

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	7CXO
Title	:	Crystal structure of Arabinose isomerase from hybrid AI10
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Deposited on	:	2020-09-02
Resolution	:	3.20 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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	498	78%	20%	••
1	В	498	74%	23%	•
1	С	498	73%	23%	•••
1	D	498	74%	23%	••
1	Е	498	% 71%	26%	•
1	F	498	72%	26%	



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2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23537 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		At	oms			ZeroOcc	AltConf	Trace
1	Δ	404	Total	С	Ν	0	\mathbf{S}	0	0	0
1	Л	494	3901	2478	687	715	21	0	0	0
1	В	406	Total	С	Ν	0	S	0	0	0
1	D	490	3918	2489	690	717	22		0	0
1	С	486	Total	С	Ν	0	S	0	0	0
1		400	3839	2443	673	702	21	0	0	0
1	Л	404	Total	С	Ν	0	S	0	0	0
1	D	494	3901	2478	687	715	21	0	0	U
1	F	406	Total	С	Ν	0	S	0	0	0
1	Ľ	490	3918	2489	690	717	22	0	0	0
1	F	405	Total	С	Ν	Ο	S	0	0	0
	L,	490	3910	2484	689	716	21	0	0 0	

• Molecule 1 is a protein called L-arabinose isomerase.

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Mn 1 1	0	0
3	В	1	Total Mn 1 1	0	0
3	С	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0
3	Ε	1	Total Mn 1 1	0	0
3	F	1	Total Mn 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	21	Total O 21 21	0	0
4	В	14	Total O 14 14	0	0
4	С	21	Total O 21 21	0	0
4	D	25	Total O 25 25	0	0
4	Ε	20	Total O 20 20	0	0
4	F	13	Total O 13 13	0	0



Chain C:

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.



73%

• Molecule 1: L-arabinose isomerase



23%





MET K2 <mark>W112</mark> D113 T114 I115 L17 Y18 M33 V34 P35 <mark>A36</mark> L37 L37 A40 V41 G42 N43 A44 W88 189 W9 F10 D109 V75 176 176 M3 P4 A5 Y6 A30 E58 I59 B60 361 <u>A85</u> D182 N183 M184 R185 E186 E186 V187 A188 V189 V189 T190 E191 R130 E131 Y132 G133 G133 I135 I135 I135 0139 G140 C141 V141 V141 V141 R143 R143 H127 R156 F157 V220 S221 E222 Q223 K224 R158 W150 Q215 Y216 D152 V14 121 E259 L260 D268 Q293 R294 L295 Q325 G326 G327 E332 D333 Y334 L344 V345 1238 E254 A273 <mark>62</mark> E361 K362 E492 V493 F494 W495 R496 GLY ARG S437 A438 E439 2430 8431 H448 H449 481 D41



4 Data and refinement statistics (i)

Property	Value	Source	
Space group	C 2 2 21	Depositor	
Cell constants	148.48Å 258.57Å 165.73Å	Deperitor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	48.89 - 3.20	Depositor	
Resolution (A)	48.84 - 3.15	EDS	
% Data completeness	98.0 (48.89-3.20)	Depositor	
(in resolution range)	$98.1 \ (48.84 - 3.15)$	EDS	
R _{merge}	0.19	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.12 (at 3.12 Å)	Xtriage	
Refinement program	REFMAC 5.8.0258	Depositor	
D D	0.176 , 0.270	Depositor	
$\mathbf{n}, \mathbf{n}_{free}$	0.175 , 0.261	DCC	
R_{free} test set	2606 reflections $(4.80%)$	wwPDB-VP	
Wilson B-factor $(Å^2)$	75.8	Xtriage	
Anisotropy	0.064	Xtriage	
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 43.8	EDS	
L-test for twinning ²	$< L > = 0.47, < L^2 > = 0.30$	Xtriage	
Estimated twinning fraction	0.026 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l	Vtriago	
Estimated twinning fraction	0.027 for 1/2 *h + 1/2 *k, 3/2 *h - 1/2 *k, -1	Atriage	
F_o, F_c correlation	0.95	EDS	
Total number of atoms	23537	wwPDB-VP	
Average B, all atoms $(Å^2)$	81.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.61% 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: GOL, MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	Bond	lengths	Bond angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.64	0/3993	0.77	0/5406
1	В	0.63	0/4010	0.77	0/5427
1	С	0.65	0/3929	0.77	0/5318
1	D	0.64	0/3993	0.76	0/5406
1	Е	0.64	0/4010	0.78	0/5427
1	F	0.65	0/4002	0.76	0/5417
All	All	0.64	0/23937	0.77	0/32401

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	Е	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Е	3	MET	Peptide
1	Е	362	LYS	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	3901	0	3809	72	0
1	В	3918	0	3834	81	0
1	С	3839	0	3753	87	0
1	D	3901	0	3809	87	0
1	Е	3918	0	3834	97	0
1	F	3910	0	3822	91	0
2	А	6	0	8	0	0
2	В	6	0	8	0	0
2	С	6	0	8	0	0
2	D	6	0	8	0	0
2	Ε	6	0	8	0	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
3	Ε	1	0	0	0	0
3	F	1	0	0	0	0
4	А	21	0	0	0	0
4	В	14	0	0	2	0
4	С	21	0	0	2	0
4	D	25	0	0	2	0
4	Е	20	0	0	1	0
4	F	13	0	0	1	0
All	All	23537	0	22901	450	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 10.

All (450) 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:D:7:GLU:OE1	1:D:48:ARG:NH1	1.94	1.00
1:A:421:LEU:HB2	1:C:115:ILE:HD13	1.50	0.94
1:B:3:MET:HG2	1:B:4:PRO:HD2	1.57	0.86
1:A:448:HIS:HB2	1:C:127:HIS:HB2	1.62	0.82



