

Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 11:37 AM EST

PDB ID	:	3A11
Title	:	Crystal structure of ribose-1,5-bisphosphate isomerase from Thermococcus
		kodakaraensis KOD1
Authors	:	Nakamura, A.; Fujihashi, M.; Nishiba, Y.; Yoshida, S.; Yano, A.; Atomi, H.;
		Imanaka, T.; Miki, K.
Deposited on	:	2009-03-25
Resolution	:	2.50 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
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 ch	nain	
1	А	338	63%	29% •	5%
1	В	338	% 66%	26% ·	5%
1	С	338	59%	33% •	6%
1	D	338	4%	27% •	5%
1	Е	338	% 64%	27% •	6%



Mol	Chain	Length	Quality of chain				
			4%				
1	F	338	55%	36% • 6%	J		

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEG	D	401	-	-	-	Х



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15535 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	200	Total	С	Ν	0	S	0	0	0
	A	320	2541	1631	428	470	12	0	0	0
1	р	200	Total	С	Ν	0	S	0	0	0
	D	322	2556	1636	435	472	13	0	0	0
1	C	217	Total	С	Ν	0	S	0	0	0
		517	2513	1613	424	464	12			0
1	П	200	Total	С	Ν	0	S	0	0	0
	D	320	2531	1623	428	468	12	0	0	0
1	1 E	217	Total	С	Ν	0	S	0	0	0
1		917	2513	1613	424	464	12	0	0	0
1	Б	210	Total	С	Ν	Ο	S	0	0	0
	Г	519	2529	1623	426	468	12	U	U	

• Molecule 1 is a protein called Translation initiation factor eIF-2B, delta subunit.

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-15	MET	-	expression tag	UNP Q5JFM9
А	-14	ASN	-	expression tag	UNP Q5JFM9
А	-13	HIS	-	expression tag	UNP Q5JFM9
А	-12	LYS	-	expression tag	UNP Q5JFM9
А	-11	VAL	-	expression tag	UNP Q5JFM9
А	-10	HIS	-	expression tag	UNP Q5JFM9
A	-9	HIS	-	expression tag	UNP Q5JFM9
А	-8	HIS	-	expression tag	UNP Q5JFM9
А	-7	HIS	-	expression tag	UNP Q5JFM9
А	-6	HIS	-	expression tag	UNP Q5JFM9
А	-5	HIS	-	expression tag	UNP Q5JFM9
А	-4	ILE	-	expression tag	UNP Q5JFM9
A	-3	GLU	-	expression tag	UNP Q5JFM9
А	-2	GLY	-	expression tag	UNP Q5JFM9
A	-1	ARG	-	expression tag	UNP Q5JFM9
A	0	HIS	-	expression tag	UNP Q5JFM9
В	-15	MET	-	expression tag	UNP Q5JFM9



