

Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2023 – 05:52 PM JST

PDB ID	:	7W7B
Title	:	Heme exporter HrtBA in complex with protoporphyrin IX containing man-
		ganese(III), high resolution data
Authors	:	Hisano, T.; Nakamura, H.; Rahman, M.M.; Tosha, T.; Shirouzu, M.; Shiro, Y.
Deposited on	:	2021-12-04
Resolution	:	3.00 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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	231	4%	22%	6%
1	С	231	64%	31%	6%
1	Е	231	13%	22%	6%
1	G	231	% 68%	30%	·
1	Ι	231	71%	25%	·
1	K	231	74%	21%	5%



Contr	nuea jron	i previous	page		
Mol	Chain	Length	Quality of chain		
2	В	344	7%	27%	·
2	D	344	76%	23%	
2	F	344	78%	22%	
2	Н	344	75%	24%	
2	J	344	4%	25%	
2	L	344	81%	19%	



7W7B

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25131 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	216	Total	С	Ν	0	S	0	0	0
	Л	210	1618	1010	293	312	3	0	0	0
1	С	218	Total	С	Ν	0	S	0	0	0
		210	1634	1019	296	316	3	0	0	0
1	F	217	Total	С	Ν	0	S	0	0	0
	Ľ	211	1629	1016	295	315	3	0	0	0
1	C	225	Total	С	Ν	0	S	0	0	0
	G	220	1693	1059	307	324	3	0	0	0
1	т	221	Total	С	Ν	0	S	0	0	0
	1	221	1652	1031	299	319	3	0	0	0
1	K	210	Total	С	Ν	Ο	S	0	0	0
	n	219	1639	1022	297	317	3		U	U

• Molecule 1 is a protein called Putative ABC transport system, ATP-binding protein.

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	222	LYS	-	expression tag	UNP Q6NEF2
А	223	LEU	-	expression tag	UNP Q6NEF2
А	224	TRP	-	expression tag	UNP Q6NEF2
А	225	SER	-	expression tag	UNP Q6NEF2
А	226	HIS	-	expression tag	UNP Q6NEF2
A	227	PRO	-	expression tag	UNP Q6NEF2
А	228	GLN	-	expression tag	UNP Q6NEF2
А	229	PHE	-	expression tag	UNP Q6NEF2
А	230	GLU	-	expression tag	UNP Q6NEF2
А	231	LYS	-	expression tag	UNP Q6NEF2
С	222	LYS	-	expression tag	UNP Q6NEF2
С	223	LEU	-	expression tag	UNP Q6NEF2
С	224	TRP	-	expression tag	UNP Q6NEF2
С	225	SER	-	expression tag	UNP Q6NEF2
С	226	HIS	-	expression tag	UNP Q6NEF2
С	227	PRO	-	expression tag	UNP Q6NEF2
С	228	GLN	-	expression tag	UNP Q6NEF2



$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Continu	ied from pre	vious page			
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Chain	Residue	Modelled	Actual	Comment	Reference
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	С	229	PHE	-	expression tag	UNP Q6NEF2
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	С	230	GLU	-	expression tag	UNP Q6NEF2
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	С	231	LYS	-	expression tag	UNP Q6NEF2
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Е	222	LYS	-	expression tag	UNP Q6NEF2
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Е	223	LEU	-	expression tag	UNP Q6NEF2
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Е	224	TRP	-	expression tag	UNP Q6NEF2
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Е	225	SER	_	expression tag	UNP Q6NEF2
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Е	226	HIS	-	expression tag	UNP Q6NEF2
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Е	227	PRO	-	expression tag	UNP Q6NEF2
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Е	228	GLN	-	expression tag	UNP Q6NEF2
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Е	229	PHE	-	expression tag	UNP Q6NEF2
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Е	230	GLU	-	expression tag	UNP Q6NEF2
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Е	231	LYS	-	expression tag	UNP Q6NEF2
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	G	222	LYS	-	expression tag	UNP Q6NEF2
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	G	223	LEU	-	expression tag	UNP Q6NEF2
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	G	224	TRP	-	expression tag	UNP Q6NEF2
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	G	225	SER	-	expression tag	UNP Q6NEF2
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	G	226	HIS	-	expression tag	UNP Q6NEF2
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	G	227	PRO	-	expression tag	UNP Q6NEF2
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	G	228	GLN	-	expression tag	UNP Q6NEF2
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	G	229	PHE	-	expression tag	UNP Q6NEF2
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	G	230	GLU	-	expression tag	UNP Q6NEF2
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	G	231	LYS	-	expression tag	UNP Q6NEF2
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Ι	222	LYS	-	expression tag	UNP Q6NEF2
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Ι	223	LEU	-	expression tag	UNP Q6NEF2
I225SER-expression tagUNP Q6NEF2I226HIS-expression tagUNP Q6NEF2I227PRO-expression tagUNP Q6NEF2I228GLN-expression tagUNP Q6NEF2I229PHE-expression tagUNP Q6NEF2I230GLU-expression tagUNP Q6NEF2I231LYS-expression tagUNP Q6NEF2K222LYS-expression tagUNP Q6NEF2K223LEU-expression tagUNP Q6NEF2K224TRP-expression tagUNP Q6NEF2K225SER-expression tagUNP Q6NEF2K226HIS-expression tagUNP Q6NEF2K227PRO-expression tagUNP Q6NEF2K228GLN-expression tagUNP Q6NEF2K229PHE-expression tagUNP Q6NEF2K229PHE-expression tagUNP Q6NEF2K229PHE-expression tagUNP Q6NEF2K230GLU-expression tagUNP Q6NEF2	Ι	224	TRP	_	expression tag	UNP Q6NEF2
I226HIS-expression tagUNP Q6NEF2I227PRO-expression tagUNP Q6NEF2I228GLN-expression tagUNP Q6NEF2I229PHE-expression tagUNP Q6NEF2I230GLU-expression tagUNP Q6NEF2I231LYS-expression tagUNP Q6NEF2K222LYS-expression tagUNP Q6NEF2K223LEU-expression tagUNP Q6NEF2K224TRP-expression tagUNP Q6NEF2K225SER-expression tagUNP Q6NEF2K226HIS-expression tagUNP Q6NEF2K227PRO-expression tagUNP Q6NEF2K228GLN-expression tagUNP Q6NEF2K229PHE-expression tagUNP Q6NEF2K230GLU-expression tagUNP Q6NEF2K230GLU-expression tagUNP Q6NEF2	Ι	225	SER	-	expression tag	UNP Q6NEF2
I227PRO-expression tagUNP Q6NEF2I228GLN-expression tagUNP Q6NEF2I229PHE-expression tagUNP Q6NEF2I230GLU-expression tagUNP Q6NEF2I231LYS-expression tagUNP Q6NEF2K222LYS-expression tagUNP Q6NEF2K223LEU-expression tagUNP Q6NEF2K224TRP-expression tagUNP Q6NEF2K225SER-expression tagUNP Q6NEF2K226HIS-expression tagUNP Q6NEF2K227PRO-expression tagUNP Q6NEF2K228GLN-expression tagUNP Q6NEF2K229PHE-expression tagUNP Q6NEF2K230GLU-expression tagUNP Q6NEF2	Ι	226	HIS	_	expression tag	UNP Q6NEF2
I228GLN-expression tagUNP Q6NEF2I229PHE-expression tagUNP Q6NEF2I230GLU-expression tagUNP Q6NEF2I231LYS-expression tagUNP Q6NEF2K222LYS-expression tagUNP Q6NEF2K223LEU-expression tagUNP Q6NEF2K224TRP-expression tagUNP Q6NEF2K225SER-expression tagUNP Q6NEF2K226HIS-expression tagUNP Q6NEF2K227PRO-expression tagUNP Q6NEF2K228GLN-expression tagUNP Q6NEF2K229PHE-expression tagUNP Q6NEF2K230GLU-expression tagUNP Q6NEF2	Ι	227	PRO	-	expression tag	UNP Q6NEF2
I229PHE-expression tagUNP Q6NEF2I230GLU-expression tagUNP Q6NEF2I231LYS-expression tagUNP Q6NEF2K222LYS-expression tagUNP Q6NEF2K223LEU-expression tagUNP Q6NEF2K224TRP-expression tagUNP Q6NEF2K225SER-expression tagUNP Q6NEF2K226HIS-expression tagUNP Q6NEF2K227PRO-expression tagUNP Q6NEF2K228GLN-expression tagUNP Q6NEF2K229PHE-expression tagUNP Q6NEF2K230GLU-expression tagUNP Q6NEF2	Ι	228	GLN	_	expression tag	UNP Q6NEF2
I230GLU-expression tagUNP Q6NEF2I231LYS-expression tagUNP Q6NEF2K222LYS-expression tagUNP Q6NEF2K223LEU-expression tagUNP Q6NEF2K224TRP-expression tagUNP Q6NEF2K225SER-expression tagUNP Q6NEF2K226HIS-expression tagUNP Q6NEF2K227PRO-expression tagUNP Q6NEF2K228GLN-expression tagUNP Q6NEF2K229PHE-expression tagUNP Q6NEF2K230GLU-expression tagUNP Q6NEF2	Ι	229	PHE	_	expression tag	UNP Q6NEF2
I231LYS-expression tagUNP Q6NEF2K222LYS-expression tagUNP Q6NEF2K223LEU-expression tagUNP Q6NEF2K224TRP-expression tagUNP Q6NEF2K225SER-expression tagUNP Q6NEF2K226HIS-expression tagUNP Q6NEF2K227PRO-expression tagUNP Q6NEF2K228GLN-expression tagUNP Q6NEF2K229PHE-expression tagUNP Q6NEF2K230GLU-expression tagUNP Q6NEF2	Ι	230	GLU	_	expression tag	UNP Q6NEF2
K222LYS-expression tagUNP Q6NEF2K223LEU-expression tagUNP Q6NEF2K224TRP-expression tagUNP Q6NEF2K225SER-expression tagUNP Q6NEF2K226HIS-expression tagUNP Q6NEF2K227PRO-expression tagUNP Q6NEF2K228GLN-expression tagUNP Q6NEF2K229PHE-expression tagUNP Q6NEF2K230GLU-expression tagUNP Q6NEF2	Ι	231	LYS	_	expression tag	UNP Q6NEF2
K223LEU-expression tagUNP Q6NEF2K224TRP-expression tagUNP Q6NEF2K225SER-expression tagUNP Q6NEF2K226HIS-expression tagUNP Q6NEF2K227PRO-expression tagUNP Q6NEF2K228GLN-expression tagUNP Q6NEF2K229PHE-expression tagUNP Q6NEF2K230GLU-expression tagUNP Q6NEF2	K	222	LYS	_	expression tag	UNP Q6NEF2
K224TRP-expression tagUNP Q6NEF2K225SER-expression tagUNP Q6NEF2K226HIS-expression tagUNP Q6NEF2K227PRO-expression tagUNP Q6NEF2K228GLN-expression tagUNP Q6NEF2K229PHE-expression tagUNP Q6NEF2K230GLU-expression tagUNP Q6NEF2	K	223	LEU	_	expression tag	UNP Q6NEF2
K225SER-expression tagUNP Q6NEF2K226HIS-expression tagUNP Q6NEF2K227PRO-expression tagUNP Q6NEF2K228GLN-expression tagUNP Q6NEF2K229PHE-expression tagUNP Q6NEF2K230GLU-expression tagUNP Q6NEF2	K	224	TRP	-	expression tag	UNP Q6NEF2
K226HIS-expression tagUNP Q6NEF2K227PRO-expression tagUNP Q6NEF2K228GLN-expression tagUNP Q6NEF2K229PHE-expression tagUNP Q6NEF2K230GLU-expression tagUNP Q6NEF2	K	225	SER	_	expression tag	UNP Q6NEF2
K227PRO-expression tagUNP Q6NEF2K228GLN-expression tagUNP Q6NEF2K229PHE-expression tagUNP Q6NEF2K230GLU-expression tagUNP Q6NEF2	K	226	HIS	_	expression tag	UNP Q6NEF2
K228GLN-expression tagUNP Q6NEF2K229PHE-expression tagUNP Q6NEF2K230GLU-expression tagUNP Q6NEF2	K	227	PRO	_	expression tag	UNP Q6NEF2
K229PHE-expression tagUNP Q6NEF2K230GLU-expression tagUNP Q6NEF2	K	228	GLN	_	expression tag	UNP Q6NEF2
K 230 GLU - expression tag UNP Q6NEF2	K	229	PHE	_	expression tag	UNP Q6NEF2
	K	230	GLU	-	expression tag	UNP Q6NEF2