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:115:ILE:HG21	1:C:418:MET:HG2	1.66	0.78
1:A:493:VAL:HG11	1:C:493:VAL:HG12	1.66	0.77
1:B:3:MET:SD	4:B:703:HOH:O	2.41	0.77
1:E:348:SER:HB2	1:E:424:ALA:O	1.87	0.75
1:F:351:LEU:HD12	1:F:352:GLU:HG3	1.69	0.75
1:A:217:ILE:CD1	1:A:258:ILE:HA	2.18	0.74
1:E:229:LEU:HD11	1:E:253:ARG:HA	1.69	0.74
1:D:380:ARG:HD2	1:D:422:PRO:O	1.87	0.73
1:A:185:ARG:HG2	1:E:206:ASN:HB3	1.69	0.73
1:C:124:GLN:O	1:C:126:ALA:N	2.21	0.73
1:E:1:MET:HG2	1:E:298:GLN:O	1.89	0.73
1:D:220:VAL:HG11	1:D:257:ARG:HG3	1.72	0.71
1:D:72:CYS:SG	1:D:97:LYS:HG3	2.31	0.71
1:B:229:LEU:HD21	1:B:253:ARG:HA	1.75	0.68
1:D:438:ALA:HB3	1:F:147:VAL:HG11	1.76	0.67
1:C:7:GLU:OE2	1:C:48:ARG:NE	2.28	0.67
1:D:52:VAL:HG23	1:D:54:LYS:HE3	1.76	0.67
1:E:127:HIS:HB3	1:F:333:ASP:O	1.95	0.67
1:C:124:GLN:HE21	1:C:124:GLN:HA	1.59	0.67
1:E:1:MET:CG	1:E:299:GLY:HA3	2.24	0.67
1:E:494:PHE:HA	1:F:493:VAL:HG21	1.76	0.66
1:F:135:ILE:HG13	1:F:139:MET:HE3	1.77	0.66
1:F:6:TYR:HB3	1:F:73:ALA:HB2	1.75	0.66
1:A:206:ASN:HB3	1:E:185:ARG:HG2	1.78	0.65
1:A:217:ILE:HD12	1:A:258:ILE:HA	1.78	0.65
1:C:380:ARG:HD2	1:C:422:PRO:O	1.96	0.65
1:F:363:PRO:HB3	1:F:383:PHE:HB3	1.80	0.64
1:E:60:ARG:HD2	1:E:90:ARG:HD3	1.80	0.64
1:C:217:ILE:HD13	1:C:258:ILE:HA	1.80	0.63
1:B:127:HIS:HB2	1:C:448:HIS:HB2	1.80	0.63
1:F:59:ILE:HG21	1:F:88:TRP:HA	1.79	0.63
1:D:106:PHE:O	1:D:149:HIS:NE2	2.31	0.63
1:D:183:ASN:ND2	1:D:191:GLU:OE2	2.32	0.63
1:B:179:ARG:NH1	1:D:182:ASP:OD2	2.32	0.62
1:E:320:MET:O	1:E:460:GLN:NE2	2.32	0.62
1:D:333:ASP:O	1:F:127:HIS:HB3	1.99	0.62
1:C:179:ARG:NH2	1:C:183:ASN:OD1	2.32	0.62
1:D:448:HIS:HB2	1:F:127:HIS:HB2	1.79	0.62
1:E:3:MET:CB	1:E:4:PRO:HD3	2.29	0.62
1:B:185:ARG:HG2	1:D:206:ASN:HB3	1.81	0.62
1:F:139:MET:HB3	1:F:141:VAL:HG13	1.83	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:198:GLN:HG3	1:E:203:TRP:O	2.01	0.60
1:E:1:MET:HB2	1:E:2:LYS:HD2	1.84	0.60
1:D:177:VAL:HA	1:D:273:ALA:O	2.02	0.59
1:C:68:ALA:HA	1:E:64:LEU:HD23	1.83	0.59
1:D:38:GLN:O	1:D:42:GLY:HA3	2.02	0.59
1:E:38:GLN:O	1:E:42:GLY:HA3	2.02	0.59
1:E:441:TRP:HE3	1:E:475:ILE:HD11	1.68	0.59
1:F:233:GLU:HG3	1:F:238:ILE:HD12	1.85	0.58
1:B:52:VAL:HG23	1:B:54:LYS:HE3	1.85	0.58
1:E:56:ALA:O	1:E:60:ARG:HG3	2.02	0.58
1:A:475:ILE:HG23	1:A:479:THR:HG21	1.86	0.58
1:E:60:ARG:O	1:E:64:LEU:HD13	2.02	0.58
1:A:38:GLN:HG2	1:A:47:LEU:HB2	1.85	0.57
1:F:177:VAL:HG22	1:F:273:ALA:HB3	1.87	0.57
1:D:127:HIS:HB2	1:E:448:HIS:HB2	1.85	0.57
1:F:189:VAL:O	1:F:309:LYS:NZ	2.38	0.57
1:F:221:SER:HG	1:F:224:LYS:HB2	1.69	0.57
1:A:448:HIS:CB	1:C:127:HIS:HB2	2.33	0.57
1:F:61:ARG:O	1:F:65:GLU:HG2	2.05	0.57
1:F:325:GLN:O	1:F:327:GLY:N	2.38	0.56
1:D:168:ALA:CB	1:D:320:MET:HG3	2.36	0.56
1:C:52:VAL:HG13	1:C:54:LYS:HE3	1.88	0.56
1:F:315:ARG:O	1:F:319:VAL:HG23	2.06	0.56
1:D:349:HIS:ND1	1:D:352:GLU:OE1	2.38	0.55
1:E:349:HIS:ND1	1:E:352:GLU:OE1	2.37	0.55
1:C:214:VAL:HA	1:C:217:ILE:HG22	1.88	0.55
1:E:315:ARG:NH2	1:E:319:VAL:HG11	2.22	0.55
1:D:384:ASP:CG	1:D:414:PRO:HG2	2.26	0.55
1:C:34:VAL:HG21	1:C:49:TRP:HB2	1.89	0.55
1:D:48:ARG:HG3	1:D:48:ARG:HH11	1.72	0.55
1:D:152:ASP:OD2	1:E:435:ARG:NH1	2.38	0.55
1:B:198:GLN:HG2	1:B:203:TRP:O	2.08	0.54
1:D:158:ARG:NE	1:D:459:GLU:OE2	2.39	0.54
1:E:34:VAL:HB	1:E:35:PRO:HD3	1.88	0.54
1:E:301:GLY:HA2	1:E:314:LEU:HD12	1.90	0.54
1:A:103:HIS:HA	1:A:129:ASP:OD2	2.08	0.54
1:E:3:MET:HB3	1:E:4:PRO:HD3	1.88	0.54
1:B:72:CYS:HB3	1:B:97:LYS:HE3	1.89	0.54
1:C:60:ARG:HD2	1:C:90:ARG:HG3	1.90	0.54
1:C:190:THR:HG23	1:C:307:ASP:HA	1.90	0.54
1:E:115:ILE:HD13	1:F:421:LEU:HB2	1.88	0.54