Chain	Residue	Modelled	Actual	Comment	Reference
В	-14	ASN	-	expression tag	UNP Q5JFM9
В	-13	HIS	-	expression tag	UNP Q5JFM9
В	-12	LYS	-	expression tag	UNP Q5JFM9
В	-11	VAL	-	expression tag	UNP Q5JFM9
В	-10	HIS	-	expression tag	UNP Q5JFM9
В	-9	HIS	-	expression tag	UNP Q5JFM9
В	-8	HIS	-	expression tag	UNP Q5JFM9
В	-7	HIS	-	expression tag	UNP Q5JFM9
В	-6	HIS	-	expression tag	UNP Q5JFM9
В	-5	HIS	-	expression tag	UNP Q5JFM9
В	-4	ILE	-	expression tag	UNP Q5JFM9
В	-3	GLU	-	expression tag	UNP Q5JFM9
В	-2	GLY	-	expression tag	UNP Q5JFM9
В	-1	ARG	-	expression tag	UNP Q5JFM9
В	0	HIS	-	expression tag	UNP Q5JFM9
С	-15	MET	-	expression tag	UNP Q5JFM9
С	-14	ASN	-	expression tag	UNP Q5JFM9
С	-13	HIS	-	expression tag	UNP Q5JFM9
С	-12	LYS	-	expression tag	UNP Q5JFM9
С	-11	VAL	-	expression tag	UNP Q5JFM9
С	-10	HIS	-	expression tag	UNP Q5JFM9
С	-9	HIS	-	expression tag	UNP Q5JFM9
С	-8	HIS	-	expression tag	UNP Q5JFM9
С	-7	HIS	-	expression tag	UNP Q5JFM9
С	-6	HIS	-	expression tag	UNP Q5JFM9
С	-5	HIS	-	expression tag	UNP Q5JFM9
С	-4	ILE	-	expression tag	UNP Q5JFM9
С	-3	GLU	-	expression tag	UNP Q5JFM9
С	-2	GLY	-	expression tag	UNP Q5JFM9
С	-1	ARG	-	expression tag	UNP Q5JFM9
С	0	HIS	-	expression tag	UNP Q5JFM9
D	-15	MET	-	expression tag	UNP Q5JFM9
D	-14	ASN	-	expression tag	UNP Q5JFM9
D	-13	HIS	-	expression tag	UNP Q5JFM9
D	-12	LYS	-	expression tag	UNP Q5JFM9
D	-11	VAL	-	expression tag	UNP Q5JFM9
D	-10	HIS	-	expression tag	UNP Q5JFM9
D	-9	HIS	-	expression tag	UNP Q5JFM9
D	-8	HIS		expression tag	UNP $Q5\overline{JFM9}$
D	-7	HIS	-	expression tag	UNP Q5JFM9
D	-6	HIS	-	expression tag	UNP $Q5\overline{JFM9}$
D	-5	HIS	-	expression tag	UNP Q5JFM9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	ILE	-	expression tag	UNP Q5JFM9
D	-3	GLU	-	expression tag	UNP Q5JFM9
D	-2	GLY	-	expression tag	UNP Q5JFM9
D	-1	ARG	-	expression tag	UNP Q5JFM9
D	0	HIS	-	expression tag	UNP Q5JFM9
Е	-15	MET	-	expression tag	UNP Q5JFM9
E	-14	ASN	-	expression tag	UNP Q5JFM9
E	-13	HIS	-	expression tag	UNP Q5JFM9
E	-12	LYS	-	expression tag	UNP Q5JFM9
E	-11	VAL	-	expression tag	UNP Q5JFM9
E	-10	HIS	-	expression tag	UNP Q5JFM9
E	-9	HIS	-	expression tag	UNP Q5JFM9
E	-8	HIS	-	expression tag	UNP Q5JFM9
E	-7	HIS	-	expression tag	UNP Q5JFM9
E	-6	HIS	-	expression tag	UNP Q5JFM9
E	-5	HIS	-	expression tag	UNP Q5JFM9
E	-4	ILE	-	expression tag	UNP Q5JFM9
E	-3	GLU	-	expression tag	UNP Q5JFM9
E	-2	GLY	-	expression tag	UNP Q5JFM9
E	-1	ARG	-	expression tag	UNP Q5JFM9
E	0	HIS	-	expression tag	UNP Q5JFM9
F	-15	MET	-	expression tag	UNP Q5JFM9
F	-14	ASN	-	expression tag	UNP Q5JFM9
F	-13	HIS	-	expression tag	UNP Q5JFM9
F	-12	LYS	-	expression tag	UNP Q5JFM9
F	-11	VAL	-	expression tag	UNP Q5JFM9
F	-10	HIS	-	expression tag	UNP Q5JFM9
F	-9	HIS	-	expression tag	UNP Q5JFM9
F	-8	HIS	-	expression tag	UNP Q5JFM9
F	-7	HIS	-	expression tag	UNP Q5JFM9
F	-6	HIS	-	expression tag	UNP Q5JFM9
F	-5	HIS	-	expression tag	UNP Q5JFM9
F	-4	ILE	-	expression tag	UNP Q5JFM9
F	-3	GLU	-	expression tag	UNP Q5JFM9
F	-2	GLY	-	expression tag	UNP Q5JFM9
F	-1	ARG	-	expression tag	UNP Q5JFM9
F	0	HIS	-	expression tag	UNP Q5JFM9

• Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
2	Ε	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
2	F	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Mg 1 1	0	0
3	Е	1	Total Mg 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atom	\mathbf{s}	ZeroOcc	AltConf
4	А	59	Total 59	O 59	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	87	Total O 87 87	0	0
4	С	34	$\begin{array}{cc} \text{Total} & \text{O} \\ 34 & 34 \end{array}$	0	0
4	D	54	$\begin{array}{cc} \text{Total} & \text{O} \\ 54 & 54 \end{array}$	0	0
4	Е	46	$\begin{array}{cc} \text{Total} & \text{O} \\ 46 & 46 \end{array}$	0	0
4	F	28	TotalO2828	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Translation initiation factor eIF-2B, delta subunit



Chain C:

59%

33%

6%



• Molecule 1: Translation initiation factor eIF-2B, delta subunit

D W I D E DATA BANK





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	117.29Å 130.81Å 132.81Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	43.66 - 2.50	Depositor
Resolution (A)	43.66 - 2.50	EDS
% Data completeness	99.8 (43.66-2.50)	Depositor
(in resolution range)	99.9 (43.66 - 2.50)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	$4.54 (at 2.51 \text{\AA})$	Xtriage
Refinement program	CNS 1.2	Depositor
P. P.	0.204 , 0.266	Depositor
Π, Π_{free}	0.198 , 0.259	DCC
R_{free} test set	3638 reflections $(5.10%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	37.2	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 58.6	EDS
L-test for $twinning^2$	$< L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15535	wwPDB-VP
Average B, all atoms $(Å^2)$	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.23% 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: MG, PEG

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	
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.35	0/2595	0.60	0/3514
1	В	0.37	0/2610	0.61	0/3530
1	С	0.31	0/2566	0.57	0/3473
1	D	0.34	0/2584	0.57	0/3498
1	Е	0.31	0/2566	0.56	0/3473
1	F	0.32	0/2582	0.55	0/3495
All	All	0.34	0/15503	0.58	0/20983

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	2541	0	2583	112	0
1	В	2556	0	2591	106	0
1	С	2513	0	2553	115	0
1	D	2531	0	2566	97	0
1	Е	2513	0	2553	95	0
1	F	2529	0	2568	133	0
2	А	7	0	10	2	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	7	0	10	2	0
2	С	7	0	10	0	0
2	D	7	0	10	2	0
2	Е	7	0	10	1	0
2	F	7	0	10	2	0
3	В	1	0	0	0	0
3	Ε	1	0	0	0	0
4	А	59	0	0	1	0
4	В	87	0	0	2	0
4	С	34	0	0	3	0
4	D	54	0	0	2	0
4	Ē	46	0	0	2	0
4	F	28	0	0	0	0
All	All	15535	0	15474	605	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 20.

All (605) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:292:THR:HG22	1:E:294:ARG:H	1.13	1.09
1:C:164:GLN:H	1:C:164:GLN:HE21	1.06	1.02
1:B:270:LYS:HE3	1:B:270:LYS:H	1.21	0.99
1:C:218:LEU:HD22	1:D:218:LEU:HD22	1.46	0.97
1:B:292:THR:HG22	1:B:294:ARG:H	1.29	0.96
1:F:214:ILE:HD12	1:F:277:PRO:HG2	1.46	0.95
1:B:318:GLU:HG3	1:B:319:PRO:HD2	1.49	0.94
1:E:181:TYR:HB3	1:F:274:VAL:HG12	1.52	0.91
1:B:270:LYS:H	1:B:270:LYS:CE	1.84	0.91
1:E:186:ALA:HB2	1:F:214:ILE:HD11	1.53	0.91
1:D:164:GLN:H	1:D:164:GLN:HE21	1.14	0.88
1:E:211:ILE:HD11	1:E:244:MET:HG3	1.53	0.88
1:C:164:GLN:H	1:C:164:GLN:NE2	1.72	0.87
1:A:164:GLN:H	1:A:164:GLN:HE21	1.17	0.87
1:E:318:GLU:HG3	1:E:319:PRO:HD2	1.55	0.86
1:D:264:GLU:O	1:D:267:THR:HG22	1.74	0.86
1:F:199:MET:HE1	1:F:216:THR:HG23	1.59	0.84
1:E:164:GLN:H	1:E:164:GLN:HE21	1.26	0.84
1:D:288:ASP:OD2	2:D:401:PEG:H21	1.77	0.83
1:E:187:ALA:HB3	1:F:218:LEU:HD11	1.62	0.81



