

Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 05:44 PM EST

PDB ID	:	4FOI
Title	:	Crystal Structure of recombinant human Hexokinase type I mutant D413N
		with Glucose 1,6-bisphosphate
Authors	:	Shen, L.; Honzatko, R.B.
Deposited on	:	2012-06-20
Resolution	:	2.40 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	:	2.36
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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	917	6%	28%	•••
1	В	917	6% 74%	22%	•••

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
5	CIT	А	1007	-	-	-	Х



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14495 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 Hexokinase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	899	Total 7032	C 4407	N 1241	0 1331	${ m S}{53}$	0	0	0
1	В	899	Total 7032	C 4407	N 1241	0 1331	S 53	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual Comment		Reference
А	413	ASN	ASP	engineered mutation	UNP P19367
В	413	ASN	ASP	engineered mutation	UNP P19367

• Molecule 2 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	А	1	Total 12	С 6	O 6	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total C O 12 6 6	0	0
2	В	1	Total C O 12 6 6	0	0
2	В	1	Total C O 12 6 6	0	0

• Molecule 3 is 1,6-di-O-phosphono-alpha-D-glucopyranose (three-letter code: G16) (formula: $C_6H_{13}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	Δ	1	Total	С	Ο	Р	0	0
0	Π	T	20	6	12	2	0	0
3	Δ	1	Total	С	Ο	Р	0	0
0	Л	1	20	6	12	2	0	0
3	В	1	Total	С	Ο	Р	0	0
0	D	1	20	6	12	2	0	0
2	Р	1	Total	С	Ο	Р	0	0
0	D		20	6	12	2	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	2	Total Na 2 2	0	0
4	В	2	Total Na 2 2	0	0



• Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total C O 13 6 7	0	0
5	В	1	Total C O 13 6 7	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	130	Total O 130 130	0	0
6	В	143	Total O 143 143	0	0



Chain B:

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.



74%

22%

• Molecule 1: Hexokinase-1

MET ILE ALA ALA GLN LEU	LEU ALA TYR TYR	PHE THR GLU	LEU LYS D16	D17 Q18	V19 K20 K21	122 D23 V24	N24 Y25 L26	Y27	T35	D38	K03	N50 P57 T58	A59	T66	171 P72	D73	6) A		VQ7	● 86N	E100 • K101 • N107	Q103	
H106 S109 Y112	V119 H120 G121	F137	K142 1143	K1 <mark>46</mark> K147 148	L148 T153 ●	0159 0160	HIDO E165	R174	F175 K176		7198 7199	V204	D209 T210	V211	M215	<mark>q222</mark>	7220	1230	T234	A236 C237	L242	12 <mark>45</mark> D246	
C256 W261 Q262 S269	L270 E271 R274	R279 E280	I281 F293	E294	V29/ S298 G299	T305	L308	K312 M313	G317	L318 L319 T200	F320 E321	63 22 R3 23	E327	K3 <mark>33</mark> F334	N335 T336	S337	1342 E343 V244	N345 N345	E347	N3 <mark>51</mark>	I355 L356	V361 E362 D363	L'OCO
V371 1376 1376 1380	R381 S382 A383 N384	L385 V386	R405 L406 R407	S415	H420 P421	Q422 Y423 S423	5424 R425 R426	L431	P436	D437	F 44.2	5449 G450 K461	M455	V456 T457	H478	L479 T480	K481 D482 M402		T CELI	E496	R500 K501	V508 Me11	ттеп
E524 N525 D532	R539 V540 L541 L542	<mark>V543</mark> K544 I545	R546 S547 ● G548 ●	K549 K550	E554	M555 H556 MEE7	K558 I559	P563	I564 E565	1566 M567		Lo(4 F575	1578 V579	1582	L586	D587 Y588	6590 1590	1031 K592 G503	P594	L598	F602 S603	I615	•
W619 T620 K621 K624	H631 D632 V633	K642 R643 R644	E645 • E646 • F647	D648 L649	V651 V652 V652	V655 Weee		E669	P670 T671	V674	1677 1677	00100 0679	S682	Y686	K691 N692	V693 E694	M695		D7 19 D7 20	1721	N735	S746	•
K763 L767 F768 R769 G770	Q771 1772 K777	T778	F782	06/1	R794 ● L795	A796 L797 1708	L / 98 Q 799 V 800	R801	0805 0806				D843 K844	I845	D852	L854 N855	V 856 T 857 VI 96 9		KRRF	6683	L903 T 004	T905	OTEU
L911 R912 T913 B14 ALA SER	SER																						



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	82.38Å 120.77Å 120.59Å	Deneriten
a, b, c, α , β , γ	90.00° 92.80° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	35.41 - 2.40	Depositor
Resolution (A)	$35.41 \ - \ 2.40$	EDS
% Data completeness	98.5 (35.41-2.40)	Depositor
(in resolution range)	98.5(35.41-2.40)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.08 (at 2.39 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
P. P.	0.247 , 0.273	Depositor
Π, Π_{free}	0.244 , 0.269	DCC
R_{free} test set	4524 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	45.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 40.0	EDS
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.34$	Xtriage
	0.009 for -h,-l,-k	
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
	0.018 for h,-k,-l	
F_o, F_c correlation	0.93	EDS
Total number of atoms	14495	wwPDB-VP
Average B, all atoms $(Å^2)$	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.20% 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: CIT, G16, NA, BGC

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		
1VIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.26	1/7138~(0.0%)	0.47	1/9606~(0.0%)	
1	В	0.27	1/7138~(0.0%)	0.47	1/9606~(0.0%)	
All	All	0.27	2/14276~(0.0%)	0.47	2/19212~(0.0%)	

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	В	0	3

All (2) bond length outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	914	GLU	C-O	8.47	1.39	1.23
1	В	914	GLU	C-O	6.13	1.35	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	914	GLU	CA-C-O	17.38	156.60	120.10
1	В	914	GLU	CA-C-O	13.91	149.32	120.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	102	ASN	Peptide



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Mol	Chain	Res	Type	Group
1	В	345	ASN	Peptide
1	В	99	HIS	Peptide

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	7032	0	7092	258	0
1	В	7032	0	7092	242	0
2	А	24	0	24	0	0
2	В	24	0	24	2	0
3	А	40	0	20	2	0
3	В	40	0	20	1	0
4	А	2	0	0	0	0
4	В	2	0	0	0	0
5	А	13	0	5	0	0
5	В	13	0	5	1	0
6	А	130	0	0	8	0
6	В	143	0	0	14	0
All	All	14495	0	14282	499	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 18.

All (499) 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)
1:B:99:HIS:N	1:B:100:GLU:HB3	1.29	1.47
1:A:496:GLU:HG3	1:A:500:ARG:NH1	1.13	1.45
1:B:323:ARG:NH1	1:B:362:GLU:HB2	1.38	1.34
1:A:496:GLU:CG	1:A:500:ARG:HH12	1.39	1.32
1:A:94:ARG:NH1	1:A:143:ILE:HD11	1.57	1.17
1:B:159:GLN:HG2	6:B:1204:HOH:O	1.44	1.15
1:B:563:PRO:HG2	1:B:566:ILE:HD12	1.25	1.11
1:B:595:ARG:HD2	1:B:648:ASP:OD2	1.50	1.10
1:B:103:GLN:OE1	1:B:103:GLN:HA	1.51	1.10