	to as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:185:ARG:CG	1:E:206:ASN:HB3	2.37	0.54
1:D:41:VAL:HG21	1:D:160:ALA:HB2	1.88	0.54
1:E:40:ALA:O	1:E:41:VAL:HG22	2.08	0.54
1:A:124:GLN:HA	1:B:334:TYR:O	2.07	0.54
1:D:185:ARG:NH2	1:D:279:GLU:HB3	2.22	0.54
1:B:255:GLN:HG3	1:B:379:ALA:HB3	1.89	0.53
1:C:179:ARG:NH1	1:F:182:ASP:OD2	2.42	0.53
1:D:7:GLU:O	1:D:72:CYS:O	2.27	0.53
1:B:214:VAL:HA	1:B:217:ILE:HG22	1.90	0.53
1:C:120:MET:O	1:C:124:GLN:NE2	2.42	0.53
1:B:421:LEU:HD13	1:B:425:ARG:HD2	1.89	0.53
1:C:126:ALA:O	1:C:130:ARG:NE	2.40	0.53
1:D:493:VAL:HG11	1:F:493:VAL:HG12	1.91	0.53
1:D:493:VAL:HG21	1:F:494:PHE:HA	1.90	0.53
1:D:112:TRP:HA	1:D:115:ILE:HD11	1.89	0.53
1:E:55:ASP:HB2	1:E:58:GLU:HB2	1.91	0.53
1:C:72:CYS:O	1:C:97:LYS:HE2	2.09	0.53
1:C:475:ILE:HG23	1:C:479:THR:HG21	1.90	0.52
1:D:410:ASP:OD2	1:D:431:ARG:NH1	2.41	0.52
1:F:85:ALA:HB1	1:F:135:ILE:HB	1.90	0.52
1:E:230:ASP:O	1:E:234:GLU:HG2	2.09	0.52
1:C:220:VAL:HG11	1:C:257:ARG:HG3	1.91	0.52
1:D:351:LEU:HD12	1:D:352:GLU:HG3	1.92	0.52
1:B:134:PHE:CD1	1:C:189:VAL:HG23	2.44	0.52
1:E:127:HIS:HB2	1:F:448:HIS:HB2	1.92	0.52
1:E:214:VAL:HA	1:E:217:ILE:HG12	1.91	0.52
1:F:488:LEU:O	1:F:492:GLU:HB2	2.09	0.52
1:E:493:VAL:HG12	1:F:493:VAL:HG11	1.92	0.52
1:A:493:VAL:HG12	1:B:493:VAL:HG11	1.91	0.52
1:A:115:ILE:HD12	1:B:421:LEU:HD12	1.91	0.52
1:B:328:THR:HG23	1:B:453:SER:HB2	1.92	0.52
1:B:296:MET:HE2	1:B:354:CYS:HB2	1.91	0.51
1:E:178:ALA:O	1:E:274:PHE:HA	2.11	0.51
1:C:410:ASP:OD2	1:C:431:ARG:NH1	2.43	0.51
1:F:421:LEU:HD23	1:F:425:ARG:HD2	1.92	0.51
1:B:152:ASP:OD2	1:C:435:ARG:NH2	2.43	0.51
1:F:286:GLN:HA	1:F:375:LYS:HB3	1.93	0.51
1:E:60:ARG:HD2	1:E:90:ARG:HB3	1.92	0.51
1:A:61:ARG:NH2	1:D:70:ASP:OD2	2.44	0.51
1:C:344:LEU:HD13	1:C:427:LEU:HD22	1.93	0.51
1:F:112:TRP:O	1:F:115:ILE:HG22	2.11	0.51



	lo uo pugo	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:301:GLY:HA2	1:F:314:LEU:HD12	1.93	0.51
1:C:217:ILE:HD11	1:C:257:ARG:HG2	1.93	0.51
1:E:132:TYR:O	1:E:135:ILE:HG22	2.10	0.51
1:D:54:LYS:O	1:D:87:MET:SD	2.69	0.51
1:A:53:LEU:HD13	1:A:59:ILE:HA	1.92	0.50
1:B:171:GLU:HG3	1:B:319:VAL:HG21	1.92	0.50
1:B:53:LEU:HD13	1:B:59:ILE:HA	1.93	0.50
1:C:208:TYR:CZ	1:F:185:ARG:HD3	2.47	0.50
1:A:425:ARG:HD3	1:A:425:ARG:N	2.27	0.50
1:C:69:ASP:OD1	1:C:71:VAL:HG12	2.11	0.50
1:A:255:GLN:HE21	1:A:286:GLN:HG3	1.76	0.50
1:B:103:HIS:ND1	1:C:442:ILE:HD11	2.27	0.50
1:C:296:MET:HE2	1:C:354:CYS:HB2	1.94	0.50
1:B:90:ARG:CZ	1:F:173:ARG:HD2	2.42	0.49
1:B:302:PHE:HE2	1:B:352:GLU:HG3	1.77	0.49
1:B:353:VAL:HG23	1:B:383:PHE:CZ	2.46	0.49
1:A:336:TYR:O	1:C:105:GLN:NE2	2.45	0.49
1:D:320:MET:CE	1:D:460:GLN:HB3	2.43	0.49
1:D:266:LEU:HD13	1:D:300:TYR:CD2	2.47	0.49
1:E:177:VAL:HG22	1:E:273:ALA:HB3	1.93	0.49
1:A:248:VAL:HG13	1:A:367:VAL:CG1	2.42	0.49
1:A:179:ARG:NH1	1:E:182:ASP:OD2	2.46	0.49
1:C:442:ILE:HA	4:C:709:HOH:O	2.11	0.49
1:E:318:LYS:NZ	1:E:354:CYS:SG	2.86	0.49
1:D:3:MET:HB3	1:D:4:PRO:HD3	1.95	0.49
1:A:471:GLU:HG3	1:A:491:ASN:HD22	1.78	0.49
1:B:177:VAL:HG22	1:B:273:ALA:HB3	1.94	0.49
1:B:211:GLY:O	1:B:214:VAL:HG12	2.13	0.49
1:C:59:ILE:HG21	1:C:88:TRP:HA	1.93	0.49
1:C:177:VAL:HG22	1:C:273:ALA:HB3	1.95	0.49
1:D:378:PRO:O	1:D:380:ARG:NH2	2.45	0.49
1:A:147:VAL:HG11	1:B:438:ALA:HB3	1.94	0.49
1:A:248:VAL:HG13	1:A:367:VAL:HG11	1.94	0.49
1:D:132:TYR:O	1:D:135:ILE:HG22	2.12	0.49
1:A:317:MET:HG2	1:A:456:VAL:HG21	1.94	0.48
1:A:282:HIS:NE2	1:E:212:ASP:OD1	2.46	0.48
1:B:3:MET:HG2	1:B:4:PRO:CD	2.36	0.48
1:B:206:ASN:HB3	1:D:185:ARG:HG2	1.94	0.48
1:C:284:LEU:HD23	1:C:288:PRO:HD3	1.95	0.48
1:D:42:GLY:O	1:D:43:ASN:HB2	2.14	0.48
1:D:353:VAL:CG1	1:D:424:ALA:HB3	2.44	0.48



