	C2'-C3'-C4'	2.17	114.63	109.68
2	В	1102	UMQ	O3-C3-C4	2.16	115.34	110.35
2	В	1103	UMQ	O1-C4'-C5'	2.14	115.32	109.45
2	В	1101	UMQ	O2'-C2'-C3'	-2.07	105.56	110.35
2	В	1101	UMQ	C1'-O5'-C5'	2.07	117.75	113.69
2	В	1102	UMQ	C6'-C5'-C4'	-2.06	107.32	113.33
2	В	1102	UMQ	O1-C4'-C3'	2.05	112.73	107.28

There are no chirality outliers.

All ((35)) torsion	outliers	are	listed	below:
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Mol	Chain	\mathbf{Res}	Type	Atoms
2	В	1102	UMQ	O5-C1-O1-C4'
2	В	1102	UMQ	C2'-C1'-O1'-CA
2	В	1102	UMQ	O5'-C1'-O1'-CA
2	В	1101	UMQ	O5-C5-C6-O6
2	В	1102	UMQ	O5-C5-C6-O6
2	В	1101	UMQ	C4-C5-C6-O6
2	В	1102	UMQ	C4-C5-C6-O6
2	В	1103	UMQ	O5-C5-C6-O6
2	В	1103	UMQ	CC-CD-CF-CG
2	В	1102	UMQ	O5'-C5'-C6'-O6'
2	В	1103	UMQ	C4-C5-C6-O6
2	В	1101	UMQ	CF-CG-CH-CI
2	В	1101	UMQ	CB-CC-CD-CF
2	В	1103	UMQ	CB-CC-CD-CF
2	В	1101	UMQ	CA-CB-CC-CD
2	В	1101	UMQ	CB-CA-O1'-C1'
2	В	1103	UMQ	CB-CA-O1'-C1'
2	В	1102	UMQ	O1'-CA-CB-CC
2	В	1102	UMQ	CC-CD-CF-CG



Mol	Chain	Res	Type	Atoms
2	В	1102	UMQ	CH-CI-CJ-CK
2	В	1103	UMQ	CF-CG-CH-CI
3	В	1104	PG4	O4-C7-C8-O5
2	В	1101	UMQ	CG-CH-CI-CJ
2	В	1102	UMQ	CB-CC-CD-CF
2	В	1103	UMQ	CH-CI-CJ-CK
2	В	1103	UMQ	O1'-CA-CB-CC
2	В	1102	UMQ	CB-CA-O1'-C1'
2	В	1103	UMQ	CD-CF-CG-CH
2	В	1102	UMQ	CA-CB-CC-CD
3	В	1104	PG4	C5-C6-O4-C7
2	В	1103	UMQ	CA-CB-CC-CD
3	В	1104	PG4	O1-C1-C2-O2
3	В	1104	PG4	O3-C5-C6-O4
2	В	1101	UMQ	CC-CD-CF-CG
3	В	1104	PG4	O2-C3-C4-O3

Continued from previous page...

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1101	UMQ	1	0
3	В	1104	PG4	1	0
2	В	1102	UMQ	4	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	1019/1051~(96%)	0.43	91 (8%) 9 8	68, 120, 184, 336	0
1	В	1024/1051~(97%)	0.39	77 (7%) 14 12	72, 110, 147, 206	0
1	С	1018/1051~(96%)	0.57	111 (10%) 5 5	72, 125, 190, 294	0
All	All	3061/3153~(97%)	0.46	279 (9%) 9 7	68, 116, 176, 336	0

All (279) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	501	PRO	14.3
1	С	633	TYR	13.7
1	В	500	ILE	11.4
1	С	635	GLN	9.3
1	С	1026	VAL	8.6
1	В	502	GLN	8.1
1	А	713	GLY	7.6
1	С	639	SER	7.6
1	В	423	GLU	7.3
1	С	800	PHE	7.1
1	В	499	PRO	6.8
1	А	425	LEU	6.4
1	В	498	LYS	6.1
1	С	641	GLN	5.9
1	С	638	SER	5.6
1	С	636	ARG	5.6
1	С	642	LYS	5.6
1	А	435	MET	5.4
1	А	829	GLN	5.3
1	А	951	LEU	5.3
1	С	802	ALA	5.3
1	С	966	ALA	5.2
1	В	348	ILE	5.1