Chain	Residue	Modelled	Actual	Comment	Reference
Κ	231	LYS	-	expression tag	UNP Q6NEF2

• Molecule 2 is a protein called Putative ABC transport system integral membrane protein.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
2	В	341	Total	С	Ν	Ο	S	0	1	0
		041	2518	1617	425	471	5	0	1	0
2	Л	343	Total	С	Ν	Ο	\mathbf{S}	0	1	0
	D	040	2530	1624	427	474	5	0	1	0
2	F	349	Total	С	Ν	Ο	\mathbf{S}	0	1	0
	T,	042	2523	1620	426	472	5	0	1	0
0	Ц	241	Total	С	Ν	Ο	S	0	0	0
	11	041	2510	1612	422	471	5	0	0	0
0	т	242	Total	С	Ν	0	S	0	1	0
	J	040	2530	1624	427	474	5	0	I	0
2	т	343	Total	С	Ν	Ο	S	0	0	0
		040	2522	1619	424	474	5		0	U

• Molecule 3 is (1S)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHO RYL]OXY}-1-[(PENTANOYLOXY)METHYL]ETHYL OCTANOATE (three-letter code: AGA) (formula: C₁₉H₃₆O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	В	1	Total 23	C 14	0 8	Р 1	0	0

• Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	В	1	Total 10	С 6	0 4	0	0

• Molecule 5 is PROTOPORPHYRIN IX CONTAINING MN (three-letter code: MNR) (formula: $C_{34}H_{32}MnN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf
5	Л	1	Total	С	Mn	Ν	Ο	0	0
0	5 D	1	43	34	1	4	4	0	0
5	Ц	1	Total	С	Mn	Ν	0	0	0
0	11	1	43	34	1	4	4	0	U



• Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	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: Putative ABC transport system, ATP-binding protein

• Molecule 1: Putative ABC transport system, ATP-binding protein







• Molecule 1: Putative ABC transport system, ATP-binding protein







• Molecule 2: Putative ABC transport system integral membrane protein







• Molecule 2: Putative ABC transport system integral membrane protein







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	82.00Å 133.49Å 159.34Å	Deperitor
a, b, c, α , β , γ	111.65° 99.69° 94.64°	Depositor
Bosolution (Å)	49.39 - 3.00	Depositor
Resolution (A)	49.39 - 2.99	EDS
% Data completeness	96.5 (49.39-3.00)	Depositor
(in resolution range)	80.2 (49.39-2.99)	EDS
R _{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.26 (at 3.01 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R R.	0.266 , 0.299	Depositor
Λ, Λ_{free}	0.266 , 0.299	DCC
R_{free} test set	3785 reflections $(3.14%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	78.3	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.26 , 55.2	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	25131	wwPDB-VP
Average B, all atoms $(Å^2)$	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.35% 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: PEG, MNR, PGE, AGA

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	
WIOI		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.30	0/1637	0.54	0/2216
1	С	0.29	0/1653	0.54	0/2238
1	Ε	0.26	0/1648	0.50	0/2230
1	G	0.30	0/1716	0.52	0/2325
1	Ι	0.30	0/1671	0.53	0/2263
1	Κ	0.29	0/1658	0.53	0/2245
2	В	0.26	0/2567	0.51	0/3509
2	D	0.29	0/2579	0.53	0/3526
2	F	0.26	0/2572	0.50	0/3516
2	Η	0.27	0/2556	0.52	0/3495
2	J	0.27	0/2579	0.50	0/3526
2	L	0.26	0/2568	0.50	0/3512
All	All	0.28	0/25404	0.52	0/34601

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1618	0	1664	37	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	1634	0	1679	53	0
1	Е	1629	0	1675	37	0
1	G	1693	0	1737	45	0
1	Ι	1652	0	1697	46	0
1	K	1639	0	1684	36	0
2	В	2518	0	2601	75	0
2	D	2530	0	2613	58	0
2	F	2523	0	2606	56	0
2	Н	2510	0	2588	61	0
2	J	2530	0	2613	59	0
2	L	2522	0	2600	42	0
3	В	23	0	19	2	0
4	В	10	0	14	1	0
5	D	43	0	30	8	0
5	Н	43	0	30	5	0
6	D	7	0	10	0	0
6	Н	7	0	10	0	0
All	All	25131	0	25870	575	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 11.

All (575) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
2:F:79:ARG:HH12	2:F:198:GLN:HB2	1.31	0.93
1:I:198:HIS:HB3	1:K:198:HIS:CE1	2.07	0.90
1:A:53:LEU:HD11	1:A:162:LEU:HB3	1.56	0.87
1:E:59:LEU:HD13	2:F:340:LEU:HD11	1.55	0.86
1:E:127:VAL:HG13	1:E:181:LEU:HD21	1.58	0.86
1:E:53:LEU:HD11	1:E:162:LEU:HB3	1.60	0.83
2:F:304:LEU:HD21	2:F:309:VAL:HG23	1.59	0.82
2:D:253:ILE:HD13	2:D:331:VAL:HG23	1.63	0.81
2:H:180:THR:HG22	2:H:182:ALA:H	1.46	0.80
1:I:132:LEU:HB3	1:I:135:ARG:HD3	1.62	0.79
2:B:253:ILE:HD13	2:B:331:VAL:HG23	1.64	0.79
1:K:55:ILE:HG23	1:K:67:VAL:HG21	1.64	0.79
1:G:127:VAL:HG13	1:G:181:LEU:HD21	1.64	0.78
1:I:127:VAL:HG13	1:I:181:LEU:HD21	1.66	0.77
1:A:127:VAL:HG13	1:A:181:LEU:HD21	1.67	0.77
2:H:193:PRO:HG3	2:H:203:VAL:HG11	1.68	0.76



	A 4 arra 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:L:79:ARG:HH12	2:L:198:GLN:HB2	1.50	0.75
1:I:95:LEU:O	1:I:103:GLN:NE2	2.20	0.74
2:B:72:ILE:HG12	2:B:187:LEU:HG	1.70	0.74
1:C:104:LEU:HB3	1:C:155:MET:HG3	1.69	0.73
1:G:53:LEU:HD11	1:G:162:LEU:HB3	1.70	0.73
1:K:41:ILE:HD11	1:K:194:LEU:HD22	1.71	0.72
1:E:49:LYS:HD2	1:E:196:VAL:HG13	1.72	0.72
2:H:56:VAL:HG22	2:H:203:VAL:HG22	1.72	0.71
2:D:185:THR:HG23	2:D:186:VAL:HG23	1.72	0.71
2:D:180:THR:HG22	2:D:182:ALA:H	1.56	0.71
1:G:55:ILE:HG22	1:G:67:VAL:HG21	1.73	0.71
1:C:53:LEU:HD11	1:C:162:LEU:HB3	1.73	0.70
2:H:88:VAL:HG22	2:H:105:MET:HG2	1.73	0.70
2:F:253:ILE:HD13	2:F:331:VAL:HG23	1.74	0.70
1:E:14:VAL:HG23	1:E:55:ILE:HD11	1.73	0.69
2:J:253:ILE:HD13	2:J:331:VAL:HG13	1.73	0.69
1:G:7:LEU:HB3	1:G:33:ILE:HG22	1.73	0.69
2:B:305:GLY:HA2	4:B:502:PGE:H2	1.74	0.69
1:K:132:LEU:HD22	1:K:135:ARG:HE	1.57	0.69
2:H:42:GLN:HG3	2:H:163:HIS:HA	1.72	0.69
1:E:7:LEU:HD23	1:E:33:ILE:HD13	1.75	0.68
2:D:108:PRO:HG2	2:D:111:THR:HG21	1.74	0.68
2:B:42:GLN:HG3	2:B:163:HIS:HA	1.74	0.68
2:B:26:THR:HG21	2:B:282:VAL:HG22	1.74	0.68
2:D:56:VAL:HG22	2:D:203:VAL:HG22	1.75	0.67
1:C:127:VAL:HG13	1:C:181:LEU:HD21	1.76	0.67
1:C:14:VAL:HG23	1:C:55:ILE:HD11	1.75	0.67
1:G:51:THR:O	1:G:55:ILE:HG12	1.96	0.66
2:L:326:ILE:O	2:L:329:ARG:NH1	2.26	0.66
1:K:42:VAL:HG11	1:K:200:ARG:HE	1.60	0.66
1:A:33:ILE:HD11	1:A:194:LEU:HG	1.76	0.66
1:C:55:ILE:HG23	1:C:67:VAL:HG21	1.76	0.65
1:A:171:ASP:HB2	1:C:214:ASP:OD1	1.97	0.65
1:C:47:SER:O	1:C:215:GLY:N	2.24	0.65
2:H:41:LYS:NZ	2:H:48:GLU:OE1	2.30	0.65
2:F:304:LEU:CD2	2:F:309:VAL:HG23	2.26	0.65
1:G:108:ASP:OD1	1:G:111:ARG:NH2	2.30	0.64
2:H:32:LEU:HD12	2:H:227:GLN:HG2	1.79	0.64
2:H:108:PRO:HD2	2:H:111:THR:HG21	1.80	0.64
1:I:182:LEU:O	1:I:186:THR:HG23	1.98	0.64
1:K:82:ARG:HB2	2:L:260:GLY:HA3	1.80	0.63