		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:361:VAL:HB	6:A:1192:HOH:O	1.52	1.09		
1:A:668:GLU:HG3	6:A:1204:HOH:O	0.90	1.07		
1:A:101:LYS:HD2	1:A:101:LYS:N	1.66	1.05		
1:A:820:LYS:NZ	6:A:1198:HOH:O	1.67	1.05		
1:A:595:ARG:HD2	1:A:648:ASP:OD2	1.53	1.04		
1:B:99:HIS:N	1:B:100:GLU:CB	2.21	1.03		
1:A:176:LYS:HE2	6:A:1216:HOH:O	1.58	1.02		
1:A:496:GLU:CG	1:A:500:ARG:NH1	2.09	1.01		
1:B:99:HIS:H	1:B:100:GLU:CB	1.74	0.99		
1:B:564:ILE:H	1:B:564:ILE:CD1	1.74	0.98		
1:A:565:GLU:HG3	1:A:566:ILE:N	1.80	0.96		
1:B:564:ILE:HD12	1:B:564:ILE:N	1.81	0.95		
1:B:335:ASN:OD1	6:B:1150:HOH:O	1.85	0.95		
1:A:98:ASN:OD1	1:A:101:LYS:HD3	1.65	0.95		
1:B:345:ASN:N	1:B:346:LYS:HB3	1.82	0.95		
1:B:563:PRO:CG	1:B:566:ILE:HD12	1.96	0.94		
1:B:323:ARG:NH1	1:B:362:GLU:CB	2.30	0.93		
1:B:797:LEU:HD11	1:B:817:ILE:HD11	1.49	0.93		
1:A:913:THR:HG22	1:A:913:THR:O	1.65	0.93		
1:B:795:LEU:HD11	1:B:799:GLN:HG2	1.51	0.92		
1:B:323:ARG:HH12	1:B:362:GLU:HB2	1.37	0.89		
1:B:323:ARG:HH11	1:B:362:GLU:HB2	1.20	0.89		
1:B:564:ILE:H	1:B:564:ILE:HD12	1.34	0.89		
1:A:97:VAL:HG22	1:A:105:VAL:HA	1.55	0.88		
1:B:103:GLN:HG3	1:B:106:HIS:HB2	1.54	0.88		
1:B:345:ASN:N	1:B:346:LYS:CB	2.36	0.88		
1:A:343:GLU:HG3	1:A:420:HIS:CE1	2.10	0.87		
1:B:99:HIS:H	1:B:100:GLU:HB3	1.06	0.87		
1:A:591:ILE:HG22	1:A:591:ILE:O	1.74	0.87		
1:B:321:GLU:CG	1:B:323:ARG:NH2	2.38	0.86		
1:A:143:ILE:HG21	1:A:148:LEU:CD1	2.05	0.86		
1:B:431:LEU:HD22	1:B:442:PHE:HZ	1.40	0.86		
1:A:563:PRO:HG2	1:A:566:ILE:HD12	1.56	0.86		
1:B:591:ILE:O	1:B:591:ILE:HG22	1.74	0.85		
1:A:94:ARG:CZ	1:A:143:ILE:HD11	2.07	0.85		
1:A:51:LEU:HD21	1:A:257:ILE:HD13	1.58	0.85		
1:A:767:LEU:HG	1:A:818:LEU:HD23	1.57	0.85		
1:B:563:PRO:HG2	1:B:566:ILE:CD1	2.07	0.85		
1:B:102:ASN:HA	1:B:104:ASN:N	1.93	0.83		
1:A:101:LYS:N	1:A:101:LYS:CD	2.40	0.83		
1:A:518:ARG:HH21	1:A:910:ARG:HH22	1.26	0.83		



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:768:PHE:HA	1:B:769:ARG:NH2	1.94	0.83	
1:B:650:ASP:OD2	1:B:912:ARG:NH2	2.12	0.83	
1:A:143:ILE:HG21	1:A:148:LEU:HD12	1.59	0.82	
1:A:320:PHE:CG	1:A:361:VAL:HG11	2.14	0.82	
1:B:420:HIS:HD2	1:B:423:TYR:H	1.24	0.82	
1:B:99:HIS:CA	1:B:100:GLU:HB3	2.10	0.81	
1:A:518:ARG:HH21	1:A:910:ARG:NH2	1.80	0.80	
1:B:98:ASN:HB2	1:B:100:GLU:HG2	1.64	0.80	
1:A:763:LYS:HG3	1:A:772:ILE:HD11	1.65	0.79	
1:B:323:ARG:HH11	1:B:362:GLU:CB	1.92	0.79	
1:A:160:GLN:HG2	1:A:165:GLU:O	1.83	0.78	
1:A:565:GLU:CG	1:A:566:ILE:N	2.46	0.78	
1:A:380:PHE:HD2	1:A:426:ARG:HD3	1.49	0.77	
1:A:79:ASP:OD1	1:A:148:LEU:HD22	1.82	0.77	
1:B:356:LEU:HD11	1:B:371:VAL:HG21	1.65	0.77	
1:B:321:GLU:HG3	1:B:323:ARG:NH2	1.99	0.77	
1:A:143:ILE:HG22	1:A:143:ILE:O	1.82	0.77	
1:A:431:LEU:HD23	1:A:442:PHE:HZ	1.47	0.76	
1:B:103:GLN:OE1	1:B:103:GLN:CA	2.33	0.76	
1:A:281:ILE:HD12	6:A:1229:HOH:O	1.85	0.75	
1:B:321:GLU:CG	1:B:323:ARG:HH21	2.00	0.74	
1:A:343:GLU:HG3	1:A:420:HIS:HE1	1.52	0.74	
1:A:380:PHE:CD2	1:A:426:ARG:HD3	2.23	0.73	
1:A:145:ASP:O	1:A:146:LYS:CB	2.37	0.72	
1:A:320:PHE:CD1	1:A:361:VAL:HG11	2.24	0.72	
1:B:344:LYS:HB3	1:B:346:LYS:HG2	1.71	0.71	
1:A:40:MET:HG3	1:A:388:ALA:O	1.91	0.71	
1:B:778:THR:O	1:B:781:ILE:HG12	1.91	0.71	
1:B:546:ARG:O	1:B:551:ARG:HA	1.92	0.70	
1:B:508:VAL:HG22	6:B:1242:HOH:O	1.91	0.70	
1:B:405:ARG:HB3	1:B:405:ARG:HH11	1.56	0.70	
1:B:321:GLU:CB	1:B:323:ARG:HH21	2.05	0.69	
1:A:309:ILE:O	1:A:313:MET:HG3	1.91	0.69	
1:B:346:LYS:HG3	1:B:347:GLU:HG2	1.75	0.69	
1:B:160:GLN:HG2	1:B:165:GLU:O	1.92	0.69	
1:A:769:ARG:NH2	1:A:815:ASP:OD2	2.25	0.69	
1:A:437:ASP:OD1	1:A:437:ASP:N	2.25	0.68	
1:B:595:ARG:CD	1:B:648:ASP:OD2	2.36	0.68	
1:B:674:VAL:HB	1:B:858:VAL:HG22	1.76	0.68	
1:A:145:ASP:O	1:A:146:LYS:HG3	1.92	0.68	
1:B:797:LEU:CD1	1:B:817:ILE:HD11	2.23	0.67	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:159:GLN:HB3	1:A:167:ILE:HB	1.74	0.67
1:A:420:HIS:HD2	1:A:423:TYR:N	1.92	0.67
1:A:913:THR:O	1:A:913:THR:CG2	2.38	0.67
1:B:344:LYS:HB3	1:B:346:LYS:HB3	1.76	0.67
1:B:21:LYS:NZ	1:B:21:LYS:HB3	2.09	0.67
1:B:102:ASN:HA	1:B:104:ASN:H	1.58	0.67
1:B:602:PHE:CE2	1:B:633:VAL:HG11	2.30	0.66
1:A:591:ILE:O	1:A:591:ILE:CG2	2.43	0.66
1:B:405:ARG:HD2	1:B:437:ASP:HB3	1.77	0.66
1:B:345:ASN:H	1:B:346:LYS:CB	2.09	0.66
1:A:786:PHE:CD2	1:A:807:LEU:HD11	2.31	0.66
1:A:145:ASP:O	1:A:146:LYS:HB2	1.95	0.66
1:A:245:ILE:HG12	1:A:257:ILE:HD11	1.75	0.66
1:A:100:GLU:C	1:A:101:LYS:HD2	2.15	0.65
1:B:103:GLN:O	1:B:104:ASN:C	2.34	0.65
1:B:98:ASN:HB2	1:B:100:GLU:CG	2.25	0.65
1:B:524:GLU:O	1:B:547:SER:HB3	1.96	0.65
1:B:174:ARG:NH1	6:B:1177:HOH:O	2.29	0.65
1:A:565:GLU:CG	1:A:566:ILE:H	2.10	0.65
1:B:345:ASN:H	1:B:346:LYS:HB2	1.62	0.64
1:B:575:PHE:O	1:B:579:VAL:HG23	1.97	0.64
1:B:415:SER:HB2	6:B:1239:HOH:O	1.98	0.64
1:B:813:CYS:O	1:B:817:ILE:HG12	1.98	0.64
1:A:420:HIS:HD2	1:A:423:TYR:H	1.46	0.63
1:B:565:GLU:OE1	1:B:565:GLU:N	2.20	0.63
1:B:782:PHE:HD1	1:B:786:PHE:CE1	2.16	0.63
1:B:345:ASN:N	1:B:346:LYS:HB2	2.12	0.63
1:A:786:PHE:CZ	1:A:790:ILE:HG13	2.34	0.63
1:B:159:GLN:CG	6:B:1204:HOH:O	2.20	0.63
1:B:344:LYS:C	1:B:346:LYS:HB3	2.19	0.63
1:B:347:GLU:HB2	1:B:351:ASN:ND2	2.14	0.63
1:A:356:LEU:HD11	1:A:371:VAL:HG21	1.81	0.62
1:A:768:PHE:HE1	1:A:811:SER:HB3	1.65	0.62
1:B:346:LYS:CE	1:B:346:LYS:HA	2.29	0.62
1:B:598:LEU:HD23	1:B:598:LEU:C	2.20	0.62
1:B:321:GLU:HB2	1:B:323:ARG:HH21	1.64	0.62
1:A:431:LEU:CD2	1:A:442:PHE:HZ	2.13	0.62
1:A:176:LYS:CE	6:A:1216:HOH:O	2.30	0.62
1:B:914:GLU:C	1:B:914:GLU:OE1	2.39	0.62
1:B:79:ASP:HB3	1:B:148:LEU:HD22	1.82	0.61
1:B:346:LYS:HA	1:B:346:LYS:HE3	1.81	0.61