Mol	Chain	Res	Type	RSRZ
1	А	439	THR	5.1
1	С	640	ASP	5.0
1	С	568	GLN	4.9
1	С	281	TYR	4.9
1	С	603	ASP	4.8
1	В	640	ASP	4.8
1	С	417	GLU	4.8
1	С	799	PRO	4.8
1	С	1028	VAL	4.7
1	С	149	MET	4.6
1	С	961	GLU	4.6
1	А	675	THR	4.5
1	С	607	SER	4.5
1	A	712	ARG	4.5
1	А	416	VAL	4.4
1	С	801	SER	4.4
1	С	429	GLU	4.2
1	А	402	ILE	4.2
1	С	609	PHE	4.2
1	В	347	GLY	4.2
1	С	604	ILE	4.1
1	В	198	LEU	4.1
1	С	790	VAL	4.0
1	В	424	GLY	4.0
1	А	830	ALA	3.9
1	А	540	TRP	3.9
1	В	351	VAL	3.8
1	С	259	GLN	3.8
1	С	618	GLY	3.8
1	В	182	TYR	3.8
1	С	786	ASN	3.7
1	С	517	ARG	3.7
1	А	537	SER	3.7
1	В	300	LEU	3.7
1	А	952	GLN	3.7
1	С	570	LEU	3.7
1	В	425	LEU	3.7
1	С	803	PHE	3.6
1	С	634	SER	3.6
1	В	959	PRO	3.6
1	A	866	ILE	3.6
1	В	960	ILE	3.6



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Mol	Chain	Res	Type	RSRZ
1	А	230	LEU	3.6
1	С	964	LEU	3.6
1	В	183	ALA	3.5
1	С	419	VAL	3.5
1	С	142	PHE	3.5
1	А	429	GLU	3.5
1	С	431	THR	3.5
1	В	137	LEU	3.5
1	А	3	LYS	3.5
1	В	866	ILE	3.5
1	С	141	ALA	3.5
1	С	798	VAL	3.5
1	В	426	PRO	3.4
1	С	148	SER	3.4
1	А	535	LYS	3.4
1	В	268	ILE	3.4
1	С	960	ILE	3.4
1	С	531	HIS	3.4
1	А	426	PRO	3.4
1	С	963	ALA	3.4
1	С	739	VAL	3.4
1	С	797	MET	3.4
1	В	140	LEU	3.3
1	А	716	PRO	3.3
1	А	832	PRO	3.3
1	С	198	LEU	3.3
1	А	860	GLY	3.3
1	А	437	GLN	3.3
1	С	327	TYR	3.3
1	A	438	ILE	3.3
1	С	516	ASN	3.3
1	А	423	GLU	3.3
1	A	442	LEU	3.3
1	А	348	ILE	3.2
1	В	848	LYS	3.2
1	В	664	PRO	3.2
1	А	710	THR	3.2
1	A	884	PHE	3.2
1	С	4	PHE	3.2
1	А	405	LEU	3.2
1	С	519	PHE	3.2
1	A	6	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	В	199	THR	3.2
1	В	290	GLY	3.2
1	А	362	LEU	3.2
1	В	289	LEU	3.2
1	В	362	LEU	3.2
1	А	515	PHE	3.2
1	А	441	ALA	3.2
1	С	710	THR	3.2
1	В	645	ALA	3.1
1	С	787	ILE	3.1
1	В	291	ILE	3.1
1	В	849	LYS	3.1
1	C	701	LEU	3.0
1	С	616	PHE	3.0
1	В	264	ASP	3.0
1	В	588	ARG	3.0
1	С	1024	PHE	3.0
1	А	352	PHE	2.9
1	С	266	ALA	2.9
1	С	737	LEU	2.9
1	С	49	TYR	2.9
1	В	405	LEU	2.9
1	А	680	ASP	2.9
1	В	193	LEU	2.9
1	С	707	LYS	2.9
1	С	569	GLY	2.9
1	С	226	PRO	2.9
1	С	285	PRO	2.8
1	С	169	ILE	2.8
1	В	790	VAL	2.8
1	В	138	LEU	2.8
1	С	370	ILE	2.8
1	В	188	LEU	2.8
1	В	269	GLY	2.8
1	В	402	ILE	2.8
1	C	147	GLY	2.8
1	С	410	ILE	2.8
1	A	431	THR	2.8
1	В	141	ALA	2.7
1	A	847	ALA	2.7
1	C	959	PRO	2.7
1	A	827	GLN	2.7