	louo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:294:ARG:HH21	1:C:315:LYS:HD2	1.47	0.79
1:D:69:LEU:HB3	1:D:70:PRO:HD3	1.65	0.79
1:D:224:LYS:HA	2:D:401:PEG:H12	1.65	0.78
1:C:8:LEU:HD12	1:C:8:LEU:H	1.48	0.77
1:A:313:ALA:HB3	1:A:316:TYR:HB2	1.66	0.77
1:A:271:ASN:HD22	1:A:271:ASN:H	1.31	0.76
1:C:10:ILE:HD12	1:C:32:ALA:HB2	1.67	0.76
1:F:3:VAL:HG21	1:F:58:ILE:HD12	1.68	0.76
1:A:243:THR:HG22	1:A:245:LEU:H	1.48	0.76
1:A:52:MET:HE1	1:A:97:ILE:HG21	1.67	0.76
1:B:244:MET:HB2	1:D:122:ARG:HH12	1.51	0.76
1:B:227:ARG:HE	1:E:227:ARG:HG2	1.51	0.76
1:C:164:GLN:HE21	1:C:164:GLN:N	1.84	0.76
1:F:256:PRO:HB3	1:F:274:VAL:HG23	1.68	0.76
1:F:259:VAL:HG12	1:F:260:ILE:HG13	1.68	0.75
1:A:251:ILE:HG22	1:A:252:GLU:N	2.01	0.75
1:A:33:LEU:HD11	1:A:73:LEU:HD12	1.69	0.74
1:D:247:GLN:CD	1:F:122:ARG:HG3	2.08	0.74
1:D:318:GLU:HG2	1:D:320:TRP:CZ2	2.22	0.74
1:B:89:ASP:OD2	1:B:92:GLN:HG3	1.88	0.74
1:E:254:ARG:HB2	1:E:276:ASN:ND2	2.02	0.74
1:D:164:GLN:H	1:D:164:GLN:NE2	1.85	0.74
1:A:164:GLN:HE21	1:A:164:GLN:N	1.86	0.74
1:B:318:GLU:HG2	1:B:320:TRP:CH2	2.23	0.73
1:A:251:ILE:HG22	1:A:252:GLU:H	1.53	0.73
1:A:5:LYS:HD3	1:A:5:LYS:N	2.03	0.73
1:A:183:VAL:HG21	1:B:160:ARG:HB3	1.69	0.73
1:F:164:GLN:H	1:F:164:GLN:HE21	1.36	0.73
1:A:224:LYS:HA	2:A:401:PEG:H41	1.70	0.73
1:B:270:LYS:HE3	1:B:270:LYS:N	2.01	0.73
1:C:297:ILE:HD13	1:C:305:ILE:HD11	1.70	0.72
1:A:139:ILE:HG22	1:A:143:LYS:HE2	1.71	0.72
1:A:221:LEU:HD13	1:B:221:LEU:HD13	1.71	0.71
1:D:297:ILE:HD13	1:D:305:ILE:HD11	1.71	0.71
1:B:318:GLU:HG2	1:B:320:TRP:CZ2	2.25	0.71
1:E:318:GLU:HG2	1:E:320:TRP:CH2	2.24	0.71
1:C:93:LEU:O	1:C:97:ILE:HG12	1.91	0.70
1:F:260:ILE:HD13	1:F:268:TRP:CH2	2.26	0.70
1:F:288:ASP:OD2	2:F:401:PEG:H32	1.91	0.70
1:E:69:LEU:HB3	1:E:70:PRO:HD3	1.74	0.70
1:F:171:GLU:HG2	1:F:175:TYR:HE2	1.56	0.70