	At any 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:D:326:ILE:O	2:D:329:ARG:NH1	2.29	0.63
1:G:73:GLU:HG2	1:K:84:HIS:HE1	1.62	0.63
2:D:102:THR:HG21	2:D:131:LEU:HD22	1.81	0.63
1:A:167:THR:HB	1:A:175:SER:HB3	1.81	0.63
2:D:156:VAL:HG12	2:D:157:LYS:H	1.64	0.62
2:H:125:ALA:HA	2:H:169:VAL:HG12	1.81	0.62
2:H:253:ILE:HG22	2:H:334:VAL:HG11	1.82	0.62
2:F:32:LEU:O	2:F:36:THR:HG23	1.99	0.62
2:L:72:ILE:HG12	2:L:187:LEU:HG	1.81	0.62
2:B:128:PRO:HB3	2:B:158:THR:HG22	1.81	0.61
2:L:8:ILE:HD11	2:L:273:GLN:HG3	1.82	0.61
1:K:127:VAL:HG13	1:K:181:LEU:HD21	1.80	0.61
2:B:219:GLU:HB2	5:D:401:MNR:C2C	2.30	0.61
2:D:42:GLN:HG3	2:D:163:HIS:HA	1.83	0.60
2:F:196:GLN:HG3	2:F:197:PRO:HD2	1.82	0.60
2:D:74:GLU:HG3	2:D:183:VAL:HG21	1.83	0.60
2:D:26:THR:HG21	2:D:282:VAL:HG22	1.82	0.60
2:F:246:THR:HG21	2:F:328:VAL:HG22	1.84	0.60
2:J:72:ILE:HG12	2:J:187:LEU:HG	1.83	0.60
1:I:7:LEU:HB3	1:I:33:ILE:HG22	1.84	0.60
2:B:239:VAL:HG12	2:D:17:LEU:HD21	1.83	0.60
2:H:117:VAL:HG13	2:H:156:VAL:HB	1.84	0.60
1:K:55:ILE:CG2	1:K:67:VAL:HG21	2.32	0.59
2:B:97:GLN:HG3	2:B:136:HIS:HB2	1.84	0.59
1:C:81:ARG:NH1	2:D:257:ALA:O	2.29	0.59
2:H:26:THR:HG21	2:H:282:VAL:HG22	1.83	0.59
2:J:32:LEU:O	2:J:36:THR:HG23	2.02	0.59
2:B:253:ILE:HG22	2:B:334:VAL:HG11	1.84	0.59
1:A:44:GLU:OE1	1:A:198:HIS:NE2	2.35	0.59
2:J:80:TRP:HA	2:J:195:ILE:HD12	1.84	0.59
2:H:73:SER:OG	2:H:76:GLN:HB2	2.03	0.58
2:D:125:ALA:HA	2:D:169:VAL:HG12	1.85	0.58
2:B:156:VAL:HG12	2:B:157:LYS:N	2.18	0.58
2:J:92:ARG:NH1	2:J:94:GLU:OE1	2.36	0.58
2:L:116:SER:OG	2:L:159:GLU:OE2	2.22	0.58
1:G:10:THR:HG21	1:K:73:GLU:HG2	1.86	0.58
2:B:17:LEU:HD21	2:D:239:VAL:HG12	1.86	0.58
2:L:31:MET:HE1	2:L:292:LEU:HD23	1.85	0.58
2:B:219:GLU:HB2	5:D:401:MNR:C1C	2.34	0.57
1:I:33:ILE:HG12	1:I:192:ALA:HB1	1.86	0.57
1:A:127:VAL:O	1:A:147:ARG:HD3	2.05	0.57



	A A	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:141:SER:OG	1:C:144:GLN:HG3	2.05	0.57
1:E:26:LEU:HD11	1:E:29:ALA:HB2	1.87	0.57
1:C:190:ALA:HB1	1:K:66:THR:HG23	1.85	0.57
1:G:141:SER:O	1:G:145:ARG:HG3	2.04	0.57
2:H:32:LEU:O	2:H:36:THR:HG23	2.05	0.57
1:I:126:ARG:NH2	1:I:188:GLU:OE1	2.36	0.57
2:B:94:GLU:HB3	2:B:144:THR:HB	1.86	0.57
2:F:26:THR:HG22	2:F:316:ILE:HG21	1.87	0.57
1:I:55:ILE:HG22	1:I:67:VAL:HG21	1.87	0.56
2:J:205:ASP:OD1	2:J:206:LEU:N	2.34	0.56
2:J:326:ILE:O	2:J:329:ARG:NH1	2.37	0.56
2:H:137:VAL:HG13	2:H:141:ASP:HB2	1.87	0.56
2:B:36:THR:HG22	2:B:223:LEU:HB3	1.87	0.56
1:K:212:MET:HG2	1:K:217:ALA:HA	1.87	0.56
2:J:245:TRP:NE1	2:J:273:GLN:OE1	2.38	0.56
2:B:116:SER:OG	2:B:159:GLU:OE2	2.24	0.56
1:C:141:SER:O	1:C:145:ARG:HG3	2.06	0.56
2:B:145:LEU:HG	2:B:177:VAL:HG11	1.88	0.56
2:D:80:TRP:HA	2:D:195:ILE:HD13	1.88	0.55
1:C:33:ILE:HG22	1:C:192:ALA:HB1	1.88	0.55
1:K:141:SER:OG	1:K:144:GLN:HG3	2.07	0.55
2:F:302:PHE:CE2	2:F:304:LEU:HD12	2.41	0.55
2:F:108:PRO:HG2	2:F:111:THR:HG21	1.89	0.55
2:H:94:GLU:HG3	2:H:99:ALA:HB2	1.89	0.55
2:H:335:ASP:OD1	2:H:336:PRO:HD2	2.07	0.55
1:I:127:VAL:HG12	1:I:147:ARG:HB3	1.88	0.55
2:B:86:LEU:HD22	2:B:188:LEU:HD11	1.89	0.55
2:F:244:VAL:HG12	2:H:244:VAL:HG12	1.88	0.55
2:L:125:ALA:HA	2:L:169:VAL:HG12	1.88	0.54
1:K:127:VAL:HG12	1:K:147:ARG:HB3	1.89	0.54
2:L:87:GLY:O	2:L:105:MET:HA	2.07	0.54
2:L:108:PRO:HD2	2:L:111:THR:HG21	1.89	0.54
1:A:123:LEU:O	1:A:127:VAL:HG23	2.06	0.54
1:A:198:HIS:O	1:A:198:HIS:ND1	2.40	0.54
1:C:41:ILE:HD13	1:C:52:LEU:HD23	1.89	0.54
1:C:44:GLU:OE2	1:C:198:HIS:NE2	2.40	0.54
1:G:38:LEU:HD11	1:G:195:MET:HE2	1.89	0.54
2:J:59:THR:N	2:J:200:ASN:O	2.36	0.54
1:K:40:ALA:HB3	1:K:209:PHE:HB3	1.89	0.54
1:C:41:ILE:CD1	1:C:194:LEU:HD11	2.37	0.54
2:L:302:PHE:CE1	2:L:304:LEU:HD13	2.42	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:13:SER:OG	1:E:28:SER:N	2.26	0.54
2:J:116:SER:OG	2:J:159:GLU:OE2	2.24	0.54
2:D:26:THR:HG22	2:D:316:ILE:HD13	1.89	0.54
1:I:107:THR:O	1:I:111:ARG:HG3	2.08	0.54
2:J:186:VAL:HG12	2:J:187:LEU:N	2.23	0.54
2:B:55:VAL:O	2:B:204:THR:HG22	2.08	0.54
1:C:15:VAL:HG22	1:C:24:THR:HA	1.89	0.54
2:D:100:ASN:OD1	2:D:101:THR:N	2.40	0.54
2:D:186:VAL:HG12	2:D:187:LEU:N	2.23	0.54
1:A:147:ARG:NH2	1:A:177:GLU:OE1	2.40	0.53
2:H:197:PRO:HB2	2:H:201:GLU:HB2	1.89	0.53
1:K:14:VAL:CG2	1:K:55:ILE:HD11	2.38	0.53
1:C:127:VAL:HG11	1:C:147:ARG:O	2.09	0.53
2:J:95:SER:HB3	2:J:135:LEU:HD13	1.89	0.53
2:L:290:ALA:HB2	2:L:309:VAL:HG21	1.89	0.53
2:F:72:ILE:HG23	2:F:76:GLN:HB3	1.91	0.53
1:I:11:ASN:O	1:I:65:GLY:HA3	2.08	0.53
1:I:203:LEU:HB3	1:I:209:PHE:CE1	2.43	0.53
2:J:15:PHE:CD1	2:J:277:ILE:HG13	2.43	0.53
2:J:26:THR:HG22	2:J:316:ILE:HD13	1.89	0.53
1:E:6:VAL:O	1:E:69:LEU:HD12	2.08	0.53
1:E:14:VAL:CG2	1:E:55:ILE:HD11	2.38	0.53
1:A:42:VAL:HG21	1:A:203:LEU:HD11	1.91	0.53
2:F:24:LEU:HD12	2:H:236:LEU:HD12	1.89	0.53
1:I:51:THR:O	1:I:55:ILE:HG12	2.09	0.53
1:A:127:VAL:HG21	1:A:151:ALA:HB2	1.91	0.53
1:C:108:ASP:OD2	1:C:116:ARG:HG2	2.08	0.53
1:E:129:LEU:HD22	1:E:132:LEU:HD12	1.91	0.53
1:I:200:ARG:HA	1:I:203:LEU:HG	1.91	0.53
1:C:93:ASN:OD1	2:D:251:ARG:NH2	2.35	0.53
1:C:42:VAL:CG2	1:C:203:LEU:HD21	2.39	0.52
2:F:72:ILE:HG12	2:F:187:LEU:HG	1.90	0.52
2:H:128:PRO:HG2	2:H:131:LEU:HB3	1.91	0.52
2:B:36:THR:HG22	2:B:223:LEU:HD13	1.91	0.52
2:B:52:PRO:HD2	2:B:206:LEU:HD13	1.90	0.52
2:F:215:ALA:HB2	5:H:401:MNR:HMD2	1.91	0.52
2:B:117:VAL:HG13	2:B:156:VAL:HG11	1.92	0.52
2:D:186:VAL:HG12	2:D:187:LEU:H	1.75	0.52
1:A:9:ILE:O	1:A:30:ASN:HA	2.08	0.52
1:K:127:VAL:HG11	1:K:147:ARG:O	2.09	0.52
2:J:26:THR:HG21	2:J:282:VAL:HG22	1.91	0.52