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:644:ARG:C	1:B:645:GLU:HG3	2.20	0.61
1:A:143:ILE:HG21	1:A:148:LEU:HD11	1.82	0.61
1:A:320:PHE:HB3	1:A:361:VAL:CG1	2.30	0.61
1:A:56:ASN:N	1:A:57:PRO:HD2	2.14	0.61
1:B:420:HIS:HD2	1:B:423:TYR:N	1.97	0.61
1:B:420:HIS:CD2	1:B:423:TYR:H	2.13	0.61
1:A:144:LYS:HD3	1:A:199:TYR:HB3	1.81	0.61
1:A:176:LYS:HG3	1:A:286:LEU:HG	1.83	0.61
1:A:361:VAL:HG12	1:A:362:GLU:N	2.15	0.61
1:B:772:ILE:HG22	1:B:777:LYS:HD2	1.83	0.61
1:A:529:LEU:HD11	1:A:586:LEU:HD21	1.83	0.61
1:B:541:LEU:HG	1:B:557:ASN:HB3	1.83	0.60
1:A:143:ILE:O	1:A:145:ASP:O	2.19	0.60
1:B:587:ASP:OD1	1:B:592:LYS:HD2	2.01	0.60
1:A:268:GLY:HA2	1:A:271:GLU:HG2	1.82	0.60
1:A:778:THR:HB	1:A:781:ILE:HD13	1.83	0.60
1:A:167:ILE:HD12	1:A:167:ILE:N	2.17	0.60
1:B:346:LYS:HG3	1:B:347:GLU:H	1.66	0.60
1:A:913:THR:O	A:913:THR:O 1:A:914:GLU:CD		0.60
1:B:644:ARG:HD3	1:B:646:GLU:OE1	2.02	0.59
1:A:143:ILE:O	1:A:143:ILE:CG2	2.48	0.59
1:B:491:MET:O	1:B:495:MET:HG3	2.01	0.59
1:B:361:VAL:O	1:B:363:PRO:HD3	2.01	0.59
1:A:795:LEU:HD11	1:A:799:GLN:HG2	1.83	0.59
1:B:344:LYS:HB3	1:B:346:LYS:CG	2.31	0.59
1:B:564:ILE:H	1:B:564:ILE:HD13	1.64	0.59
1:B:102:ASN:HB2	1:B:104:ASN:ND2	2.17	0.59
1:A:798:LEU:HD23	1:A:798:LEU:C	2.23	0.59
1:B:59:ALA:HB1	6:B:1110:HOH:O	2.03	0.59
1:B:767:LEU:HG	1:B:818:LEU:HD23	1.85	0.59
1:A:93:LEU:N	1:A:93:LEU:HD12	2.18	0.59
1:A:320:PHE:O	1:A:323:ARG:HG3	2.02	0.58
1:B:431:LEU:HD22	1:B:442:PHE:CZ	2.31	0.58
1:A:119:VAL:HG13	1:A:175:PHE:CD1	2.38	0.58
1:A:431:LEU:HD23	1:A:442:PHE:CZ	2.36	0.58
1:B:335:ASN:ND2	1:B:337:SER:HB2	2.18	0.58
1:B:735:ASN:HB2	1:B:738:LYS:HE3	1.84	0.58
1:A:145:ASP:O	1:A:146:LYS:CG	2.52	0.58
1:A:315:LYS:HA	1:A:324:ILE:HD11	1.86	0.58
1:B:582:ILE:O	1:B:586:LEU:HG	2.03	0.58
1:A:786:PHE:CE2	1:A:790:ILE:HD11	2.40	0.57