	i agein	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:122:LEU:HD12	1:E:123:ASN:OD1	2.13	0.48
1:F:183:ASN:HD22	1:F:190:THR:HG23	1.78	0.48
1:C:34:VAL:HB	1:C:35:PRO:HD3	1.96	0.48
1:C:410:ASP:CG	1:C:431:ARG:HH12	2.16	0.48
1:A:315:ARG:O	1:A:319:VAL:HG12	2.14	0.48
1:B:184:MET:HB2	1:B:305:GLU:HB3	1.95	0.48
1:D:334:TYR:O	1:F:124:GLN:HA	2.14	0.48
1:E:248:VAL:HG13	1:E:367:VAL:HG11	1.95	0.48
1:E:351:LEU:HD12	1:E:352:GLU:HG3	1.96	0.48
1:E:353:VAL:CG1	1:E:424:ALA:HB3	2.42	0.48
1:F:115:ILE:HG23	1:F:115:ILE:O	2.14	0.48
1:F:194:LYS:HE2	1:F:308:TRP:CD1	2.48	0.48
1:F:221:SER:OG	1:F:224:LYS:HB2	2.14	0.48
1:D:190:THR:HG23	1:D:307:ASP:HA	1.96	0.48
1:E:348:SER:O	1:E:348:SER:OG	2.31	0.48
1:D:49:TRP:CZ2	1:D:51:GLY:HA2	2.49	0.48
1:D:248:VAL:HG13	1:D:367:VAL:HG11	1.95	0.48
1:C:331:MET:HG3	1:C:452:PHE:HB2	1.95	0.47
1:D:66:ALA:O	1:D:72:CYS:SG	2.61	0.47
1:B:493:VAL:HG12	1:C:493:VAL:HG11	1.95	0.47
1:B:54:LYS:O	1:B:87:MET:SD	2.73	0.47
1:B:59:ILE:HG21	1:B:88:TRP:HA	1.97	0.47
1:D:391:VAL:HG13	1:D:406:VAL:HG13	1.96	0.47
1:D:41:VAL:HG23	1:D:41:VAL:O	2.14	0.47
1:E:183:ASN:ND2	1:E:191:GLU:OE2	2.47	0.47
1:A:302:PHE:H	1:A:314:LEU:HD23	1.78	0.47
1:C:214:VAL:HA	1:C:217:ILE:CG2	2.45	0.47
1:D:12:VAL:HA	1:D:78:TRP:O	2.15	0.47
1:F:9:TRP:HB2	1:F:75:VAL:HG22	1.96	0.47
1:B:347:GLY:HA3	1:B:428:TRP:CZ3	2.50	0.47
1:C:465:ALA:CB	1:C:472:CYS:HB2	2.45	0.47
1:E:12:VAL:HA	1:E:78:TRP:O	2.15	0.47
1:E:33:MET:HG2	1:E:150:TRP:CD2	2.50	0.47
1:E:475:ILE:HA	1:E:479:THR:OG1	2.15	0.47
1:A:214:VAL:HG12	1:A:284:LEU:HD12	1.97	0.47
1:B:103:HIS:CD2	1:B:129:ASP:OD2	2.67	0.47
1:B:117:MET:HE2	1:C:422:PRO:HG2	1.96	0.47
1:E:17:LEU:O	1:E:17:LEU:HD23	2.15	0.47
1:E:309:LYS:HE2	4:E:702:HOH:O	2.14	0.47
1:F:3:MET:HB3	1:F:4:PRO:HD3	1.97	0.46
1:F:228:LEU:HD22	1:F:260:LEU:HD23	1.96	0.46



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:33:MET:HG2	1:E:150:TRP:CE2	2.50	0.46
1:B:337:HIS:HB3	1:B:344:LEU:HB2	1.98	0.46
1:C:36:ALA:HB3	1:C:150:TRP:HZ3	1.80	0.46
1:C:62:LEU:HD13	1:C:62:LEU:C	2.36	0.46
1:F:430:PRO:HB2	1:F:437:SER:OG	2.15	0.46
1:B:103:HIS:HA	1:B:129:ASP:OD2	2.15	0.46
1:B:430:PRO:HG2	1:B:434:LEU:HA	1.98	0.46
1:E:45:HIS:NE2	1:E:167:VAL:HG21	2.31	0.46
1:E:1:MET:HG3	1:E:299:GLY:HA3	1.93	0.46
1:E:41:VAL:O	1:E:41:VAL:HG23	2.15	0.46
1:F:114:THR:O	1:F:116:ASP:N	2.48	0.46
1:B:111:PRO:HB2	1:B:114:THR:HG22	1.97	0.46
1:C:438:ALA:O	1:C:442:ILE:HD12	2.16	0.46
1:D:328:THR:HG23	1:D:453:SER:HB2	1.98	0.46
1:F:17:LEU:HD22	1:F:18:TYR:CE1	2.50	0.46
1:B:132:TYR:O	1:B:135:ILE:HG22	2.14	0.46
1:D:442:ILE:HD13	1:F:130:ARG:HA	1.97	0.46
1:E:367:VAL:HG22	1:E:367:VAL:O	2.15	0.46
1:B:350:MET:O	1:B:423:VAL:HG11	2.15	0.46
1:E:87:MET:HG3	1:F:186:GLU:HG2	1.98	0.46
1:A:274:PHE:O	1:A:302:PHE:HA	2.16	0.46
1:A:338:PHE:HA	1:A:343:ASP:OD1	2.16	0.46
1:B:193:ASP:OD1	1:B:195:VAL:HG22	2.16	0.46
1:D:315:ARG:O	1:D:319:VAL:HG12	2.16	0.46
1:E:14:SER:HA	1:E:81:THR:OG1	2.16	0.46
1:C:14:SER:O	1:C:54:LYS:HA	2.16	0.46
1:C:175:LEU:HD23	1:C:203:TRP:CD1	2.51	0.46
1:C:273:ALA:HA	1:C:301:GLY:O	2.15	0.46
1:A:93:LEU:HG	1:A:139:MET:CE	2.46	0.45
1:B:45:HIS:NE2	1:B:167:VAL:HG21	2.31	0.45
1:D:80:HIS:CE1	1:D:122:LEU:HD13	2.51	0.45
1:E:1:MET:SD	1:E:299:GLY:HA3	2.56	0.45
1:C:362:LYS:N	1:C:363:PRO:HD3	2.31	0.45
1:E:3:MET:HB2	1:E:4:PRO:HD3	1.97	0.45
1:F:34:VAL:HB	1:F:35:PRO:HD3	1.98	0.45
1:C:368:GLN:O	1:C:380:ARG:NH2	2.49	0.45
1:E:328:THR:HG23	1:E:453:SER:HB2	1.98	0.45
1:A:206:ASN:HB3	1:E:185:ARG:CG	2.45	0.45
1:D:82:PHE:HA	1:D:128:GLY:HA2	1.98	0.45
1:D:471:GLU:HB2	1:D:495:TRP:CD1	2.51	0.45
1:E:236:TYR:HD1	1:E:363:PRO:HB2	1.80	0.45