	the pagette	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:F:52:PRO:HD2	2:F:206:LEU:HD13	1.92	0.52
2:H:36:THR:HG22	2:H:223:LEU:HD13	1.92	0.52
2:J:278:LEU:HD13	2:J:320:GLY:HA3	1.92	0.52
2:B:24:LEU:HD12	2:D:236:LEU:HD12	1.91	0.52
1:G:171:ASP:OD1	1:G:174:LEU:HB2	2.10	0.52
5:D:401:MNR:HBB1	5:D:401:MNR:HMB1	1.91	0.51
2:F:241:PHE:HD2	2:F:242:LEU:HD22	1.74	0.51
2:J:113:LEU:HD21	2:J:121:ILE:HD11	1.92	0.51
2:L:26:THR:HG21	2:L:282:VAL:HG22	1.90	0.51
1:A:41:ILE:HD11	1:A:194:LEU:HD22	1.92	0.51
2:F:17:LEU:HD21	2:H:239:VAL:HG12	1.91	0.51
1:G:199:ASP:OD2	1:G:202:GLN:HG3	2.11	0.51
2:L:15:PHE:CD1	2:L:277:ILE:HG13	2.46	0.51
2:F:302:PHE:CZ	2:F:304:LEU:HD12	2.45	0.51
2:H:104:VAL:HG22	2:H:167:VAL:HB	1.92	0.51
2:J:25:ILE:HG21	2:J:234:SER:HB3	1.90	0.51
2:J:117:VAL:HG13	2:J:156:VAL:HB	1.91	0.51
1:A:95:LEU:O	1:A:103:GLN:NE2	2.43	0.51
2:B:32:LEU:O	2:B:36:THR:HG23	2.10	0.51
1:I:55:ILE:CG2	1:I:67:VAL:HG21	2.41	0.51
1:K:21:SER:OG	1:K:22:THR:N	2.43	0.51
1:K:95:LEU:O	1:K:103:GLN:NE2	2.44	0.51
2:H:145:LEU:HG	2:H:177:VAL:HG11	1.93	0.51
1:I:132:LEU:HD22	1:I:135:ARG:HH11	1.76	0.51
2:H:161:TYR:O	2:H:164:THR:OG1	2.27	0.51
1:A:129:LEU:HD22	1:A:132:LEU:HD12	1.91	0.50
1:A:135:ARG:HD2	1:A:139:GLN:HB3	1.93	0.50
2:H:86:LEU:O	2:H:185:THR:HG22	2.11	0.50
2:B:205:ASP:OD1	2:B:206:LEU:N	2.43	0.50
1:C:119:ARG:NH1	1:C:155:MET:O	2.44	0.50
1:E:82:ARG:NH1	2:F:260:GLY:O	2.44	0.50
1:E:127:VAL:HG21	1:E:151:ALA:HB2	1.93	0.50
2:L:106:GLY:HA2	2:L:169:VAL:O	2.12	0.50
1:A:21:SER:OG	1:A:22:THR:N	2.44	0.50
2:L:14:ARG:O	2:L:18:ILE:HG13	2.12	0.50
1:C:42:VAL:HG21	1:C:203:LEU:HD21	1.94	0.50
1:E:41:ILE:HD13	1:E:52:LEU:HD23	1.93	0.50
1:I:171:ASP:HB2	1:K:214:ASP:OD1	2.11	0.50
2:D:17:LEU:O	2:D:20:SER:OG	2.24	0.50
1:E:38:LEU:HD21	1:E:195:MET:HE3	1.94	0.50
2:F:304:LEU:HD23	2:F:308:SER:HB3	1.93	0.50



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:211:GLN:HG2	2:B:217:LYS:HD2	1.93	0.50
1:C:126:ARG:HH22	1:C:184:ASP:HB3	1.77	0.50
1:C:167:THR:HB	1:C:175:SER:HB3	1.94	0.50
1:C:198:HIS:O	1:C:198:HIS:ND1	2.35	0.50
1:E:6:VAL:HG11	1:E:159:GLN:O	2.12	0.50
1:E:33:ILE:HG22	1:E:192:ALA:HB1	1.94	0.50
1:E:135:ARG:NH2	1:E:139:GLN:O	2.43	0.50
2:H:86:LEU:HD11	2:H:105:MET:HB3	1.94	0.50
1:E:175:SER:O	1:E:179:VAL:HG23	2.12	0.50
2:L:56:VAL:HG22	2:L:203:VAL:HG22	1.93	0.50
2:B:328:VAL:O	2:B:331:VAL:HG12	2.12	0.50
1:G:41:ILE:HB	1:G:196:VAL:HG22	1.92	0.50
2:H:197:PRO:HG3	2:H:203:VAL:HG23	1.94	0.50
2:D:328:VAL:HG12	2:D:328:VAL:O	2.12	0.49
1:G:101:ARG:HD3	1:G:121:ASP:OD1	2.12	0.49
1:I:203:LEU:HB3	1:I:209:PHE:HE1	1.77	0.49
2:H:26:THR:HG22	2:H:316:ILE:HD13	1.93	0.49
2:B:108:PRO:HD2	2:B:111:THR:HG21	1.92	0.49
2:B:128:PRO:HD2	2:B:131:LEU:HD23	1.95	0.49
2:B:317:TRP:CH2	2:B:321:LEU:HD11	2.47	0.49
1:E:14:VAL:HG22	1:E:62:PRO:HA	1.94	0.49
2:F:211:GLN:HG3	2:F:217:LYS:HD2	1.94	0.49
1:I:41:ILE:HD11	1:I:194:LEU:HD22	1.95	0.49
1:E:99:THR:O	1:E:103:GLN:HG2	2.11	0.49
2:D:108:PRO:HG2	2:D:111:THR:CG2	2.41	0.49
2:L:1:MET:SD	2:L:272:GLY:HA3	2.52	0.49
1:C:49:LYS:HB3	1:C:196:VAL:HG13	1.95	0.49
2:D:71:GLU:OE2	2:D:180:THR:HG21	2.13	0.49
2:F:335:ASP:OD1	2:F:336:PRO:HD2	2.13	0.49
1:G:55:ILE:CG2	1:G:67:VAL:HG21	2.40	0.49
1:I:149:ASN:ND2	1:I:152:ARG:HH21	2.11	0.49
2:B:72:ILE:HG23	2:B:76:GLN:HB3	1.94	0.49
2:J:14:ARG:O	2:J:18:ILE:HG13	2.12	0.49
1:A:141:SER:O	1:A:145:ARG:HG3	2.12	0.48
2:B:267:LEU:HD12	2:B:328:VAL:HG12	1.94	0.48
1:I:7:LEU:HD22	1:I:160:LEU:HD21	1.94	0.48
2:J:135:LEU:HB2	2:J:137:VAL:HG22	1.95	0.48
1:C:31:VAL:HG21	1:C:52:LEU:HD21	1.94	0.48
2:D:87:GLY:O	2:D:105:MET:HA	2.12	0.48
2:F:26:THR:HG22	2:F:316:ILE:HD13	1.95	0.48
2:F:116:SER:OG	2:F:159:GLU:OE2	2.31	0.48



A 4 1	A t and D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:J:76:GLN:HE21	2:J:201:GLU:HG2	1.78	0.48
2:B:88:VAL:HG22	2:B:105:MET:HG2	1.94	0.48
1:I:143:GLY:O	1:I:147:ARG:HG3	2.13	0.48
1:A:38:LEU:HD11	1:A:195:MET:HE2	1.96	0.48
2:B:312:PRO:HD3	3:B:501:AGA:H131	1.95	0.48
1:I:200:ARG:HG2	1:I:203:LEU:HD11	1.96	0.48
2:B:307:VAL:HG12	3:B:501:AGA:H41	1.95	0.48
1:E:102:GLU:OE2	2:F:6:ARG:NH1	2.47	0.48
2:H:93:ILE:HA	2:H:144:THR:O	2.14	0.48
2:J:55:VAL:O	2:J:204:THR:HG22	2.13	0.48
1:A:72:ALA:HB2	1:A:84:HIS:CD2	2.49	0.48
2:B:87:GLY:HA2	2:B:185:THR:H	1.79	0.48
1:I:81:ARG:HG2	1:I:87:PHE:HZ	1.79	0.48
1:A:49:LYS:HB3	1:A:196:VAL:HG13	1.96	0.47
1:A:99:THR:HG22	1:A:136:ARG:HG2	1.94	0.47
1:C:26:LEU:HD23	1:C:55:ILE:HD12	1.96	0.47
5:D:401:MNR:HBC1	5:D:401:MNR:HMC1	1.95	0.47
1:G:165:GLU:OE2	1:G:198:HIS:NE2	2.46	0.47
2:B:185:THR:HG23	2:B:186:VAL:HG22	1.97	0.47
2:F:229:PHE:O	2:F:233:ILE:HG13	2.15	0.47
1:I:53:LEU:HD21	1:I:164:ASP:HB2	1.95	0.47
2:B:25:ILE:HG21	2:B:234:SER:HB3	1.95	0.47
1:A:55:ILE:HD13	1:A:60:GLN:O	2.15	0.47
2:J:245:TRP:O	2:J:249:ARG:HG3	2.15	0.47
1:C:16:TYR:HE1	1:C:60:GLN:HE22	1.63	0.47
2:D:161:TYR:O	2:D:164:THR:OG1	2.26	0.47
2:F:229:PHE:HE1	2:H:27:LEU:HD23	1.80	0.47
2:H:112:PRO:HA	2:H:120:PHE:CD1	2.49	0.47
1:I:127:VAL:CG1	1:I:147:ARG:HB3	2.44	0.47
1:C:104:LEU:HB3	1:C:155:MET:CG	2.42	0.47
1:C:203:LEU:HD23	1:C:203:LEU:HA	1.65	0.47
1:G:15:VAL:H	1:G:63:THR:HG21	1.80	0.47
1:G:127:VAL:HG21	1:G:151:ALA:HB2	1.97	0.47
1:G:18:ASP:HB2	1:G:23:VAL:CG1	2.45	0.47
1:K:95:LEU:N	1:K:103:GLN:HE22	2.13	0.47
2:B:117:VAL:HG13	2:B:156:VAL:CG1	2.45	0.46
2:B:87:GLY:O	2:B:105:MET:HA	2.15	0.46
2:D:88:VAL:HG22	2:D:105:MET:HG2	1.97	0.46
2:H:137:VAL:HG11	2:H:152:VAL:HG21	1.98	0.46
1:I:167:THR:HB	1:I:175:SER:HB3	1.97	0.46
2:J:161:TYR:O	2:J:164:THR:OG1	2.29	0.46