	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:496:GLU:CD	1:A:500:ARG:HH12	2.06	0.57
1:A:570:THR:OG1	1:A:573:GLU:HG3	2.04	0.57
1:A:652:VAL:HB	1:A:905:THR:HG23	1.87	0.57
1:B:99:HIS:CA	1:B:100:GLU:CB	2.80	0.57
1:A:428:HIS:O	1:A:432:ARG:HG2	2.04	0.57
1:A:497:LEU:O	1:A:503:THR:HG23	2.05	0.57
1:A:798:LEU:HD23	1:A:798:LEU:O	2.05	0.57
1:B:621:LYS:HE2	2:B:1003:BGC:O5	2.04	0.57
1:A:307:ARG:O	1:A:311:VAL:HG23	2.05	0.57
1:B:320:PHE:C	1:B:323:ARG:HH21	2.07	0.57
1:B:351:ASN:O	1:B:355:ILE:HG12	2.05	0.56
1:B:619:TRP:CD1	1:B:624:LYS:HA	2.41	0.56
1:B:693:VAL:HG12	1:B:693:VAL:O	2.05	0.56
1:A:21:LYS:HB2	1:A:21:LYS:NZ	2.20	0.56
1:A:302:LEU:HD22	1:A:378:VAL:HG12	1.87	0.56
1:A:570:THR:HA	1:A:626:THR:OG1	2.06	0.56
1:B:574:LEU:O	1:B:578:ILE:HG12	2.06	0.56
1:A:105:VAL:HG11	1:A:451:LYS:HE2	1.87	0.56
1:A:168:LEU:HD23	1:A:180:VAL:HG12	1.87	0.56
1:B:425:ARG:HH22	5:B:1007:CIT:H22	1.71	0.56
1:B:686:TYR:CD2	1:B:845:ILE:HD11	2.41	0.56
1:A:375:CYS:O	1:A:379:SER:HB3	9:SER:HB3 2.06	
1:B:578:ILE:O	1:B:582:ILE:HG13	2.05	0.55
1:B:542:LEU:HD11	1:B:544:LYS:HE3	1.86	0.55
1:B:525:ASN:HA	1:B:545:ILE:O	2.06	0.55
1:B:98:ASN:ND2	1:B:100:GLU:HG3	2.22	0.55
1:A:853:ARG:HH11	1:A:853:ARG:HG2	1.72	0.55
1:A:58:THR:OG1	1:B:799:GLN:NE2	2.40	0.54
1:B:545:ILE:HD13	1:B:903:LEU:HD23	1.89	0.54
1:A:912:ARG:O	1:A:914:GLU:N	2.37	0.54
1:B:346:LYS:HG3	1:B:347:GLU:N	2.21	0.54
1:A:760:ASP:O	1:A:764:LYS:HG2	2.07	0.54
1:B:313:MET:CB	1:B:319:LEU:HD12	2.37	0.54
1:A:98:ASN:OD1	1:A:101:LYS:CD	2.47	0.54
1:A:446:GLU:HG3	1:A:447:SER:N	2.23	0.54
1:B:98:ASN:HD21	1:B:101:LYS:HB2	1.73	0.54
1:A:307:ARG:NH2	1:A:331:ARG:HA	2.23	0.54
1:B:405:ARG:CD	1:B:437:ASP:HB3	2.38	0.54
1:B:643:ARG:O	1:B:645:GLU:CG	2.56	0.54
1:A:398:ARG:NH1	1:A:398:ARG:HB3	2.23	0.54
1:A:413:ASN:ND2	1:A:414:GLY:H	2.05	0.54



	is as page	Interatomic	Clash	
Atom-1 Atom-2		distance (Å)	overlap (Å)	
1:B:323:ARG:HH11	1:B:362:GLU:CG	2.20	0.54	
1:B:344:LYS:HB3	1:B:346:LYS:CB	2.36	0.54	
1:B:58:THR:HG22	1:B:58:THR:O	2.06	0.54	
1:A:165:GLU:HG3	1:A:184:ASP:OD2	2.08	0.53	
1:A:671:THR:OG1	1:A:857:THR:HG23	2.08	0.53	
1:A:767:LEU:CG	1:A:818:LEU:HD23	2.35	0.53	
1:B:650:ASP:CG	1:B:912:ARG:HH22	2.07	0.53	
1:A:496:GLU:HG3	1:A:500:ARG:HH11	1.51	0.53	
1:B:321:GLU:HG2	1:B:323:ARG:NH2	2.21	0.53	
1:A:240:GLU:HB3	1:A:257:ILE:HD12	1.90	0.53	
1:B:21:LYS:HB3	1:B:21:LYS:HZ2	1.72	0.53	
1:B:361:VAL:HG12	1:B:362:GLU:N	2.23	0.53	
1:A:104:ASN:O	1:A:105:VAL:C	2.47	0.53	
1:A:342:ILE:O	1:A:372:GLN:HG3	2.08	0.53	
1:B:591:ILE:O	1:B:591:ILE:CG2	2.47	0.53	
1:A:563:PRO:HG2	1:A:566:ILE:CD1	2.34	0.53	
1:A:39:ILE:HD11	1:A:273:ILE:HG12	1.90	0.53	
1:A:283:ARG:HD2	1:B:559:ILE:O	2.09	0.53	
1:B:198:ASP:HB3	1:B:199:TYR:HD1	1.74	0.53	
1:B:313:MET:HB2	1:B:319:LEU:HD12	1.91	0.53	
1:A:72:PRO:HG3	1:A:455:MET:HB3	1.90	0.53	
1:A:297:VAL:HG13	1:A:382:SER:OG	2.08	0.53	
1:A:505:ASN:HB2	6:A:1205:HOH:O	2.08	0.53	
1:B:281:ILE:HG13	1:B:305:LEU:HD13	1.90	0.52	
1:A:321:GLU:HB2	1:A:323:ARG:NH1	2.24	0.52	
1:A:414:GLY:HA2	3:A:1002:G16:O6	2.09	0.52	
1:B:679:GLY:O	1:B:746:SER:HB2	2.08	0.52	
1:A:26:LEU:HD22	1:A:29:MET:CE	2.39	0.52	
1:B:346:LYS:CG	1:B:347:GLU:H	2.21	0.52	
1:A:94:ARG:CZ	1:A:143:ILE:CD1	2.84	0.52	
1:B:782:PHE:CD1	1:B:786:PHE:CE1	2.97	0.52	
1:B:539:ARG:HG3	1:B:541:LEU:HD11	1.92	0.51	
1:B:541:LEU:HG	1:B:557:ASN:CB	2.40	0.51	
1:A:166:ALA:HB3	1:A:185:VAL:HG22	1.92	0.51	
1:B:347:GLU:HB2	1:B:351:ASN:HD21	1.74	0.51	
1:A:91:ARG:HG2	1:A:92:ILE:N	2.24	0.51	
1:A:98:ASN:CG	1:A:101:LYS:HD3	2.30	0.51	
1:B:664:THR:HG23	1:B:899:LYS:HD3	1.92	0.51	
1:B:786:PHE:CD2	1:B:807:LEU:HD11	2.45	0.51	
1:B:798:LEU:O	1:B:798:LEU:HD23	2.10	0.51	
1:A:295:LYS:HA	1:A:301:TYR:CD2	2.46	0.51	



Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:71:ILE:HA	1:B:215:MET:SD	2.51	0.51
1:B:119:VAL:CG1	1:B:175:PHE:HA	2.41	0.51
1:A:18:GLN:HE22	1:A:366:ASP:HB3	1.74	0.51
1:B:644:ARG:C	1:B:645:GLU:CG	2.78	0.51
1:B:103:GLN:O	1:B:105:VAL:N	2.44	0.51
1:B:198:ASP:HB3	1:B:199:TYR:CD1	2.46	0.51
1:B:320:PHE:O	1:B:323:ARG:NH2	2.44	0.51
1:B:655:VAL:HG12	1:B:656:ASN:O	2.11	0.51
1:B:644:ARG:NE	1:B:646:GLU:OE1	2.44	0.51
1:A:66:THR:O	1:A:67:PHE:HB2	2.11	0.50
1:B:56:ASN:N	1:B:57:PRO:HD2	2.26	0.50
1:B:910:ARG:O	1:B:914:GLU:HB3	2.12	0.50
1:B:98:ASN:ND2	1:B:101:LYS:HB2	2.25	0.50
1:B:279:ARG:HD2	6:B:1218:HOH:O	2.11	0.50
1:B:588:TYR:CD2	1:B:589:MET:CE	2.94	0.50
1:A:574:LEU:O	1:A:578:ILE:HG12	2.10	0.50
1:B:242:LEU:HD12	1:B:245:ILE:HD12	1.93	0.50
1:B:79:ASP:HB3	1:B:148:LEU:CD2	2.41	0.50
1:B:320:PHE:O	1:B:323:ARG:HB2	2.12	0.50
1:A:271:GLU:OE1	1:A:271:GLU:HA	2.11	0.50
1:B:269:SER:HB3	6:B:1230:HOH:O	2.11	0.49
1:B:615:ILE:HA	1:B:631:HIS:O	2.12	0.49
1:A:98:ASN:HB3	1:A:103:GLN:OE1	2.13	0.49
1:A:645:GLU:O	1:A:645:GLU:HG2	2.13	0.49
1:B:35:THR:O	1:B:38:ASP:HB3	2.12	0.49
1:A:786:PHE:O	1:A:790:ILE:HG12	2.12	0.49
1:B:643:ARG:O	1:B:645:GLU:HG2	2.13	0.49
1:A:541:LEU:HD22	1:A:898:GLY:HA3	1.93	0.49
1:B:549:LYS:HD2	1:B:550:LYS:HB2	1.93	0.49
1:B:671:THR:OG1	1:B:857:THR:HG23	2.13	0.49
1:A:718:LEU:C	1:A:720:ASP:N	2.66	0.49
1:B:320:PHE:O	1:B:321:GLU:HB2	2.13	0.49
1:B:588:TYR:CD2	1:B:589:MET:HE2	2.48	0.49
1:B:380:PHE:CD2	1:B:426:ARG:HD3	2.48	0.49
1:B:644:ARG:CD	1:B:646:GLU:OE1	2.61	0.49
1:A:339:VAL:O	1:A:343:GLU:HG2	2.13	0.48
1:A:612:ASP:O	1:A:634:VAL:HG21	2.13	0.48
1:B:541:LEU:HD12	1:B:541:LEU:N	2.28	0.48
1:B:854:LEU:HD12	1:B:855:ASN:N	2.28	0.48
1:A:22:ILE:HD11	1:A:370:SER:HB3	1.94	0.48
1:A:79:ASP:OD1	1:A:148:LEU:CD2	2.57	0.48