	i agem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:396:ILE:HD11	1:E:403:ARG:HD2	1.99	0.45
1:D:348:SER:OG	1:D:349:HIS:N	2.49	0.45
1:E:22:ALA:O	1:E:26:VAL:HG12	2.17	0.45
1:E:100:LEU:HD12	1:E:162:TRP:CG	2.52	0.45
1:E:103:HIS:ND1	1:E:129:ASP:OD2	2.36	0.45
1:F:214:VAL:HG21	1:F:283:GLY:HA3	1.98	0.45
1:A:127:HIS:HB2	1:B:448:HIS:HB2	1.98	0.45
1:E:353:VAL:HG13	1:E:424:ALA:HB3	1.97	0.45
1:F:220:VAL:CG2	1:F:260:LEU:HB3	2.46	0.45
1:B:198:GLN:O	1:B:202:GLY:HA2	2.16	0.45
1:C:274:PHE:O	1:C:302:PHE:HA	2.16	0.45
1:E:465:ALA:CB	1:E:472:CYS:HB2	2.47	0.45
1:A:230:ASP:O	1:A:234:GLU:HG3	2.17	0.45
1:D:286:GLN:HA	1:D:375:LYS:HB3	1.99	0.45
1:F:319:VAL:HA	1:F:322:THR:HG23	1.98	0.45
1:B:120:MET:O	1:B:124:GLN:HB3	2.17	0.44
1:B:286:GLN:OE1	1:B:378:PRO:HA	2.16	0.44
1:C:486:ASN:HB3	1:C:490:TRP:CH2	2.52	0.44
1:D:127:HIS:HB3	1:E:333:ASP:O	2.17	0.44
1:D:183:ASN:O	1:D:185:ARG:N	2.49	0.44
1:B:274:PHE:O	1:B:302:PHE:HA	2.17	0.44
1:A:188:ALA:HB1	1:C:135:ILE:HD13	2.00	0.44
1:A:263:LYS:NZ	1:A:298:GLN:OE1	2.50	0.44
1:E:168:ALA:HA	1:E:319:VAL:HG23	1.98	0.44
1:E:296:MET:HE1	1:E:330:PHE:H	1.83	0.44
1:F:233:GLU:OE2	1:F:249:ARG:NH1	2.50	0.44
1:F:254:GLU:OE1	1:F:254:GLU:HA	2.17	0.44
1:F:345:VAL:O	1:F:427:LEU:HA	2.18	0.44
1:A:33:MET:SD	1:A:78:TRP:CZ3	3.11	0.44
1:D:108:ARG:HG2	1:D:149:HIS:CE1	2.52	0.44
1:F:315:ARG:O	1:F:315:ARG:HD3	2.18	0.44
1:A:315:ARG:O	1:A:315:ARG:HD3	2.18	0.44
1:D:81:THR:HA	1:D:124:GLN:HB2	1.98	0.44
1:E:214:VAL:HG21	1:E:283:GLY:HA3	2.00	0.44
1:B:168:ALA:HA	1:B:319:VAL:HG13	2.00	0.44
1:D:347:GLY:HA3	1:D:428:TRP:CZ3	2.53	0.44
1:E:60:ARG:CD	1:E:90:ARG:HB3	2.48	0.44
1:F:42:GLY:O	1:F:44:ALA:N	2.50	0.44
1:A:211:GLY:O	1:A:214:VAL:HG22	2.18	0.44
1:A:483:SER:O	1:A:487:GLU:HG3	2.18	0.44
1:D:329:SER:HB2	1:D:354:CYS:HB3	2.00	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:334:TYR:HE2	1:D:349:HIS:HA	1.83	0.44
1:F:115:ILE:HD12	1:F:119:PHE:CD1	2.53	0.44
1:C:82:PHE:H	1:C:124:GLN:HG3	1.83	0.43
1:C:184:MET:O	1:C:186:GLU:N	2.51	0.43
1:C:328:THR:HG23	1:C:453:SER:HB2	1.99	0.43
1:F:89:ILE:HD11	1:F:135:ILE:HD11	1.99	0.43
1:A:13:GLY:HA3	1:A:79:MET:SD	2.57	0.43
1:E:66:ALA:O	1:E:97:LYS:NZ	2.49	0.43
1:A:90:ARG:HG3	4:D:710:HOH:O	2.17	0.43
1:D:178:ALA:HB2	1:D:271:PHE:CE1	2.53	0.43
1:E:198:GLN:CG	1:E:203:TRP:O	2.65	0.43
1:F:216:TYR:HE2	1:F:268:ASP:OD2	2.01	0.43
1:B:84:PRO:HB2	1:C:186:GLU:O	2.18	0.43
1:C:69:ASP:CG	1:C:71:VAL:HG12	2.38	0.43
1:F:439:GLU:CD	1:F:481:VAL:HG11	2.39	0.43
1:B:38:GLN:OE1	1:B:47:LEU:N	2.48	0.43
1:C:175:LEU:HD12	1:C:272:THR:OG1	2.19	0.43
1:C:124:GLN:HE21	1:C:124:GLN:CA	2.29	0.43
1:D:435:ARG:NH2	1:F:152:ASP:OD2	2.51	0.43
1:E:483:SER:O	1:E:487:GLU:HG3	2.19	0.43
1:F:410:ASP:OD1	1:F:431:ARG:NH1	2.50	0.43
1:B:233:GLU:OE1	1:B:249:ARG:NH1	2.50	0.43
1:B:241:ALA:O	1:B:248:VAL:CG1	2.66	0.43
1:F:232:TYR:CE1	1:F:294:ARG:HD2	2.53	0.43
1:A:255:GLN:NE2	1:A:286:GLN:HG3	2.34	0.43
1:C:211:GLY:O	1:C:214:VAL:HG12	2.19	0.43
1:F:475:ILE:HG23	1:F:479:THR:HG21	2.00	0.43
1:A:18:TYR:CE1	1:A:121:ASN:HB2	2.53	0.43
1:B:79:MET:HE3	1:B:88:TRP:CE2	2.53	0.43
1:B:282:HIS:CG	1:D:211:GLY:HA3	2.54	0.43
1:E:72:CYS:O	1:E:97:LYS:HE2	2.19	0.43
1:C:13:GLY:HA3	1:C:79:MET:SD	2.59	0.43
1:E:391:VAL:HG22	1:E:406:VAL:HG13	2.01	0.43
1:F:332:GLU:HG3	1:F:449:HIS:HD2	1.83	0.43
1:F:417:ASP:OD1	1:F:418:MET:N	2.52	0.43
1:A:422:PRO:CG	1:C:117:MET:HG2	2.49	0.42
1:F:3:MET:HB3	1:F:4:PRO:CD	2.49	0.42
1:F:3:MET:CB	1:F:4:PRO:CD	2.97	0.42
1:F:184:MET:HB2	1:F:305:GLU:HB3	1.99	0.42
1:A:89:ILE:HG12	1:A:135:ILE:HD11	2.01	0.42
1:B:112:TRP:O	1:B:115:ILE:HG22	2.19	0.42