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:E:127:VAL:HG12	1:E:147:ARG:HB3	1.96	0.46	
2:F:223:LEU:HD21	5:H:401:MNR:CMB	2.45	0.46	
2:H:53:HIS:HD2	2:H:192:GLU:HA	1.80	0.46	
2:J:128:PRO:HG3	2:J:165:PRO:HB2	1.97	0.46	
2:J:189:LEU:HD13	2:J:193:PRO:HB3	1.97	0.46	
1:A:26:LEU:HD11	1:A:29:ALA:HB2	1.98	0.46	
2:D:128:PRO:HD2	2:D:167:VAL:HG22	1.96	0.46	
2:H:53:HIS:N	2:H:189:LEU:O	2.42	0.46	
2:L:56:VAL:HB	2:L:187:LEU:HB2	1.98	0.46	
1:A:187:LYS:NZ	1:A:207:ASP:OD2	2.29	0.46	
1:E:118:ASP:O	1:E:122:GLU:HG3	2.14	0.46	
1:I:88:VAL:HB	1:I:163:ALA:HA	1.98	0.46	
2:J:29:ILE:CG1	2:J:230:LEU:HB3	2.46	0.46	
2:J:74:GLU:HG2	2:J:183:VAL:HG13	1.98	0.46	
2:L:161:TYR:O	2:L:164:THR:OG1	2.28	0.46	
2:L:29:ILE:HD11	2:L:230:LEU:HB2	1.98	0.46	
2:B:161:TYR:O	2:B:164:THR:OG1	2.33	0.46	
1:C:180:GLU:HG2	1:C:205:TYR:CE1	2.50	0.46	
1:G:208:ARG:NH2	1:G:219:GLN:OE1	2.49	0.46	
1:C:98:LEU:HD11	1:C:106:ILE:HD12	1.98	0.46	
2:J:18:ILE:HG12	2:J:241:PHE:CD1	2.51	0.46	
2:J:29:ILE:HG12	2:J:230:LEU:HB3	1.97	0.46	
1:K:41:ILE:HG22	1:K:49:LYS:HG2	1.97	0.46	
1:A:18:ASP:HB2	1:A:23:VAL:CG1	2.46	0.46	
1:G:141:SER:OG	1:G:144:GLN:HG3	2.15	0.46	
1:G:218:LEU:HG	1:G:220:THR:HG23	1.97	0.46	
1:I:73:GLU:H	1:I:73:GLU:CD	2.16	0.46	
1:I:154:LEU:HD11	1:I:185:VAL:HG11	1.98	0.46	
2:B:56:VAL:HB	2:B:187:LEU:HB2	1.98	0.46	
1:C:11:ASN:N	1:C:30:ASN:OD1	2.48	0.46	
2:F:309:VAL:HG12	2:F:310:LEU:HD23	1.97	0.46	
1:G:59:LEU:HD12	2:H:340:LEU:HD11	1.98	0.46	
2:D:43:ASN:HD22	2:D:216:TYR:HA	1.80	0.45	
2:D:253:ILE:HG22	2:D:334:VAL:HG11	1.97	0.45	
2:F:241:PHE:CE1	2:H:244:VAL:HG21	2.51	0.45	
1:G:72:ALA:HB2	1:G:84:HIS:CD2	2.51	0.45	
2:L:223:LEU:O	2:L:227:GLN:HG3	2.16	0.45	
2:F:8:ILE:HA	2:F:15:PHE:CD2	2.51	0.45	
1:G:127:VAL:HG11	1:G:147:ARG:O	2.16	0.45	
2:J:87:GLY:O	2:J:105:MET:HA	2.16	0.45	
1:C:99:THR:O	1:C:103:GLN:HG2	2.17	0.45	



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:D:80:TRP:CZ2	2:D:197:PRO:HB3	2.51	0.45
1:G:185:VAL:HG13	1:G:189:PHE:CD2	2.51	0.45
1:K:129:LEU:HD11	1:K:147:ARG:HB2	1.98	0.45
2:L:26:THR:HG21	2:L:282:VAL:HA	1.98	0.45
2:B:39:LEU:HD12	2:B:223:LEU:HD11	1.98	0.45
1:E:127:VAL:O	1:E:147:ARG:HD3	2.16	0.45
2:F:245:TRP:O	2:F:248:GLN:HB3	2.16	0.45
1:E:49:LYS:HD2	1:E:196:VAL:CG1	2.42	0.45
2:H:112:PRO:HA	2:H:120:PHE:HD1	1.81	0.45
2:J:15:PHE:HD1	2:J:277:ILE:HG13	1.81	0.45
2:B:125:ALA:HA	2:B:169:VAL:HG12	1.98	0.45
2:F:88:VAL:HG22	2:F:105:MET:HG2	1.99	0.45
1:G:180:GLU:HG2	1:G:205:TYR:CE1	2.51	0.45
2:J:293:GLY:O	2:J:297:ALA:N	2.50	0.45
2:B:36:THR:CG2	2:B:223:LEU:HB3	2.47	0.45
2:D:114:PRO:O	2:D:117:VAL:N	2.45	0.45
2:D:229:PHE:O	2:D:233:ILE:HG13	2.17	0.45
1:E:127:VAL:HG11	1:E:147:ARG:O	2.17	0.45
2:F:108:PRO:HG2	2:F:111:THR:CG2	2.47	0.45
2:L:18:ILE:HG12	2:L:241:PHE:CD1	2.52	0.45
1:G:99:THR:O	1:G:103:GLN:HG2	2.17	0.45
2:H:26:THR:O	2:H:30:VAL:HG23	2.17	0.45
2:L:192:GLU:HG3	2:L:193:PRO:HD2	1.99	0.45
1:A:42:VAL:CG2	1:A:203:LEU:HD21	2.47	0.45
2:B:102:THR:HG21	2:B:131:LEU:CD2	2.46	0.45
1:C:116:ARG:HG2	1:C:116:ARG:H	1.59	0.45
2:F:253:ILE:HG22	2:F:334:VAL:HG11	1.99	0.45
2:H:145:LEU:HD23	2:H:177:VAL:HG21	1.99	0.45
1:K:167:THR:HB	1:K:175:SER:HB3	1.99	0.45
2:D:26:THR:O	2:D:30:VAL:HG23	2.16	0.45
2:D:106:GLY:HA2	2:D:169:VAL:O	2.17	0.45
2:D:85:PRO:HD2	2:D:108:PRO:HG3	1.99	0.44
2:D:156:VAL:HG12	2:D:157:LYS:N	2.30	0.44
1:K:185:VAL:HG13	1:K:189:PHE:CD2	2.52	0.44
2:B:26:THR:HG22	2:B:316:ILE:HG21	2.00	0.44
1:K:169:ALA:O	1:K:170:LEU:HD23	2.17	0.44
2:B:156:VAL:HG12	2:B:157:LYS:H	1.83	0.44
1:G:75:LEU:HD22	1:G:79:SER:HB2	1.99	0.44
1:G:132:LEU:HD23	1:G:135:ARG:HE	1.81	0.44
1:G:173:ARG:O	1:G:177:GLU:HG3	2.17	0.44
1:I:14:VAL:HG21	1:I:55:ILE:HD11	1.99	0.44



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:J:26:THR:OG1	2:J:285:GLY:HA3	2.17	0.44	
1:C:6:VAL:HG23	1:C:35:PRO:HG3	1.99	0.44	
1:E:49:LYS:NZ	1:E:165:GLU:OE2	2.39	0.44	
1:E:209:PHE:CE1	1:E:221:ALA:HB3	2.53	0.44	
2:F:95:SER:HB2	2:F:135:LEU:HB3	2.00	0.44	
2:H:233:ILE:O	2:H:237:VAL:HG23	2.18	0.44	
2:L:43:ASN:HD22	2:L:216:TYR:HA	1.83	0.44	
2:D:107:LEU:HB3	2:D:108:PRO:HD2	1.98	0.44	
1:K:132:LEU:HD22	1:K:135:ARG:NE	2.27	0.44	
2:L:278:LEU:HD13	2:L:320:GLY:HA3	1.99	0.44	
2:B:15:PHE:CD1	2:B:277:ILE:HG13	2.53	0.44	
2:B:141:ASP:O	2:B:152:VAL:HG23	2.18	0.44	
2:D:214:PRO:HG2	5:D:401:MNR:O1D	2.18	0.44	
2:F:288:ILE:O	2:F:292:LEU:HB2	2.18	0.44	
1:G:170:LEU:HD22	1:G:174:LEU:HD13	1.98	0.44	
2:H:331:VAL:O	2:H:334:VAL:HG12	2.17	0.44	
1:C:42:VAL:HG21	1:C:203:LEU:HD11	1.99	0.44	
2:F:223:LEU:HD21	5:H:401:MNR:HMB1	1.99	0.44	
2:H:169:VAL:CG2	2:H:174:TRP:HB2	2.48	0.44	
1:I:44:GLU:HA	1:I:44:GLU:OE1	2.17	0.44	
2:D:270:ALA:HB3	2:D:328:VAL:HG11	1.99	0.43	
2:D:293:GLY:HA3	2:D:302:PHE:CE2	2.53	0.43	
2:L:173:THR:O	2:L:177:VAL:HG23	2.18	0.43	
2:B:106:GLY:HA2	2:B:169:VAL:O	2.18	0.43	
2:F:60:ALA:HB1	2:H:97:GLN:O	2.18	0.43	
2:F:233:ILE:O	2:F:237:VAL:HG23	2.18	0.43	
2:F:302:PHE:CE2	2:F:304:LEU:HB2	2.53	0.43	
2:H:85:PRO:HD2	2:H:108:PRO:CG	2.47	0.43	
2:H:192:GLU:HG2	2:H:193:PRO:HD2	2.00	0.43	
2:J:36:THR:CG2	2:J:223:LEU:HB3	2.48	0.43	
2:J:185:THR:HG23	2:J:186:VAL:HG23	2.00	0.43	
2:B:15:PHE:HA	2:B:18:ILE:HG22	2.01	0.43	
1:E:132:LEU:HD22	1:E:135:ARG:NE	2.33	0.43	
1:I:82:ARG:HB2	2:J:260:GLY:HA3	2.00	0.43	
2:J:277:ILE:HD13	2:J:277:ILE:HA	1.84	0.43	
2:B:293:GLY:HA2	2:B:296:ILE:HG22	2.00	0.43	
2:D:219:GLU:HB2	5:D:401:MNR:C3A	2.48	0.43	
2:J:76:GLN:NE2	2:J:201:GLU:HG2	2.33	0.43	
2:J:290:ALA:HB2	2:J:309:VAL:HG21	2.01	0.43	
2:L:86:LEU:O	2:L:185:THR:HG22	2.18	0.43	
1:C:15:VAL:HA	1:C:23:VAL:O	2.18	0.43	