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:152:PHE:HB3	1:A:206:VAL:HG22	1.95	0.48	
1:B:234:THR:HG22	1:B:294:GLU:HG3	1.94	0.48	
1:A:69:ARG:O	1:A:70:SER:HB3	2.14	0.48	
1:B:105:VAL:HG11	1:B:451:LYS:HE2	1.94	0.48	
1:B:320:PHE:CG	1:B:361:VAL:HG11	2.48	0.48	
1:A:390:LEU:HD23	1:A:431:LEU:HD22	1.96	0.48	
1:B:143:ILE:HD12	1:B:148:LEU:HD12	1.96	0.48	
1:B:98:ASN:C	1:B:100:GLU:HB3	2.20	0.48	
1:B:786:PHE:O	1:B:790:ILE:HG22	2.13	0.48	
1:A:35:THR:O	1:A:39:ILE:HG12	2.14	0.48	
1:A:39:ILE:HD13	1:A:42:ARG:HH21	1.78	0.48	
1:A:230:ILE:HD11	1:A:386:VAL:HG11	1.96	0.48	
1:B:420:HIS:CD2	1:B:423:TYR:HB2	2.49	0.48	
1:B:335:ASN:HD22	1:B:337:SER:HB2	1.78	0.47	
1:B:480:THR:OG1	1:B:483:MET:HG3	2.14	0.47	
1:A:598:LEU:C	1:A:598:LEU:HD23	2.34	0.47	
1:A:80:PHE:CZ	1:A:458:ALA:HB2	2.50	0.47	
1:A:412:VAL:HG12	1:A:413:ASN:N	2.28	0.47	
1:B:691:LYS:HB2	6:B:1213:HOH:O	2.14	0.47	
1:A:601:THR:HA	1:A:655:VAL:O	2.14	0.47	
1:B:93:LEU:HG	LEU:HG 1:B:109:SER:HB2		0.47	
1:A:144:LYS:NZ	1:A:198:ASP:OD2	2.44	0.47	
1:A:398:ARG:HB3	1:A:398:ARG:HH11	1.79	0.47	
1:B:71:ILE:HB	1:B:72:PRO:HD2	1.97	0.47	
1:A:667:TYR:CE2	1:A:668:GLU:OE2	2.67	0.47	
1:B:327:GLU:O	1:B:333:LYS:HG3	2.15	0.47	
1:A:265:GLY:HA2	1:A:269:SER:HB2	1.96	0.47	
1:A:278:ASP:O	1:A:281:ILE:HG22	2.15	0.47	
1:A:361:VAL:CG1	1:A:362:GLU:N	2.77	0.47	
1:A:353:LYS:HA	1:A:368:CYS:SG	2.55	0.47	
1:A:338:ASP:O	1:A:342:ILE:HD13	2.14	0.46	
1:A:405:ARG:NE	1:A:439:ASP:OD2	2.47	0.46	
1:A:145:ASP:C	1:A:146:LYS:HG3	2.35	0.46	
1:A:240:GLU:CB	1:A:257:ILE:HD12	2.46	0.46	
1:B:549:LYS:HD2	1:B:550:LYS:N	2.30	0.46	
1:B:669:GLU:OE2	1:B:670:PRO:HD2	2.15	0.46	
1:A:33:ASP:O	1:A:37:ILE:HG12	2.16	0.46	
1:B:478:HIS:HB2	6:B:1227:HOH:O	2.16	0.46	
1:A:258:ASN:C	1:A:258:ASN:OD1	2.53	0.46	
1:A:307:ARG:HB2	1:A:334:PHE:HB3	1.98	0.46	
1:A:66:THR:HG21	1:A:211:VAL:HG21	1.97	0.46	



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:155:SER:HB3	1:A:209:ASP:OD2	2.16	0.46
1:A:393:ILE:O	1:A:396:ARG:HB3	2.16	0.46
1:A:320:PHE:CB	1:A:361:VAL:HG11	2.45	0.45
1:B:495:MET:HB3	1:B:511:MET:HE2	1.98	0.45
1:A:168:LEU:CD2	1:A:180:VAL:HG12	2.46	0.45
1:A:515:PHE:HA	1:A:703:MET:SD	2.56	0.45
1:A:518:ARG:HH22	1:A:907:VAL:HG22	1.81	0.45
1:A:518:ARG:NH2	1:A:907:VAL:HG22	2.31	0.45
1:A:619:TRP:HB3	1:A:623:PHE:O	2.16	0.45
1:A:782:PHE:CD1	1:A:786:PHE:CE1	3.04	0.45
1:A:913:THR:O	1:A:914:GLU:OE2	2.34	0.45
1:B:230:ILE:HD11	1:B:386:VAL:HG11	1.97	0.45
1:B:550:LYS:HD2	1:B:550:LYS:HA	1.66	0.45
1:A:367:ASP:O	1:A:371:VAL:HG23	2.17	0.45
1:B:772:ILE:CG2	1:B:777:LYS:HD2	2.47	0.45
1:A:231:GLY:O	1:A:298:SER:HB2	2.17	0.45
1:A:342:ILE:O	1:A:342:ILE:CG2	2.65	0.45
1:A:354:GLU:O	1:A:358:ARG:HG3	2.17	0.45
1:A:541:LEU:N	1:A:541:LEU:HD12	2.31	0.45
1:A:663:MET:HG3	1:A:904:ILE:HD11	1.99	0.45
1:A:565:GLU:HG3	1:A:566:ILE:H	1.67	0.45
1:B:323:ARG:HB2	1:B:323:ARG:HE	1.62	0.45
1:B:854:LEU:HD12	1:B:855:ASN:H	1.82	0.45
1:A:655:VAL:HG12	1:A:656:ASN:O	2.17	0.45
1:A:62:LYS:HB3	1:A:64:LEU:HD21	1.98	0.45
1:A:546:ARG:O	1:A:551:ARG:HA	2.17	0.45
1:B:53:ARG:HB3	1:B:246:ASP:HB3	1.99	0.45
1:B:146:LYS:HB2	1:B:148:LEU:HG	1.99	0.45
1:B:593:GLY:N	1:B:594:PRO:CD	2.80	0.45
1:A:23:ASP:OD1	1:A:373:HIS:NE2	2.39	0.44
1:A:44:ARG:HA	1:A:47:MET:HE2	1.99	0.44
1:B:376:THR:O	1:B:380:PHE:HB2	2.16	0.44
1:B:738:LYS:HE3	6:B:1107:HOH:O	2.17	0.44
1:B:798:LEU:HD23	1:B:798:LEU:C	2.38	0.44
1:A:134:LEU:O	1:A:138:MET:HG3	2.17	0.44
1:A:119:VAL:HG13	1:A:175:PHE:CG	2.52	0.44
1:B:801:ARG:O	1:B:805:GLN:HB2	2.17	0.44
1:A:853:ARG:HH11	1:A:853:ARG:CG	2.29	0.44
1:B:271:GLU:OE2	1:B:274:ARG:HD3	2.18	0.44
1:B:323:ARG:HH11	1:B:362:GLU:HG3	1.82	0.44
1:B:718:LEU:C	1:B:720:ASP:N	2.71	0.44