Mol	Chain	Res	Type	RSRZ
1	С	337	ILE	2.7
1	С	943	LEU	2.7
1	С	250	LEU	2.7
1	С	409	ALA	2.7
1	С	366	ILE	2.7
1	В	662	VAL	2.7
1	А	984	GLY	2.7
1	А	533	VAL	2.6
1	В	422	GLU	2.6
1	С	785	MET	2.6
1	А	845	THR	2.6
1	В	429	GLU	2.6
1	А	641	GLN	2.6
1	С	258	SER	2.6
1	В	304	LYS	2.6
1	А	936	LEU	2.6
1	В	97	GLY	2.6
1	С	426	PRO	2.6
1	А	262	LEU	2.6
1	А	854	ILE	2.5
1	А	841	THR	2.5
1	В	631	LYS	2.5
1	А	1010	MET	2.5
1	В	142	PHE	2.5
1	В	421	ALA	2.5
1	С	791	ARG	2.5
1	А	434	ALA	2.5
1	А	134	SER	2.5
1	А	542	ILE	2.5
1	С	433	LYS	2.5
1	С	333	VAL	2.5
1	С	962	ALA	2.5
1	С	427	PRO	2.5
1	А	831	ALA	2.5
1	С	629	LYS	2.5
1	С	497	LEU	2.5
1	С	606	GLU	2.4
1	В	162	VAL	2.4
1	В	513	GLY	2.4
1	С	371	ALA	2.4
1	В	266	ALA	2.4
1	А	531	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	В	497	LEU	2.4
1	А	265	VAL	2.4
1	С	261	ARG	2.4
1	С	1025	PHE	2.4
1	А	534	ILE	2.4
1	С	140	LEU	2.4
1	С	356	TYR	2.4
1	А	840	MET	2.4
1	С	632	ASP	2.4
1	С	565	ASP	2.4
1	А	744	ILE	2.4
1	С	731	ARG	2.4
1	А	538	GLY	2.4
1	А	810	TYR	2.4
1	С	228	THR	2.4
1	А	674	GLY	2.3
1	А	325	TYR	2.3
1	В	630	LEU	2.3
1	В	370	ILE	2.3
1	А	609	PHE	2.3
1	А	422	GLU	2.3
1	А	539	ARG	2.3
1	В	263	LYS	2.3
1	В	609	PHE	2.3
1	С	778	PHE	2.3
1	А	428	LYS	2.3
1	С	534	ILE	2.3
1	В	259	GLN	2.3
1	В	689	LEU	2.3
1	А	387	GLY	2.3
1	В	616	PHE	2.3
1	С	947	PHE	2.3
1	В	850	LEU	2.3
1	А	638	SER	2.2
1	А	659	ASP	2.2
1	А	30	LEU	2.2
1	С	533	VAL	2.2
1	С	834	LYS	2.2
1	А	266	ALA	2.2
1	В	964	LEU	2.2
1	С	352	PHE	2.2
1	С	704	MET	2.2



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Mol	Chain	Res	Type	RSRZ
1	А	419	VAL	2.2
1	А	747	THR	2.2
1	В	239	LEU	2.2
1	А	790	VAL	2.2
1	А	418	ARG	2.2
1	С	608	ALA	2.2
1	С	284	GLN	2.2
1	С	689	LEU	2.2
1	С	520	ASN	2.2
1	В	327	TYR	2.2
1	А	630	LEU	2.1
1	С	193	LEU	2.1
1	А	494	ALA	2.1
1	A	714	VAL	2.1
1	А	247	GLY	2.1
1	С	425	LEU	2.1
1	А	13	TRP	2.1
1	В	149	MET	2.1
1	С	420	MET	2.1
1	А	82	SER	2.1
1	А	842	ALA	2.1
1	С	994	ALA	2.1
1	А	863	PHE	2.1
1	С	255	GLN	2.1
1	В	128	SER	2.1
1	А	850	LEU	2.1
1	В	344	LEU	2.1
1	В	404	LEU	2.1
1	В	641	GLN	2.1
1	A	859	THR	2.1
1	A	846	LEU	2.1
1	В	324	LYS	2.1
1	С	157	TYR	2.1
1	В	865	GLU	2.1
1	С	154	LEU	2.0
1	B	126	GLY	2.0
1	В	371	ALA	2.0
1	A	541	LEU	2.0
1	A	849	LYS	2.0
1	A	828	GLY	2.0
1	C	526	TYR	2.0
1	В	575	VAL	2.0



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Mol	Chain	Res	Type	RSRZ
1	В	768	LYS	2.0
1	В	643	VAL	2.0
1	А	433	LYS	2.0
1	А	867	GLN	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
2	UMQ	В	1102	34/34	0.69	0.24	111,120,129,131	0
2	UMQ	В	1101	34/34	0.80	0.38	97,113,121,124	0
3	PG4	В	1104	13/13	0.84	0.30	99,103,117,119	0
2	UMQ	В	1103	34/34	0.89	0.34	104,121,125,128	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.