	h h o	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:D:52:PRO:HG3	2:D:188:LEU:HD22	2.00	0.43	
1:E:6:VAL:HG23	1:E:35:PRO:HG3	1.99	0.43	
1:E:78:THR:HA	1:E:81:ARG:CZ	2.49	0.43	
2:F:113:LEU:HD21	2:F:121:ILE:HD11	2.00	0.43	
2:L:47:ILE:HG13	2:L:213:MET:HE2	2.01	0.43	
2:H:215:ALA:HB2	5:H:401:MNR:O1D	2.18	0.43	
1:K:59:LEU:HD13	2:L:340:LEU:HD11	2.00	0.43	
2:L:233:ILE:O	2:L:237:VAL:HG23	2.19	0.43	
1:E:167:THR:HB	1:E:175:SER:HB2	2.00	0.43	
1:G:15:VAL:H	1:G:63:THR:CG2	2.31	0.43	
1:G:220:THR:HG21	1:G:224:TRP:CD1	2.54	0.43	
1:I:127:VAL:HG21	1:I:151:ALA:HB2	2.00	0.43	
2:B:278:LEU:HD13	2:B:320:GLY:HA3	2.00	0.43	
2:H:46:ALA:HB2	2:H:166:VAL:HG21	2.01	0.43	
1:I:165:GLU:HB3	1:I:168:SER:HG	1.83	0.43	
2:J:26:THR:HG22	2:J:316:ILE:CD1	2.48	0.43	
1:A:18:ASP:CG	1:C:141:SER:HB2	2.38	0.43	
2:B:156:VAL:CG1	2:B:157:LYS:N	2.80	0.43	
2:D:246:THR:HG21	2:D:328:VAL:HG22	2.01	0.43	
2:J:197:PRO:HB2	2:J:201:GLU:HB2	2.01	0.43	
1:A:18:ASP:HB2	1:A:23:VAL:HG12	2.01	0.43	
2:B:244:VAL:HG11	2:D:244:VAL:HG13	2.00	0.43	
1:C:171:ASP:OD1	1:C:174:LEU:HD12	2.18	0.43	
1:I:160:LEU:HD12	1:I:192:ALA:O	2.19	0.43	
2:L:277:ILE:HD13	2:L:277:ILE:HA	1.84	0.43	
2:B:223:LEU:HD21	5:D:401:MNR:CMB	2.49	0.42	
2:H:72:ILE:O	2:H:182:ALA:HB1	2.19	0.42	
2:J:22:VAL:O	2:J:26:THR:HG23	2.18	0.42	
2:B:255:VAL:O	2:B:259:LEU:HG	2.19	0.42	
2:F:278:LEU:HD23	2:F:278:LEU:HA	1.89	0.42	
2:H:270:ALA:HB3	2:H:328:VAL:HG11	2.00	0.42	
2:F:26:THR:O	2:F:30:VAL:HG23	2.18	0.42	
1:I:147:ARG:NH2	1:I:177:GLU:OE1	2.53	0.42	
1:K:161:LEU:O	1:K:193:THR:HA	2.19	0.42	
2:B:26:THR:HG22	2:B:316:ILE:HD13	1.99	0.42	
1:C:38:LEU:HD11	1:C:195:MET:HE2	2.00	0.42	
2:D:230:LEU:HD23	2:D:230:LEU:HA	1.83	0.42	
2:H:143:ILE:O	2:H:149:THR:HA	2.19	0.42	
1:E:200:ARG:NH2	1:E:211:GLU:OE2	2.53	0.42	
1:G:49:LYS:HE3	1:G:49:LYS:HB2	1.74	0.42	
1:K:42:VAL:HG11	1:K:200:ARG:NE	2.32	0.42	



	A la C	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:L:22:VAL:O	2:L:26:THR:HG23	2.20	0.42	
1:I:19:GLY:HA2	1:K:138:ALA:O	2.20	0.42	
2:J:173:THR:O	2:J:177:VAL:HG23	2.19	0.42	
1:K:37:GLU:HA	1:K:207:ASP:OD2	2.19	0.42	
1:K:210:VAL:HG22	1:K:219:GLN:HG2	2.01	0.42	
2:B:266:LEU:HB3	2:B:331:VAL:HG22	2.01	0.42	
1:G:42:VAL:HG13	1:G:227:PRO:HB3	2.01	0.42	
2:J:125:ALA:HA	2:J:169:VAL:HG12	2.01	0.42	
2:H:223:LEU:O	2:H:227:GLN:HG3	2.19	0.42	
1:A:106:ILE:HD11	2:B:3:LEU:HB2	2.02	0.42	
2:B:8:ILE:HD11	2:B:273:GLN:HG3	2.01	0.42	
2:F:277:ILE:HD13	2:F:277:ILE:HA	1.91	0.42	
1:G:9:ILE:HG23	1:G:67:VAL:HG22	2.02	0.42	
2:H:87:GLY:O	2:H:105:MET:HA	2.20	0.42	
2:H:229:PHE:O	2:H:233:ILE:HG13	2.19	0.42	
2:L:192:GLU:CG	2:L:193:PRO:HD2	2.50	0.42	
2:F:128:PRO:HG2	2:F:131:LEU:HB3	2.02	0.42	
1:G:62:PRO:HB2	1:G:64:SER:O	2.20	0.42	
2:J:67:PHE:CE1	2:J:186:VAL:HG21	2.55	0.42	
2:B:76:GLN:O	2:B:80:TRP:HD1	2.03	0.41	
2:F:330:ASN:OD1	2:F:333:LYS:HD2	2.21	0.41	
1:G:182:LEU:HD23	1:G:182:LEU:HA	1.93	0.41	
2:B:54:SER:HB3	2:B:203:VAL:HG13	2.02	0.41	
2:F:22:VAL:O	2:F:26:THR:HG23	2.20	0.41	
2:F:87:GLY:O	2:F:105:MET:HA	2.19	0.41	
2:B:98:ASN:OD1	2:D:60:ALA:HB3	2.20	0.41	
1:C:199:ASP:OD2	1:C:201:SER:HB3	2.19	0.41	
2:D:215:ALA:HB2	5:D:401:MNR:CGD	2.50	0.41	
2:D:315:GLY:O	2:D:319:LEU:HD23	2.19	0.41	
1:E:98:LEU:HB3	1:E:102:GLU:HB2	2.02	0.41	
1:G:75:LEU:HD22	1:G:79:SER:CB	2.50	0.41	
1:I:186:THR:HG22	1:I:193:THR:OG1	2.20	0.41	
2:J:186:VAL:CG1	2:J:187:LEU:N	2.83	0.41	
1:A:118:ASP:O	1:A:122:GLU:HG3	2.20	0.41	
1:G:55:ILE:HD13	1:G:60:GLN:HG3	2.01	0.41	
1:I:53:LEU:HD11	1:I:162:LEU:HB3	2.03	0.41	
2:J:253:ILE:HG21	2:J:331:VAL:HG13	2.03	0.41	
2:B:102:THR:HG21	2:B:131:LEU:HD21	2.03	0.41	
1:C:127:VAL:O	1:C:147:ARG:HD3	2.19	0.41	
1:C:180:GLU:HG2	1:C:205:TYR:HE1	1.85	0.41	
2:H:29:ILE:HG12	2:H:230:LEU:HB3	2.03	0.41	



	h i o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:146:GLY:HA3	2:H:177:VAL:HG13	2.03	0.41
1:I:73:GLU:OE1	1:I:73:GLU:N	2.44	0.41
2:L:229:PHE:O	2:L:233:ILE:HG13	2.20	0.41
1:C:41:ILE:HD12	1:C:194:LEU:HD11	2.01	0.41
2:D:50:LEU:HA	2:D:114:PRO:HG3	2.02	0.41
2:D:233:ILE:O	2:D:237:VAL:HG23	2.21	0.41
2:D:242:LEU:HD23	2:D:242:LEU:HA	1.86	0.41
1:I:126:ARG:HH22	1:I:184:ASP:CG	2.23	0.41
1:K:174:LEU:O	1:K:178:ILE:HG12	2.20	0.41
1:C:55:ILE:CG2	1:C:67:VAL:HG21	2.47	0.41
2:F:56:VAL:HB	2:F:187:LEU:HB2	2.03	0.41
2:F:88:VAL:HB	2:F:185:THR:HG21	2.03	0.41
2:F:321:LEU:HD12	2:F:321:LEU:HA	1.81	0.41
1:G:203:LEU:HD23	1:G:223:LEU:HD11	2.03	0.41
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.83	0.41
1:E:8:SER:HA	1:E:32:GLU:HG3	2.02	0.41
2:J:26:THR:O	2:J:30:VAL:HG23	2.20	0.41
2:J:53:HIS:HB2	2:J:190:ASN:O	2.21	0.41
1:A:33:ILE:HD11	1:A:194:LEU:CG	2.46	0.41
1:A:82:ARG:HB2	2:B:260:GLY:HA3	2.03	0.41
1:A:110:LEU:HA	2:B:265:TYR:CE1	2.55	0.41
2:B:60:ALA:HB1	2:D:97:GLN:O	2.20	0.41
1:C:161:LEU:O	1:C:193:THR:HG23	2.21	0.41
2:F:219:GLU:HB2	5:H:401:MNR:C1C	2.50	0.41
1:G:161:LEU:O	1:G:193:THR:HA	2.20	0.41
2:H:137:VAL:CG1	2:H:152:VAL:HG21	2.51	0.41
2:J:21:VAL:CG1	2:J:237:VAL:HG11	2.50	0.41
2:J:223:LEU:O	2:J:227:GLN:HG3	2.20	0.41
2:J:337:GLN:O	2:J:337:GLN:HG3	2.21	0.41
1:K:141:SER:O	1:K:145:ARG:HG3	2.21	0.41
2:B:277:ILE:HD13	2:B:277:ILE:HA	1.87	0.41
2:B:278:LEU:HD23	2:B:278:LEU:HA	1.87	0.41
1:C:179:VAL:HG21	1:C:202:GLN:CD	2.41	0.41
1:E:13:SER:HB2	1:E:64:SER:OG	2.21	0.41
2:F:117:VAL:HG13	2:F:156:VAL:HB	2.02	0.41
1:I:81:ARG:HG2	1:I:87:PHE:CZ	2.56	0.41
1:K:171:ASP:OD1	1:K:174:LEU:HB2	2.21	0.41
2:L:32:LEU:HD23	2:L:32:LEU:HA	1.85	0.41
2:L:88:VAL:HB	2:L:185:THR:HG21	2.02	0.41
2:B:2:PHE:O	2:B:6:ARG:NH1	2.54	0.40
1:C:100:ALA:HB3	1:C:133:GLY:HA2	2.04	0.40