	lo ao pagom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:554:GLU:OE2	1:A:556:HIS:HE1	2.01	0.44	
1:A:852:ASP:C	1:A:853:ARG:HD2	2.38	0.44	
1:B:121:GLY:O	1:B:177:ALA:HA	2.18	0.44	
1:A:602:PHE:CE2	1:A:633:VAL:HG11	2.53	0.44	
1:A:152:PHE:O	1:A:206:VAL:HA	2.18	0.44	
1:B:19:VAL:O	1:B:23:ASP:HB2	2.17	0.44	
1:A:56:ASN:N	1:A:57:PRO:CD	2.80	0.43	
1:A:320:PHE:HB3	1:A:361:VAL:HG11	1.96	0.43	
1:B:112:TYR:OH	1:B:137:PHE:HB2	2.18	0.43	
1:A:327:GLU:N	1:A:327:GLU:OE1	2.51	0.43	
1:B:451:LYS:O	1:B:455:MET:HG2	2.18	0.43	
1:B:677:ILE:O	1:B:682:SER:HA	2.18	0.43	
1:A:62:LYS:O	1:A:63:MET:C	2.57	0.43	
1:A:104:ASN:HD22	1:A:104:ASN:HA	1.58	0.43	
1:A:422:GLN:O	1:A:426:ARG:HG3	2.17	0.43	
1:B:281:ILE:HG12	1:B:308:LEU:HD12	2.00	0.43	
1:A:405:ARG:HG3	1:A:437:ASP:O	2.18	0.43	
1:A:739:GLN:O	1:A:743:LYS:HG3	2.18	0.43	
1:B:73:ASP:OD1	1:B:73:ASP:C	2.57	0.43	
1:B:147:LYS:O	1:B:147:LYS:HG2	2.19	0.43	
1:B:644:ARG:O	1:B:645:GLU:HG3	2.18	0.43	
1:A:277:PHE:CE1	1:A:309:ILE:HA	2.53	0.43	
1:A:420:HIS:CD2	1:A:422:GLN:H	2.36	0.43	
1:B:718:LEU:HD22	1:B:721:ILE:HD11	2.00	0.43	
1:A:26:LEU:HD22	1:A:29:MET:HE3	2.01	0.43	
1:B:603:SER:HB2	2:B:1003:BGC:H4	2.01	0.43	
1:A:21:LYS:HB2	1:A:21:LYS:HZ3	1.82	0.43	
1:A:118:ILE:CG2	1:A:126:LEU:HA	2.49	0.43	
1:A:176:LYS:HD2	1:A:286:LEU:HG	2.01	0.43	
1:A:650:ASP:OD2	1:A:912:ARG:NH2	2.51	0.43	
1:B:345:ASN:CA	1:B:346:LYS:CB	2.96	0.43	
1:A:124:SER:O	1:A:125:GLN:C	2.57	0.43	
1:A:143:ILE:HD13	1:A:148:LEU:HD11	2.00	0.43	
1:A:280:GLU:HG3	1:A:283:ARG:NH2	2.33	0.43	
1:A:532:ASP:O	1:A:538:PHE:HA	2.19	0.43	
1:B:524:GLU:CD	1:B:524:GLU:H	2.22	0.43	
1:A:193:ILE:HD13	1:A:201:ALA:HB3	2.00	0.43	
1:B:25:TYR:OH	1:B:312:LYS:HG3	2.19	0.43	
1:B:763:LYS:HG3	1:B:772:ILE:HD11	2.00	0.43	
1:B:222:GLN:HA	1:B:222:GLN:NE2	2.34	0.42	
1:B:320:PHE:C	1:B:323:ARG:NH2	2.72	0.42	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:321:GLU:HB2	1:B:323:ARG:NH2	2.31	0.42
1:A:202:ASN:C	1:A:202:ASN:ND2	2.72	0.42
1:A:274:ARG:NH1	1:A:292:LEU:HD22	2.34	0.42
1:A:519:THR:HB	1:A:520:PRO:HD2	2.00	0.42
1:A:667:TYR:CD2	1:A:668:GLU:HG2	2.54	0.42
1:B:361:VAL:CG1	1:B:362:GLU:N	2.82	0.42
1:B:786:PHE:CD1	1:B:786:PHE:C	2.92	0.42
1:A:80:PHE:CE2	1:A:458:ALA:HA	2.54	0.42
1:B:532:ASP:HB3	1:B:539:ARG:HG2	2.00	0.42
1:A:763:LYS:CG	1:A:772:ILE:HD11	2.43	0.42
1:B:66:THR:OG1	1:B:256:CYS:HB3	2.18	0.42
1:A:235:ASN:HA	1:A:261:TRP:CD1	2.55	0.42
1:B:420:HIS:CD2	1:B:422:GLN:H	2.37	0.42
1:B:853:ARG:HA	1:B:885:LYS:O	2.20	0.42
1:A:167:ILE:N	1:A:167:ILE:CD1	2.83	0.42
1:A:74:GLY:O	1:A:99:HIS:HD2	2.03	0.42
1:A:141:ARG:N	1:A:141:ARG:HD2	2.35	0.42
1:A:145:ASP:C	1:A:146:LYS:CG	2.87	0.42
3:A:1002:G16:O3P	3:A:1002:G16:H5	2.20	0.42
1:B:104:ASN:H	1:B:104:ASN:ND2	2.18	0.42
1:B:320:PHE:O	1:B:323:ARG:NE	2.53	0.42
1:B:342:ILE:O	1:B:342:ILE:HG22	2.20	0.42
1:B:652:VAL:HB	1:B:905:THR:HG23	2.02	0.42
1:B:763:LYS:CG	1:B:772:ILE:HD11	2.50	0.42
1:A:44:ARG:HA	1:A:47:MET:CE	2.50	0.42
1:A:534:GLY:HA3	1:A:603:SER:HB2	2.02	0.42
1:A:811:SER:HB2	1:A:815:ASP:HB2	2.01	0.42
1:B:120:HIS:NE2	1:B:174:ARG:O	2.52	0.42
1:B:554:GLU:OE2	1:B:556:HIS:HE1	2.03	0.42
1:A:166:ALA:HB3	1:A:185:VAL:CG2	2.50	0.41
1:A:320:PHE:HB3	1:A:361:VAL:HG13	2.00	0.41
1:B:501:LYS:CB	1:B:695:MET:SD	3.08	0.41
1:B:669:GLU:CD	1:B:670:PRO:HD2	2.40	0.41
1:A:44:ARG:HG2	1:A:392:ALA:HB1	2.02	0.41
1:A:644:ARG:HG2	1:A:646:GLU:HG3	2.02	0.41
1:B:176:LYS:HB3	6:B:1206:HOH:O	2.20	0.41
1:A:811:SER:HB2	1:A:815:ASP:CB	2.51	0.41
1:A:120:HIS:NE2	1:A:174:ARG:O	2.52	0.41
1:A:420:HIS:CD2	1:A:423:TYR:HB2	2.56	0.41
1:B:105:VAL:HG11	1:B:451:LYS:HG3	2.01	0.41
1:A:342:ILE:CG2	1:A:372:GLN:HG3	2.51	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:342:ILE:O	1:B:342:ILE:CG2	2.68	0.41
1:B:346:LYS:CG	1:B:347:GLU:N	2.83	0.41
1:B:862:GLY:HA2	3:B:1004:G16:O6	2.20	0.41
1:B:102:ASN:HA	1:B:103:GLN:C	2.39	0.41
1:B:496:GLU:OE2	1:B:500:ARG:NH1	2.44	0.41
1:A:148:LEU:HA	1:A:149:PRO:HD3	1.90	0.41
1:A:26:LEU:HD21	1:A:309:ILE:CG2	2.51	0.41
1:A:281:ILE:HG23	1:A:282:ASP:N	2.36	0.41
1:A:520:PRO:HD3	1:A:663:MET:CE	2.51	0.41
1:A:595:ARG:HG3	1:A:648:ASP:O	2.21	0.41
1:A:665:CYS:HB3	1:A:891:LEU:HD23	2.03	0.41
1:A:693:VAL:HA	6:A:1207:HOH:O	2.21	0.41
1:A:767:LEU:HG	1:A:818:LEU:CD2	2.41	0.41
1:B:545:ILE:HD13	1:B:903:LEU:CD2	2.50	0.41
1:A:62:LYS:HB3	1:A:64:LEU:CD2	2.51	0.41
1:A:196:ARG:C	1:A:198:ASP:N	2.74	0.41
1:A:319:LEU:O	1:A:321:GLU:O	2.39	0.41
1:A:786:PHE:CD1	1:A:787:LEU:N	2.89	0.41
1:A:342:ILE:HG13	1:A:352:ALA:HB2	2.02	0.40
1:A:356:LEU:CD1	1:A:371:VAL:HG21	2.49	0.40
1:B:384:ASN:HD22	2 1:B:384:ASN:HA 1.67		0.40
1:A:101:LYS:O	1:A:102:ASN:CB	2.70 0.40	
1:A:167:ILE:HA	1:A:183:ALA:O	2.22	0.40
1:A:419:THR:O	1:A:420:HIS:C	2.59	0.40
1:A:798:LEU:C	1:A:798:LEU:CD2	2.89	0.40
1:A:718:LEU:C	1:A:720:ASP:H	2.23	0.40
1:B:141:ARG:O	1:B:143:ILE:HG23	2.22	0.40
1:B:204:VAL:CG2	1:B:457:THR:HG23	2.52	0.40
1:A:321:GLU:HB3	1:A:322:GLY:H	1.53	0.40
1:B:97:VAL:HA	1:B:104:ASN:O	2.21	0.40
1:B:405:ARG:HB3	1:B:405:ARG:NH1	2.29	0.40
1:A:126:LEU:O	1:A:129:HIS:HB3	2.21	0.40
1:A:196:ARG:C	1:A:198:ASP:H	2.25	0.40
1:A:353:LYS:CA	1:A:368:CYS:SG	3.10	0.40
1:A:712:PHE:HB3	1:A:741:TYR:HB2	2.03	0.40
1:A:855:ASN:OD1	1:A:887:ASN:HB3	2.21	0.40
1:A:857:THR:HA	1:A:889:SER:O	2.21	0.40
1:B:98:ASN:O	1:B:101:LYS:O	2.39	0.40
1:B:451:LYS:NZ	6:B:1238:HOH:O	2.45	0.40