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:134:PHE:CD1	1:F:189:VAL:HG23	2.55	0.42
1:F:314:LEU:HD11	1:F:318:LYS:HZ2	1.84	0.42
1:A:465:ALA:CB	1:A:472:CYS:HB2	2.50	0.42
1:D:12:VAL:O	1:D:52:VAL:HA	2.18	0.42
1:F:37:LEU:HD12	1:F:37:LEU:HA	1.84	0.42
1:A:339:GLU:O	1:A:340:LYS:C	2.58	0.42
1:A:82:PHE:HA	1:A:128:GLY:HA2	2.00	0.42
1:B:103:HIS:NE2	1:C:336:TYR:HE2	2.18	0.42
1:D:189:VAL:HG23	1:F:134:PHE:CD1	2.54	0.42
1:D:411:ALA:HB3	1:D:454:PHE:HE1	1.85	0.42
1:E:361:GLU:HG2	1:E:362:LYS:HG3	2.01	0.42
1:F:132:TYR:O	1:F:135:ILE:HG22	2.20	0.42
1:F:150:TRP:O	1:F:156:ARG:NE	2.51	0.42
1:B:149:HIS:O	1:B:152:ASP:HB3	2.20	0.42
1:B:228:LEU:HD12	1:B:228:LEU:HA	1.94	0.42
1:B:290:LEU:HD13	1:B:381:LEU:HG	2.02	0.42
1:C:33:MET:HG2	1:C:150:TRP:CD2	2.55	0.42
1:C:177:VAL:HA	1:C:273:ALA:O	2.20	0.42
1:D:40:ALA:O	1:D:41:VAL:C	2.58	0.42
1:D:302:PHE:CG	1:D:303:ALA:N	2.87	0.42
1:D:320:MET:HE3	1:D:460:GLN:HB3	2.00	0.42
1:E:38:GLN:NE2	1:E:46:VAL:HA	2.35	0.42
1:F:363:PRO:CB	1:F:383:PHE:HB3	2.50	0.42
1:A:406:VAL:CG2	1:A:461:LEU:HD13	2.50	0.42
1:B:182:ASP:OD2	1:D:179:ARG:NH1	2.53	0.42
1:F:30:ALA:O	1:F:33:MET:N	2.53	0.42
1:B:3:MET:SD	1:B:319:VAL:HG23	2.59	0.42
1:C:113:ASP:N	1:C:113:ASP:OD1	2.52	0.42
1:C:214:VAL:CA	1:C:217:ILE:HG22	2.50	0.42
1:D:41:VAL:CG2	1:D:160:ALA:HB2	2.50	0.42
1:A:353:VAL:CG1	1:A:424:ALA:HB3	2.50	0.42
1:C:45:HIS:HA	4:C:717:HOH:O	2.19	0.42
1:D:69:ASP:O	1:D:72:CYS:SG	2.78	0.42
1:D:85:ALA:HB1	1:D:135:ILE:HB	2.02	0.42
1:E:3:MET:HB3	1:E:4:PRO:CD	2.49	0.42
1:E:101:HIS:HE1	1:F:442:ILE:HD12	1.84	0.42
1:A:255:GLN:HG2	1:A:286:GLN:OE1	2.20	0.41
1:A:354:CYS:HG	1:A:356:SER:CB	2.29	0.41
1:C:168:ALA:HA	1:C:319:VAL:CG1	2.50	0.41
1:E:401:ARG:HD2	1:E:495:TRP:HB3	2.02	0.41
1:F:206:ASN:ND2	4:F:601:HOH:O	2.50	0.41



	i agem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:223:GLN:NE2	1:D:227:GLU:OE2	2.53	0.41
1:F:40:ALA:O	1:F:41:VAL:C	2.58	0.41
1:F:76:ILE:O	1:F:76:ILE:HG13	2.20	0.41
1:B:214:VAL:HA	1:B:217:ILE:CG2	2.50	0.41
1:B:391:VAL:HG22	1:B:406:VAL:HG13	2.03	0.41
1:C:296:MET:CE	1:C:354:CYS:HB2	2.50	0.41
1:C:326:GLY:HA3	1:C:455:ALA:HB2	2.01	0.41
1:D:178:ALA:O	1:D:274:PHE:HA	2.20	0.41
1:D:189:VAL:HG21	1:D:447:ALA:HA	2.02	0.41
1:D:217:ILE:HD13	1:D:258:ILE:HG12	2.03	0.41
1:E:320:MET:HG2	1:E:460:GLN:NE2	2.35	0.41
1:A:328:THR:HG23	1:A:453:SER:HB2	2.02	0.41
1:B:7:GLU:O	1:B:8:PHE:CD2	2.73	0.41
1:E:255:GLN:HA	1:E:255:GLN:NE2	2.35	0.41
1:E:284:LEU:HD23	1:E:288:PRO:HD3	2.03	0.41
1:A:54:LYS:O	1:A:87:MET:SD	2.79	0.41
1:A:321:SER:HB3	1:A:455:ALA:HB3	2.01	0.41
1:A:391:VAL:CG2	1:A:406:VAL:HG13	2.51	0.41
1:B:64:LEU:HD13	1:B:64:LEU:HA	1.93	0.41
1:B:127:HIS:HB2	1:C:448:HIS:CB	2.50	0.41
1:D:438:ALA:O	1:D:442:ILE:HG12	2.20	0.41
1:A:217:ILE:O	1:A:220:VAL:HG12	2.21	0.41
1:A:431:ARG:HE	1:A:477:GLU:HG3	1.85	0.41
1:B:133:GLY:CA	1:C:442:ILE:HG23	2.50	0.41
1:E:103:HIS:HA	1:E:129:ASP:OD2	2.20	0.41
1:E:255:GLN:HA	1:E:255:GLN:HE21	1.85	0.41
1:B:318:LYS:HE3	1:B:328:THR:O	2.21	0.41
1:B:471:GLU:OE2	1:B:491:ASN:CB	2.68	0.41
1:C:368:GLN:O	1:C:377:ASP:HB2	2.21	0.41
1:D:332:GLU:OE2	1:F:127:HIS:CE1	2.74	0.41
1:F:438:ALA:O	1:F:442:ILE:HG12	2.21	0.41
1:C:194:LYS:HB2	1:F:191:GLU:HG2	2.02	0.41
1:C:302:PHE:H	1:C:314:LEU:HD23	1.85	0.41
1:D:248:VAL:HG13	1:D:367:VAL:CG1	2.50	0.41
1:A:134:PHE:HA	1:B:445:GLY:HA2	2.03	0.41
1:B:255:GLN:HE21	1:B:286:GLN:HG3	1.86	0.41
1:B:302:PHE:H	1:B:314:LEU:HD23	1.86	0.41
1:C:124:GLN:O	1:C:125:SER:C	2.59	0.41
1:C:345:VAL:O	1:C:427:LEU:HA	2.21	0.41
1:D:6:TYR:HB3	1:D:73:ALA:HB2	2.02	0.41
1:E:130:ARG:HA	1:F:442:ILE:HD13	2.03	0.41