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:95:SER:HB2	2:D:137:VAL:CG1	2.51	0.40
1:G:78:THR:HA	1:G:81:ARG:CZ	2.51	0.40
2:J:35:LEU:O	2:J:39:LEU:HG	2.21	0.40
2:L:26:THR:O	2:L:30:VAL:HG23	2.21	0.40
2:J:66:GLU:HB2	2:J:69:SER:OG	2.21	0.40
2:L:278:LEU:HA	2:L:278:LEU:HD23	1.88	0.40
1:A:33:ILE:CD1	1:A:194:LEU:HG	2.47	0.40
1:A:141:SER:OG	1:A:142:GLY:N	2.54	0.40
2:B:145:LEU:HD23	2:B:177:VAL:HG21	2.02	0.40
1:C:5:PRO:HB3	1:C:32:GLU:HG2	2.03	0.40
1:C:127:VAL:O	1:C:127:VAL:HG12	2.22	0.40
2:H:45:SER:HB2	2:H:159:GLU:OE1	2.22	0.40
2:H:156:VAL:HG23	2:H:157:LYS:O	2.21	0.40
2:J:55:VAL:HB	2:J:204:THR:CG2	2.52	0.40
2:B:192:GLU:HG2	2:B:193:PRO:HD2	2.03	0.40
2:D:95:SER:HB3	2:D:135:LEU:HB3	2.04	0.40
2:H:100:ASN:OD1	2:H:101:THR:N	2.51	0.40
1:I:135:ARG:NH2	1:I:139:GLN:O	2.53	0.40
1:I:171:ASP:OD1	1:I:174:LEU:HB2	2.22	0.40
2:J:145:LEU:HD12	2:J:150:VAL:HG21	2.04	0.40
2:B:24:LEU:HD23	2:B:24:LEU:HA	1.87	0.40
2:D:44:THR:HB	2:D:210:PHE:CE1	2.55	0.40
1:G:185:VAL:HG13	1:G:189:PHE:HD2	1.86	0.40
2:J:100:ASN:HB2	2:J:134:PHE:HE2	1.85	0.40
2:L:109:GLU:HA	2:L:121:ILE:HG22	2.03	0.40
2:L:128:PRO:HG2	2:L:131:LEU:HB3	2.03	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	214/231~(93%)	208 (97%)	6 (3%)	0	100	100
1	С	216/231~(94%)	210 (97%)	6 (3%)	0	100	100
1	Ε	215/231~(93%)	208 (97%)	7 (3%)	0	100	100
1	G	223/231~(96%)	216 (97%)	7 (3%)	0	100	100
1	Ι	219/231~(95%)	211 (96%)	8 (4%)	0	100	100
1	Κ	217/231~(94%)	210 (97%)	7 (3%)	0	100	100
2	В	340/344~(99%)	334 (98%)	6 (2%)	0	100	100
2	D	342/344~(99%)	336 (98%)	6 (2%)	0	100	100
2	F	341/344~(99%)	331 (97%)	10 (3%)	0	100	100
2	Н	339/344~(98%)	331 (98%)	8 (2%)	0	100	100
2	J	342/344~(99%)	332 (97%)	10 (3%)	0	100	100
2	L	341/344~(99%)	335 (98%)	6 (2%)	0	100	100
All	All	3349/3450~(97%)	3262 (97%)	87 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	172/186~(92%)	171 (99%)	1 (1%)	86 95
1	С	174/186~(94%)	172~(99%)	2(1%)	73 90
1	Ε	174/186~(94%)	174 (100%)	0	100 100
1	G	180/186~(97%)	180 (100%)	0	100 100
1	Ι	175/186~(94%)	174 (99%)	1 (1%)	86 95
1	Κ	174/186~(94%)	173~(99%)	1 (1%)	86 95
2	В	265/265~(100%)	265 (100%)	0	100 100
2	D	266/265~(100%)	266 (100%)	0	100 100
2	F	265/265~(100%)	263 (99%)	2 (1%)	81 93



Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
2	Н	264/265~(100%)	264 (100%)	0	100	100
2	J	266/265~(100%)	264~(99%)	2(1%)	81	93
2	L	265/265~(100%)	264 (100%)	1 (0%)	91	97
All	All	2640/2706~(98%)	2630 (100%)	10 (0%)	91	97

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All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	198	HIS
1	С	173	ARG
1	С	197	THR
2	F	141	ASP
2	F	226	MET
1	Ι	173	ARG
2	J	67	PHE
2	J	302	PHE
1	Κ	197	THR
2	L	67	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	В	337	GLN
2	Н	53	HIS
2	J	43	ASN
1	Κ	84	HIS
1	Κ	198	HIS

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)

6 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	Bo	ond leng	$_{\rm ths}$	E	ond ang	gles
INIOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
6	PEG	Н	402	-	$6,\!6,\!6$	0.12	0	5,5,5	0.06	0
4	PGE	В	502	-	9,9,9	0.16	0	8,8,8	0.11	0
5	MNR	D	401	2	36,50,50	1.66	8 (22%)	34,82,82	1.88	11 (32%)
6	PEG	D	402	-	$6,\!6,\!6$	0.13	0	5,5,5	0.07	0
3	AGA	В	501	-	22,22,29	0.49	0	26,27,35	0.72	1 (3%)
5	MNR	Н	401	2	36,50,50	1.67	8 (22%)	34,82,82	1.99	11 (32%)

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
6	PEG	Н	402	-	-	2/4/4/4	-
4	PGE	В	502	-	-	1/7/7/7	-
5	MNR	D	401	2	-	5/12/94/94	-
6	PEG	D	402	-	-	0/4/4/4	-
3	AGA	В	501	-	-	4/24/24/34	-
5	MNR	Н	401	2	-	6/12/94/94	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
5	D	401	MNR	CHB-C4A	3.50	1.43	1.37
5	Н	401	MNR	CHB-C4A	3.48	1.43	1.37



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	401	MNR	C3B-CAB	-3.38	1.40	1.47
5	Н	401	MNR	C3B-CAB	-3.33	1.41	1.47
5	Н	401	MNR	CAA-C2A	3.11	1.56	1.51
5	Н	401	MNR	C3B-C4B	3.01	1.48	1.40
5	D	401	MNR	C3B-C4B	3.00	1.48	1.40
5	D	401	MNR	CAA-C2A	2.98	1.56	1.51
5	Н	401	MNR	CMC-C2C	2.50	1.54	1.50
5	Н	401	MNR	CAC-C3C	-2.45	1.41	1.47
5	D	401	MNR	CMC-C2C	2.43	1.54	1.50
5	D	401	MNR	CHC-C1C	2.39	1.41	1.37
5	D	401	MNR	CAC-C3C	-2.39	1.41	1.47
5	Н	401	MNR	CHC-C1C	2.35	1.41	1.37
5	D	401	MNR	C4A-NA	2.35	1.41	1.36
5	Н	401	MNR	C4A-NA	2.25	1.40	1.36

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
5	Н	401	MNR	CBD-CAD-C3D	4.31	119.87	112.60
5	Н	401	MNR	CHD-C4C-NC	4.14	124.50	120.84
5	D	401	MNR	CHD-C4C-NC	4.11	124.48	120.84
5	Н	401	MNR	CHA-C1A-NA	3.77	124.17	120.84
5	D	401	MNR	CHA-C1A-NA	3.54	123.97	120.84
5	Н	401	MNR	C1C-CHC-C4B	3.26	127.49	118.67
5	D	401	MNR	C1C-CHC-C4B	3.22	127.37	118.67
5	Н	401	MNR	CHC-C1C-NC	3.19	123.66	120.84
5	D	401	MNR	CHB-C4A-NA	3.03	123.52	120.84
5	D	401	MNR	CBD-CAD-C3D	2.99	117.64	112.60
5	Н	401	MNR	C4C-CHD-C1D	2.96	126.69	118.67
5	D	401	MNR	C4A-CHB-C1B	2.96	126.67	118.67
5	Н	401	MNR	C4A-CHB-C1B	2.95	126.65	118.67
5	D	401	MNR	C4C-CHD-C1D	2.94	126.62	118.67
5	Н	401	MNR	CHB-C4A-NA	2.92	123.42	120.84
5	D	401	MNR	CHC-C1C-NC	2.87	123.38	120.84
5	Н	401	MNR	C1A-CHA-C4D	2.84	126.34	118.67
5	D	401	MNR	C1A-CHA-C4D	2.75	126.11	118.67
3	В	501	AGA	O3-P1-O4	2.41	120.13	110.68
5	Н	401	MNR	C1A-C2A-C3A	-2.27	104.79	113.64
5	D	401	MNR	C1A-C2A-C3A	-2.21	105.05	113.64
5	Н	401	MNR	CMB-C2B-C3B	2.13	128.67	124.68
5	D	401	MNR	CMB-C2B-C3B	2.12	128.64	124.68



There are no chirality outliers.

Mol	Chain	\mathbf{Res}	Type	Atoms
5	D	401	MNR	C2D-C3D-CAD-CBD
5	D	401	MNR	C4D-C3D-CAD-CBD
5	Н	401	MNR	C1A-C2A-CAA-CBA
5	Н	401	MNR	C2D-C3D-CAD-CBD
5	Н	401	MNR	C4D-C3D-CAD-CBD
3	В	501	AGA	C13-C12-O9-C5
5	Н	401	MNR	C3A-C2A-CAA-CBA
6	Н	402	PEG	C1-C2-O2-C3
3	В	501	AGA	O10-C12-O9-C5
6	Н	402	PEG	C4-C3-O2-C2
4	В	502	PGE	O2-C3-C4-O3
5	Н	401	MNR	CAD-CBD-CGD-O1D
5	Н	401	MNR	CAD-CBD-CGD-O2D
5	D	401	MNR	CAD-CBD-CGD-O1D
5	D	401	MNR	C3D-CAD-CBD-CGD
3	В	501	AGA	O7-C7-C8-C9
5	D	401	MNR	CAD-CBD-CGD-O2D
3	В	501	AGA	O8-C7-C8-C9

All (18) torsion outliers are listed below:

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	502	PGE	1	0
5	D	401	MNR	8	0
3	В	501	AGA	2	0
5	Н	401	MNR	5	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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	216/231~(93%)	0.03	9 (4%) 36 14	94, 115, 134, 152	0
1	С	218/231~(94%)	-0.21	0 100 100	75, 100, 120, 134	0
1	Ε	217/231~(93%)	0.56	30 (13%) 2 1	110, 147, 192, 290	0
1	G	225/231~(97%)	-0.20	2 (0%) 84 63	82, 108, 145, 171	0
1	Ι	221/231~(95%)	-0.18	1 (0%) 91 75	79, 99, 117, 130	0
1	Κ	219/231~(94%)	-0.22	0 100 100	77, 92, 114, 151	0
2	В	341/344~(99%)	0.23	24 (7%) 16 5	98, 120, 183, 228	0
2	D	343/344~(99%)	0.84	58~(16%) 1 0	95,160,220,246	0
2	F	342/344~(99%)	0.10	11 (3%) 47 20	110, 133, 173, 202	0
2	Η	341/344~(99%)	0.81	64 (18%) 1 0	109, 176, 221, 267	0
2	J	343/344~(99%)	-0.02	13 (3%) 40 16	94, 149, 187, 241	0
2	L	343/344~(99%)	0.39	39 (11%) 5 1	86, 144, 191, 215	0
All	All	$336\overline{9/3450}~(97\%)$	0.22	251 (7%) 14 4	75, 128, 195, 290	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	154	GLY	12.1
2	D	155	THR	8.9
2	D	187	LEU	7.4
1	Е	21	SER	6.9
2	J	100	ASN	6.8
2	Н	154	GLY	6.7
2	Н	78	GLU	6.6
1	Е	66	THR	6.4
2	L	297	ALA	6.4
2	Н	82	ASP	6.4
2	Н	118	GLY	6.3



7	W	7	В
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Mol	Chain	Res	Type	RSRZ		
2	L	80	TRP	6.0		
2	В	155	THR	5.9		
2	L	191	GLN	5.9		
2	Н	80	TRP	5.9		
2	В	154	GLY	5.8		
2	Н	193	PRO	5.7		
2	Н	75	GLN	5.6		
2	L	190	ASN	5.5		
2	J	216	TYR	5.4		
1	А	218	LEU	5.3		
2	D	57	PHE	5.2		
2	Н	117	VAL	5.0		
2	L	156	VAL	4.9		
2	D	168	TRP	4.9		
1	Е	220	THR	4.9		
2	D	189	LEU	4.9		
2	Н	125	ALA	4.9		
2	Н	194	THR	4.9		
2	L	189	LEU	4.8		
2	D	149	THR	4.8		
2	D	127	LEU	4.7		
2	D	152	VAL	4.7		
1	Е	19	GLY	4.7		
2	D	84	THR	4.6		
2	L	194	THR	4.6		
2	L	306	TRP	4.5		
2	D	203	VAL	4.5		
2	В	118	GLY	4.5		
2	F	205	ASP	4.5		
2	Н	77	ALA	4.4		
2	Н	157	LYS	4.4		
1	Е	20	ILE	4.3		
2	J	215	ALA	4.3		
2	F	207	LYS	4.3		
1	Е	67	VAL	4.3		
2	Н	138	ARG	4.2		
2	L	195	ILE	4.2		
2	Н	162	SER	4.2		
2	Н	113	LEU	4.2		
2	Н	90	GLN	4.2		
2	L	78	GLU	4.2		
2	D	148	ALA	4.2		



Mol	Chain	Res	Type	RSRZ
1	Е	8	SER	4.1
2	В	156	VAL	4.1
2	F	206	LEU 4.1	
2	D	125	ALA	4.1
2	Н	74	GLU	4.1
2	D	55	VAL	4.0
2	D	156	VAL	4.0
2	Н	123	GLN	4.0
2	D	188	LEU	4.0
2	D	186	VAL	3.9
2	F	204	THR	3.9
2	F	54	SER	3.9
2	Н	156	VAL	3.9
2	L	100	ASN	3.9
2	D	147	GLY	3.9
2	Н	126	LEU	3.8
2	D	209	ALA	3.8
2	L	157	LYS	3.8
2	Н	203	VAL	3.8
2	D	85	PRO	3.8
2	В	127 LEU		3.7
1	Е	18	ASP	3.7
2	Н	195	ILE	3.7
2	Н	168	TRP	3.6
2	J	163	HIS	3.6
2	D	204	THR	3.6
2	Н	79	ARG	3.6
2	D	176	LEU	3.6
2	Н	46	ALA	3.6
1	Е	32	GLU	3.6
2	Н	207	LYS	3.5
2	D	151	THR	3.5
2	Н	48	GLU	3.5
2	Η	114	PRO	3.5
2	J	214	PRO	3.5
2	Н	116	SER	3.5
2	D	76	GLN	3.4
2	В	82	ASP	3.4
2	D	73	SER	3.4
1	Е	7	LEU	3.4
2	D	72	ILE	3.4
2	D	58	THR	3.4



Mol	Chain	Res Type		RSRZ
1	А	210	VAL	3.3
2	L	299	SER	3.3
2	Н	109	GLU	3.3
1	Е	5	PRO	3.3
2	D	140	GLY	3.3
2	Н	181	LYS	3.3
2	L	302	PHE	3.3
1	Е	36	GLY	3.3
2	D	123	GLN	3.3
2	L	30	VAL	3.3
2	Н	42	GLN	3.3
2	L	158	THR	3.3
2	В	306	TRP	3.2
2	L	154	GLY	3.2
2	D	133	ASP	3.2
1	А	209	PHE	3.2
2	D	56	VAL	3.2
2	D	153	ALA	3.1
2	В	191	GLN	3.1
2	D	78	GLU	3.1
1	G	224 TRP		3.1
2	D	294 TRP		3.1
2	В	203	VAL	3.1
2	В	139	ALA	3.1
2	F	210	PHE	3.1
2	L	193	PRO	3.0
2	J	217	LYS	3.0
2	D	150	VAL	3.0
2	Н	153	ALA	3.0
1	Ε	221	ALA	3.0
2	L	304	LEU	3.0
1	Е	14	VAL	3.0
2	D	67	PHE	3.0
2	F	202	VAL	2.9
2	F	203	VAL	2.9
2	L	295	LEU	2.9
2	D	132	ALA	2.9
2	В	2	PHE	2.9
2	D	157	LYS	2.9
1	G	20	ILE	2.9
1	А	217	ALA	2.9
2	В	193	PRO	2.9



Mol	Chain	Res Type		RSRZ
2	Н	1	MET	2.8
2	Н	110 GLY		2.8
1	Е	218	LEU	2.8
1	Ι	159	GLN	2.8
2	Н	238	THR	2.8
2	F	211	GLN	2.8
2	L	127	LEU	2.8
2	В	202	VAL	2.8
2	D	115	ASP	2.8
2	В	80	TRP	2.8
2	Н	164	THR	2.8
1	Е	55	ILE	2.8
2	D	116	SER	2.8
1	Е	194	LEU	2.7
2	L	93	ILE	2.7
2	J	44	THR	2.7
2	L	64	SER	2.7
2	D	80	TRP	2.7
1	Е	206	ALA	2.7
2	D	83	SER	2.7
2	Н	196	GLN	2.7
1	Е	26	LEU	2.6
2	L	196	GLN	2.6
2	В	132	ALA	2.6
2	Н	326	ILE	2.6
1	Е	205	TYR	2.6
2	Н	214	PRO	2.6
2	L	298	GLY	2.6
2	В	189	LEU	2.6
1	Е	56	ALA	2.6
1	A	18	ASP	2.6
2	D	202	VAL	2.5
1	Е	33	ILE	2.5
1	Е	37	GLU	2.5
2	D	74	GLU	2.5
2	Н	39	LEU	2.5
2	В	201	GLU	2.5
2	L	82	ASP	2.5
2	В	194	THR	2.5
2	J	48	GLU	2.5
2	D	212	ALA	2.5
1	Е	130	LYS	2.4



Mol	Chain	Res Type		RSRZ
2	J	1	MET	2.4
2	Н	139 ALA		2.4
2	L	192 GLU		2.4
2	L	296	296 ILE	
2	J	222	SER	2.4
2	Н	101	THR	2.4
2	D	129	ALA	2.4
2	Н	201	GLU	2.4
2	D	183	VAL	2.3
2	Н	81	LYS	2.3
2	L	98	ASN	2.3
2	D	47	ILE	2.3
2	D	120	PHE	2.3
1	А	97	SER	2.3
2	Н	198	GLN	2.3
2	D	159	GLU	2.3
2	F	267	LEU	2.3
2	Н	197	PRO	2.3
2	Н	76 GLN		2.3
1	Е	6 VAL		2.3
2	В	56	VAL	2.3
2	L	330	ASN	2.3
2	В	157	LYS	2.2
1	Е	15	VAL	2.2
1	Е	62	PRO	2.2
2	Н	142	HIS	2.2
2	D	54	SER	2.2
2	F	162	SER	2.2
1	Е	219	GLN	2.2
2	J	114	PRO	2.2
1	А	114	LYS	2.2
2	L	168	TRP	2.2
2	D	112	PRO	2.2
1	А	30	ASN	2.2
1	Е	70	HIS	2.2
2	Н	54	SER	2.2
2	Н	217	LYS	2.2
2	D	117	VAL	2.2
2	D	146	GLY	2.2
2	Н	40	GLY	2.2
2	J	219	GLU	2.2
2	L	201	GLU	2.2



7	W	7	В
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Mol	Chain	Res	Type	RSRZ
2	L	81	LYS	2.2
2	В	195	ILE	2.1
2	Н	56	VAL	2.1
2	D	194	THR	2.1
2	Н	241	PHE	2.1
2	L	97	GLN	2.1
2	Н	38	GLY	2.1
2	В	204	THR	2.1
2	Н	115	ASP	2.1
2	L	148	ALA	2.1
1	Е	208	ARG	2.1
2	В	117	VAL	2.1
2	Н	163	HIS	2.1
2	D	126	LEU	2.1
2	В	100	ASN	2.1
2	Н	155	THR	2.1
2	L	101	THR	2.1
2	Н	127	LEU	2.1
2	Н	183	VAL	2.1
2	J	343	THR	2.1
2	L	77	ALA	2.1
2	Н	68	THR	2.1
2	D	36	THR	2.0
2	Н	47	ILE	2.0
1	А	211	GLU	2.0
2	Н	189	LEU	2.0
2	L	267	LEU	2.0
2	L	128	PRO	2.0
2	D	81	LYS	2.0
2	Н	137	VAL	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	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
4	PGE	В	502	10/10	0.71	0.29	132,132,132,132	0
3	AGA	В	501	23/30	0.76	0.21	142,142,142,142	0
6	PEG	Н	402	7/7	0.80	0.29	172,172,172,172	0
6	PEG	D	402	7/7	0.84	0.41	172,172,172,172	0
5	MNR	Н	401	43/43	0.86	0.35	179,179,179,179	0
5	MNR	D	401	43/43	0.93	0.26	119,119,119,119	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.