There are no symmetry-related clashes.



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	897/917~(98%)	849 (95%)	45~(5%)	3~(0%)	41 55
1	В	897/917~(98%)	856~(95%)	37~(4%)	4 (0%)	34 48
All	All	1794/1834~(98%)	1705 (95%)	82 (5%)	7~(0%)	34 48

All (7) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	В	100	GLU
1	В	104	ASN
1	В	346	LYS
1	А	146	LYS
1	А	913	THR
1	А	105	VAL
1	В	593	GLY

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	774/788~(98%)	752~(97%)	22 (3%)	43	63
1	В	774/788~(98%)	747 (96%)	27 (4%)	36	55
All	All	1548/1576~(98%)	1499 (97%)	49 (3%)	39	59

All (49) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	21	LYS
1	А	33	ASP
1	А	80	PHE
1	А	93	LEU
1	А	101	LYS
1	А	104	ASN
1	А	261	TRP
1	А	321	GLU
1	А	366	ASP
1	А	399	ASP
1	А	413	ASN
1	А	437	ASP
1	А	481	LYS
1	А	531	LEU
1	А	541	LEU
1	А	542	LEU
1	А	709	TRP
1	А	769	ARG
1	А	786	PHE
1	А	843	ASP
1	А	853	ARG
1	А	914	GLU
1	В	23	ASP
1	В	99	HIS
1	В	102	ASN
1	В	103	GLN
1	В	261	TRP
1	В	281	ILE
1	В	320	PHE
1	В	323	ARG
1	В	337	SER
1	В	346	LYS
1	В	380	PHE
1	В	405	ARG
1	В	407	ARG
1	В	424	SER
1	В	481	LYS
1	В	549	LYS
1	В	550	LYS
1	В	551	ARG
1	В	557	ASN
1	В	564	ILE
1	В	645	GLU



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Mol	Chain	Res	Type
1	В	709	TRP
1	В	769	ARG
1	В	797	LEU
1	В	805	GLN
1	В	843	ASP
1	В	914	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such side chains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	18	GLN
1	А	99	HIS
1	А	104	ASN
1	А	125	GLN
1	А	159	GLN
1	А	202	ASN
1	А	222	GLN
1	А	345	ASN
1	А	384	ASN
1	А	400	ASN
1	А	413	ASN
1	А	420	HIS
1	А	466	GLN
1	А	556	HIS
1	А	631	HIS
1	А	771	GLN
1	А	805	GLN
1	А	848	ASN
1	А	887	ASN
1	В	96	GLN
1	В	102	ASN
1	В	104	ASN
1	В	202	ASN
1	В	222	GLN
1	В	351	ASN
1	В	384	ASN
1	В	400	ASN
1	В	420	HIS
1	В	466	GLN
1	В	506	ASN
1	В	556	HIS
1	В	557	ASN



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Mol	Chain	\mathbf{Res}	Type					
1	В	799	GLN					
1	В	805	GLN					
1	В	806	GLN					
1	В	810	ASN					
1	В	832	GLN					
1	В	855	ASN					
1	В	877	GLN					
1	В	887	ASN					

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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 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	Type	Chain	Dec	Tink	Bo	ond leng	$_{\rm sths}$	B	ond ang	les
	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	G16	В	1004	-	19,20,20	0.52	0	30,31,31	0.93	0
3	G16	А	1002	-	19,20,20	0.56	0	30,31,31	0.86	0
3	G16	В	1002	-	19,20,20	0.54	0	30,31,31	0.96	0
5	CIT	В	1007	-	12,12,12	1.01	0	17,17,17	1.52	1 (5%)
2	BGC	В	1003	-	12,12,12	0.42	0	17,17,17	1.28	2 (11%)



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	В	ond ang	les
INIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	А	1001	-	12,12,12	0.56	0	$17,\!17,\!17$	1.06	2 (11%)
5	CIT	А	1007	-	12,12,12	1.03	0	$17,\!17,\!17$	1.53	1 (5%)
3	G16	А	1004	-	19,20,20	0.57	0	$30,\!31,\!31$	0.95	0
2	BGC	В	1001	-	12,12,12	0.33	0	$17,\!17,\!17$	0.85	1 (5%)
2	BGC	А	1003	-	12,12,12	0.39	0	17,17,17	1.19	2 (11%)

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	G16	В	1004	-	-	1/11/31/31	0/1/1/1
3	G16	А	1002	-	-	1/11/31/31	0/1/1/1
3	G16	В	1002	-	-	1/11/31/31	0/1/1/1
5	CIT	В	1007	-	-	10/16/16/16	-
2	BGC	В	1003	-	-	0/2/22/22	0/1/1/1
2	BGC	А	1001	-	-	0/2/22/22	0/1/1/1
5	CIT	А	1007	-	-	2/16/16/16	-
3	G16	А	1004	-	-	1/11/31/31	0/1/1/1
2	BGC	В	1001	-	-	0/2/22/22	0/1/1/1
2	BGC	A	1003	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$
5	А	1007	CIT	O6-C6-C3	4.19	120.33
5	В	1007	CIT	O6-C6-C3	4.12	120.20
2	А	1003	BGC	C1-O5-C5	-3.23	107.57
2	В	1003	BGC	C1-O5-C5	-3.16	107.69

C1-O5-C5

O5-C1-C2

O5-C1-C2

C1-O5-C5

O5-C1-C2

BGC

BGC

BGC

BGC

BGC

All (9) bond angle outliers are listed below:

There are no chirality outliers.