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:E:325:GLN:HG3	1:E:326:GLY:N	2.36	0.41	
1:F:52:VAL:HG23	1:F:54:LYS:HE3	2.03	0.41	
1:F:289:GLY:HA3	1:F:351:LEU:HD13	2.03	0.41	
1:F:295:LEU:O	1:F:300:TYR:HB2	2.21	0.41	
1:A:34:VAL:HB	1:A:35:PRO:HD3	2.04	0.41	
1:A:132:TYR:O	1:A:135:ILE:HG22	2.20	0.41	
1:A:406:VAL:HG22	1:A:461:LEU:HD13	2.03	0.41	
1:C:138:ARG:HA	1:C:138:ARG:HD2	1.97	0.41	
1:C:178:ALA:O	1:C:274:PHE:HA	2.21	0.41	
1:E:26:VAL:HG23	1:E:80:HIS:ND1	2.36	0.41	
1:E:350:MET:SD	1:E:372:ILE:HG21	2.61	0.41	
1:F:293:GLN:NE2	1:F:351:LEU:O	2.54	0.41	
1:A:52:VAL:HG23	1:A:54:LYS:HE3	2.03	0.40	
1:A:85:ALA:HB1	1:A:135:ILE:HB	2.03	0.40	
1:D:168:ALA:HB2	1:D:320:MET:HG3	2.03	0.40	
1:D:353:VAL:HG13	1:D:424:ALA:HB3	2.03	0.40	
1:E:3:MET:CB	1:E:4:PRO:CD	2.96	0.40	
1:F:337:HIS:HB3	1:F:344:LEU:HB2	2.03	0.40	
1:B:483:SER:O	1:B:487:GLU:HG3	2.22	0.40	
1:D:198:GLN:HG2	4:D:703:HOH:O	2.20	0.40	
1:F:10:PHE:CD2	1:F:76:ILE:HD11	2.57	0.40	
1:A:179:ARG:HD2	1:A:308:TRP:HB3	2.04	0.40	
1:A:333:ASP:O	1:C:127:HIS:HB3	2.21	0.40	
1:B:364:ILE:HD13	4:B:714:HOH:O	2.21	0.40	
1:C:122:LEU:HD23	1:C:122:LEU:HA	1.92	0.40	
1:E:53:LEU:HD13	1:E:59:ILE:HA	2.03	0.40	
1:A:273:ALA:HA	1:A:301:GLY:O	2.22	0.40	
1:A:337:HIS:HB3	1:A:344:LEU:HB2	2.03	0.40	
1:B:147:VAL:HG11	1:C:438:ALA:HB3	2.03	0.40	
1:E:100:LEU:HD12	1:E:162:TRP:CD2	2.56	0.40	
1:F:184:MET:HB3	1:F:187:VAL:CG2	2.52	0.40	
1:A:214:VAL:HG11	1:A:283:GLY:HA3	2.03	0.40	
1:B:102:LEU:HD13	1:B:159:LEU:HD11	2.03	0.40	
1:B:353:VAL:CG2	1:B:424:ALA:HB3	2.52	0.40	
1:D:72:CYS:O	1:D:74:GLY:N	2.46	0.40	
1:F:355:PRO:HA	1:F:383:PHE:CZ	2.57	0.40	

There are no symmetry-related clashes.



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	492/498~(99%)	465 (94%)	26~(5%)	1 (0%)	47	79
1	В	494/498~(99%)	466 (94%)	25~(5%)	3(1%)	25	64
1	С	482/498~(97%)	437 (91%)	38 (8%)	7(2%)	10	44
1	D	492/498~(99%)	451 (92%)	35 (7%)	6 (1%)	13	49
1	Е	494/498~(99%)	449 (91%)	35~(7%)	10 (2%)	7	38
1	F	493/498~(99%)	453 (92%)	31 (6%)	9(2%)	8	41
All	All	2947/2988~(99%)	2721 (92%)	190 (6%)	36 (1%)	13	49

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	8	PHE
1	С	125	SER
1	D	184	MET
1	Е	3	MET
1	Е	362	LYS
1	Е	363	PRO
1	F	41	VAL
1	F	115	ILE
1	F	326	GLY
1	F	367	VAL
1	В	115	ILE
1	С	43	ASN
1	С	46	VAL
1	С	185	ARG
1	С	240	PRO
1	D	351	LEU
1	Е	350	MET
1	Е	367	VAL
1	F	359	ALA
1	D	185	ARG



Mol	Chain	Res	Type
1	Е	326	GLY
1	F	350	MET
1	F	386	GLY
1	А	362	LYS
1	С	126	ALA
1	D	350	MET
1	F	43	ASN
1	F	351	LEU
1	В	340	LYS
1	С	44	ALA
1	D	43	ASN
1	Е	116	ASP
1	Е	351	LEU
1	Ε	242	GLY
1	D	41	VAL
1	Е	89	ILE

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	Percentiles
1	А	402/405~(99%)	386~(96%)	16 (4%)	31 66
1	В	404/405~(100%)	379~(94%)	25~(6%)	18 53
1	С	396/405~(98%)	370~(93%)	26 (7%)	16 51
1	D	402/405~(99%)	382 (95%)	20 (5%)	24 60
1	Ε	404/405~(100%)	380 (94%)	24 (6%)	19 54
1	F	403/405~(100%)	384 (95%)	19 (5%)	26 62
All	All	2411/2430 (99%)	2281 (95%)	130 (5%)	22 58