А

В

А

В

А

2

 $\overline{2}$

 $\overline{2}$

2

 $\mathbf{2}$

All (16) torsion outliers are listed below:

1001

1003

1003

1001

1001



-3.14

-2.89

-2.81

-2.22

-2.08

107.73

105.13

105.26

109.48

106.58

Ideal(°)

113.05

113.05

113.66

113.66

113.66

110.28

110.28

113.66

110.28

Mol	Chain	Res	Type	Atoms
5	В	1007	CIT	C2-C3-C4-C5
5	В	1007	CIT	O7-C3-C4-C5
5	В	1007	CIT	C6-C3-C4-C5
5	В	1007	CIT	O7-C3-C6-O5
5	В	1007	CIT	O7-C3-C6-O6
5	В	1007	CIT	C4-C3-C6-O5
5	В	1007	CIT	C4-C3-C6-O6
3	А	1002	G16	C5-C6-O6-P
3	В	1004	G16	C5-C6-O6-P
5	В	1007	CIT	C1-C2-C3-C6
3	А	1004	G16	C5-C6-O6-P
3	В	1002	G16	C5-C6-O6-P
5	В	1007	CIT	C1-C2-C3-O7
5	В	1007	CIT	C1-C2-C3-C4
5	А	1007	CIT	C6-C3-C4-C5
5	А	1007	CIT	C2-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	1004	G16	1	0
3	А	1002	G16	2	0
5	В	1007	CIT	1	0
2	В	1003	BGC	2	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	899/917~(98%)	0.29	53 (5%) 22 21	26, 51, 80, 119	0
1	В	899/917~(98%)	0.29	55 (6%) 21 20	27, 51, 80, 118	0
All	All	1798/1834~(98%)	0.29	108 (6%) 21 20	26, 51, 80, 119	0

All (108) RSRZ outliers are listed below:

Mol	Chain	hain Res		RSRZ	
1	В	16	ASP	7.1	
1	А	16	ASP	6.9	
1	А	17	ASP	6.5	
1	В	100	GLU	6.0	
1	В	102	ASN	5.0	
1	А	21	LYS	5.0	
1	В	103	GLN	4.6	
1	В	101	LYS	4.6	
1	А	685	CYS	4.5	
1	В	564	ILE	4.2	
1	В	99	HIS	4.2	
1	В	548	GLY	4.0	
1	В	549	LYS	3.7	
1	В	550	LYS	3.6	
1	А	794	ARG	3.4	
1	В	798	LEU	3.3	
1	А	322	GLY	3.3	
1	В	17	ASP	3.2	
1	А	684	ALA	3.2	
1	А	404	PRO	3.2	
1	А	145	ASP	3.2	
1	А	314	ALA	3.1	
1	В	591	ILE	3.1	
1	А	709	TRP	3.1	



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Mol Chain R		Res	Type	RSRZ
1	В	297	VAL	3.1
1	А	101	LYS	3.0
1	А	549	LYS	3.0
1	В	852	ASP	3.0
1	В	234	THR	3.0
1	А	143	ILE	2.9
1	А	707	MET	2.9
1	А	142	LYS	2.9
1	В	237	CYS	2.9
1	А	550	LYS	2.8
1	А	403	THR	2.8
1	А	223	HIS	2.8
1	В	24	LYS	2.8
1	В	794	ARG	2.8
1	А	786	PHE	2.7
1	В	449	SER	2.7
1	В	229	ILE	2.7
1	А	100	GLU	2.7
1	А	841	VAL	2.6
1	В	593	GLY	2.6
1	В	786	PHE	2.6
1	А	113	ASP	2.6
1	В	98	ASN	2.6
1	В	649	LEU	2.6
1	А	406	LEU	2.6
1	В	565	GLU	2.6
1	В	645	GLU	2.6
1	А	146	LYS	2.6
1	В	18	GLN	2.6
1	В	913	THR	2.5
1	А	310	LEU	2.5
1	А	436	PRO	2.5
1	В	211	VAL	2.5
1	А	438	SER	2.5
1	В	21	LYS	2.5
1	А	24	LYS	2.5
1	А	437	ASP	2.5
1	А	198	ASP	2.5
1	В	153	THR	2.5
1	В	317	GLY	2.4
1	А	398	ARG	2.4
1	А	676	LEU	2.4



Mol	Chain	Res	Type	RSRZ
1	А	659	VAL	2.4
1	В	642	LYS	2.4
1	В	771	GLN	2.4
1	В	436	PRO	2.4
1	А	103	GLN	2.4
1	А	19	VAL	2.4
1	А	658	THR	2.3
1	В	298	SER	2.3
1	А	656	ASN	2.3
1	В	262	GLY	2.3
1	В	382	SER	2.3
1	А	700	GLN	2.3
1	В	547	SER	2.3
1	А	564	ILE	2.3
1	А	358	ARG	2.3
1	А	118	ILE	2.3
1	А	45	LYS	2.2
1	А	20	LYS	2.2
1	В	210	THR	2.2
1	В	235	ASN	2.2
1	А	502	GLN	2.2
1	А	675	GLY	2.2
1	А	686	TYR	2.2
1	В	83	LEU	2.2
1	В	236	ALA	2.1
1	А	350	HIS	2.1
1	В	27	TYR	2.1
1	В	226	VAL	2.1
1	В	386	VAL	2.1
1	В	293	PHE	2.1
1	В	305	LEU	2.1
1	В	209	ASP	2.1
1	В	646	GLU	2.1
1	В	230	ILE	2.1
1	A	706	ASN	2.1
1	В	299	GLY	2.1
1	А	80	PHE	2.0
1	В	501	LYS	2.0
1	A	252	GLU	2.0
1	A	674	VAL	2.0
1	А	682	SER	2.0
1	В	568	GLN	2.0

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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	$B-factors(Å^2)$	Q<0.9
5	CIT	В	1007	13/13	0.45	0.32	102,103,104,104	0
5	CIT	А	1007	13/13	0.80	0.43	105,106,106,106	0
4	NA	А	1006	1/1	0.87	0.13	54,54,54,54	0
2	BGC	А	1001	12/12	0.90	0.16	43,46,47,49	0
2	BGC	А	1003	12/12	0.92	0.30	33,35,35,38	0
4	NA	В	1005	1/1	0.92	0.12	53,53,53,53	0
2	BGC	В	1003	12/12	0.93	0.25	35,37,37,40	0
4	NA	В	1006	1/1	0.93	0.07	53,53,53,53	0
2	BGC	В	1001	12/12	0.94	0.33	41,43,44,46	0
4	NA	А	1005	1/1	0.95	0.15	55,55,55,55	0
3	G16	А	1002	20/20	0.95	0.11	51,53,55,55	0
3	G16	В	1002	20/20	0.97	0.21	48,50,53,53	0
3	G16	В	1004	20/20	0.97	0.14	30,32,35,35	0
3	G16	А	1004	20/20	0.98	0.17	28,30,33,34	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.