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	14	SER
1	А	54	LYS



Mol	Chain	Res	Type
1	А	121	ASN
1	А	143	ARG
1	А	221	SER
1	А	223	GLN
1	А	315	ARG
1	А	317	MET
1	А	333	ASP
1	А	334	TYR
1	А	361	GLU
1	А	380	ARG
1	А	400	HIS
1	А	425	ARG
1	А	431	ARG
1	A	492	GLU
1	В	17	LEU
1	В	54	LYS
1	В	61	ARG
1	В	62	LEU
1	В	79	MET
1	В	83	SER
1	В	108	ARG
1	В	118	ASP
1	В	138	ARG
1	В	143	ARG
1	В	157	GLU
1	В	159	LEU
1	В	198	GLN
1	В	223	GLN
1	В	268	ASP
1	В	272	THR
1	B	285	LYS
1	В	331	MET
1	В	333	ASP
1	B	334	TYR
1	В	380	ARG
1	B	421	LEU
1	В	425	ARG
1	B	433	SER
1	В	435	ARG
1	C	20	ASP
1	С	54	LYS
1	С	65	GLU



Mol	Chain	Res	Type
1	С	70	ASP
1	С	90	ARG
1	С	108	ARG
1	С	113	ASP
1	С	122	LEU
1	С	124	GLN
1	С	125	SER
1	С	143	ARG
1	С	154	GLU
1	С	182	ASP
1	С	212	ASP
1	С	270	ASN
1	С	305	GLU
1	С	320	MET
1	С	333	ASP
1	С	334	TYR
1	С	335	THR
1	С	360	GLU
1	С	415	GLU
1	С	425	ARG
1	С	482	SER
1	С	492	GLU
1	С	496	ARG
1	D	43	ASN
1	D	45	HIS
1	D	54	LYS
1	D	90	ARG
1	D	113	ASP
1	D	152	ASP
1	D	184	MET
1	D	198	GLN
1	D	218	ARG
1	D	230	ASP
1	D	315	ARG
1	D	333	ASP
1	D	372	ILE
1	D	400	HIS
1	D	413	LYS
1	D	420	LYS
1	D	425	ARG
1	D	431	ARG
1	D	457	THR



Mol	Chain	Res	Type
1	D	482	SER
1	Е	2	LYS
1	Е	38	GLN
1	Е	54	LYS
1	Е	61	ARG
1	Е	113	ASP
1	Е	143	ARG
1	Е	190	THR
1	Е	245	GLU
1	Е	251	SER
1	Е	268	ASP
1	Е	285	LYS
1	Е	315	ARG
1	Е	331	MET
1	E	333	ASP
1	E	334	TYR
1	Е	348	SER
1	Е	352	GLU
1	Е	366	ASP
1	Е	380	ARG
1	Е	415	GLU
1	Е	418	MET
1	Е	425	ARG
1	Е	437	SER
1	Е	457	THR
1	F	54	LYS
1	F	57	ASP
1	F	109	ASP
1	F	113	ASP
1	F	143	ARG
1	F	158	ARG
1	F	182	ASP
1	F	190	THR
1	F	221	SER
1	F	223	GLN
1	F	259	GLU
1	F	315	ARG
1	F	334	TYR
1	F	380	ARG
1	F	413	LYS
1	F	417	ASP
1	F	425	ARG



Continued from previous page...

Mol	Chain	Res	Type
1	F	473	VAL
1	F	492	GLU

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	407	ASN
1	В	183	ASN
1	F	183	ASN

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 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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 Turna Cl		Chain	Dec	Dec Link	Bond lengths			Bond angles				
MOI	туре	Unain	nes	nes	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	GOL	D	601	-	$5,\!5,\!5$	0.07	0	$5,\!5,\!5$	0.26	0		
2	GOL	Е	601	-	$5,\!5,\!5$	0.13	0	$5,\!5,\!5$	0.29	0		
2	GOL	С	601	-	$5,\!5,\!5$	0.12	0	$5,\!5,\!5$	0.32	0		
2	GOL	A	601	-	$5,\!5,\!5$	0.12	0	$5,\!5,\!5$	0.29	0		



Mol	Type	Chain	Res	Tink	Bond lengths			Bond angles		
					Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	GOL	В	601	-	$5,\!5,\!5$	0.09	0	$5,\!5,\!5$	0.22	0

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	GOL	D	601	-	-	2/4/4/4	-
2	GOL	Е	601	-	-	2/4/4/4	-
2	GOL	С	601	-	-	4/4/4/4	-
2	GOL	А	601	-	-	4/4/4/4	-
2	GOL	В	601	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	601	GOL	O1-C1-C2-C3
2	С	601	GOL	O1-C1-C2-C3
2	С	601	GOL	C1-C2-C3-O3
2	D	601	GOL	O1-C1-C2-C3
2	Е	601	GOL	C1-C2-C3-O3
2	Ε	601	GOL	O2-C2-C3-O3
2	А	601	GOL	O1-C1-C2-O2
2	С	601	GOL	O1-C1-C2-O2
2	С	601	GOL	O2-C2-C3-O3
2	D	601	GOL	O1-C1-C2-O2
2	А	601	GOL	O2-C2-C3-O3
2	А	601	GOL	C1-C2-C3-O3
2	В	601	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.



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	494/498~(99%)	-0.45	0 100 100	45, 70, 98, 113	0
1	В	496/498~(99%)	-0.35	1 (0%) 95 94	48, 79, 112, 150	0
1	С	486/498~(97%)	-0.25	3 (0%) 89 83	45, 81, 113, 134	0
1	D	494/498~(99%)	-0.25	3 (0%) 89 83	53, 78, 107, 134	0
1	Ε	496/498~(99%)	-0.23	4 (0%) 86 78	51, 82, 111, 176	0
1	F	495/498~(99%)	-0.15	1 (0%) 95 94	56, 89, 122, 150	0
All	All	2961/2988~(99%)	-0.28	12 (0%) 92 89	45, 79, 112, 176	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	1	MET	5.1
1	F	361	GLU	3.5
1	Е	366	ASP	2.6
1	D	342	ASN	2.5
1	С	362	LYS	2.4
1	В	1	MET	2.3
1	D	337	HIS	2.3
1	Е	365	LEU	2.2
1	Е	384	ASP	2.1
1	С	236	TYR	2.1
1	D	336	TYR	2.1
1	С	416	HIS	2.1

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

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



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	GOL	В	601	6/6	0.87	0.24	84,97,108,117	0
2	GOL	Е	601	6/6	0.87	0.20	79,84,88,89	0
2	GOL	С	601	6/6	0.89	0.16	87,92,98,99	0
2	GOL	А	601	6/6	0.91	0.14	77,79,82,82	0
2	GOL	D	601	6/6	0.94	0.14	70,74,76,83	0
3	MN	С	602	1/1	0.98	0.11	82,82,82,82	0
3	MN	В	602	1/1	0.99	0.07	77,77,77,77	0
3	MN	А	602	1/1	0.99	0.12	75,75,75,75	0
3	MN	D	602	1/1	0.99	0.10	79,79,79,79	0
3	MN	Е	602	1/1	0.99	0.12	75,75,75,75	0
3	MN	F	501	1/1	0.99	0.09	82,82,82,82	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.