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:251:ILE:HD12	1:F:251:ILE:H	1.55	0.70
1:F:224:LYS:HA	2:F:401:PEG:H41	1.74	0.70
1:F:160:ARG:HD2	1:F:161:PRO:HA	1.74	0.70
1:E:186:ALA:CB	1:F:214:ILE:HD11	2.20	0.70
1:B:264:GLU:O	1:B:267:THR:HB	1.92	0.70
1:C:257:THR:HA	1:C:260:ILE:O	1.92	0.70
1:B:47:GLU:O	1:B:51:GLU:HG3	1.91	0.69
1:E:211:ILE:CD1	1:E:244:MET:HG3	2.22	0.69
1:F:307:ARG:HD3	1:F:312:TRP:O	1.90	0.69
1:A:143:LYS:HD3	1:A:175:TYR:CE2	2.27	0.69
1:F:164:GLN:H	1:F:164:GLN:NE2	1.89	0.69
1:E:143:LYS:HE2	1:E:147:GLU:HG3	1.73	0.69
1:A:160:ARG:HD3	1:B:158:GLU:OE2	1.93	0.69
1:F:199:MET:CE	1:F:216:THR:HG23	2.23	0.68
1:C:76:VAL:HG23	1:C:77:MET:N	2.08	0.68
1:C:242:GLU:HG2	1:C:243:THR:H	1.58	0.68
1:A:144:THR:O	1:A:148:GLN:HG3	1.93	0.68
1:D:182:VAL:CG1	1:D:186:ALA:HB3	2.24	0.68
1:D:247:GLN:OE1	1:F:122:ARG:HG3	1.92	0.68
1:C:221:LEU:HD13	1:D:221:LEU:HD13	1.74	0.68
4:C:603:HOH:O	1:D:183:VAL:HG13	1.93	0.68
1:C:211:ILE:HD11	1:C:244:MET:HG2	1.77	0.67
1:C:270:LYS:HE3	1:C:270:LYS:H	1.60	0.67
1:F:114:ARG:HG3	1:F:114:ARG:HH11	1.59	0.67
1:D:243:THR:HG22	1:D:247:GLN:HG2	1.75	0.67
1:E:183:VAL:HG13	4:E:617:HOH:O	1.94	0.66
1:D:52:MET:HE2	1:D:97:ILE:HD13	1.78	0.66
1:A:210:VAL:HG21	1:A:232:ILE:HG13	1.78	0.66
1:A:305:ILE:HD11	1:C:314:LEU:HD12	1.76	0.66
1:C:144:THR:O	1:C:148:GLN:HG3	1.95	0.66
1:A:45:VAL:HG22	1:A:90:LEU:N	2.10	0.66
1:B:122:ARG:HE	1:F:246:GLY:HA2	1.61	0.66
1:E:255:ASP:OD2	1:E:257:THR:HB	1.96	0.66
1:C:145:ALA:O	1:C:150:LYS:HB2	1.95	0.65
1:B:132:HIS:HD2	1:B:157:THR:OG1	1.80	0.65
1:C:270:LYS:H	1:C:270:LYS:CE	2.09	0.65
1:E:160:ARG:HB3	1:F:183:VAL:HG21	1.79	0.65
1:B:17:MET:CE	1:B:63:ARG:HD2	2.25	0.65
1:B:247:GLN:HE22	1:B:252:GLU:HB2	1.60	0.65
1:B:236:THR:HG23	1:B:292:THR:HG23	1.79	0.65
1:F:13:LYS:HB3	1:F:19:ILE:HG13	1.79	0.65



	1	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:13:LYS:HB3	1:C:19:ILE:HG12	1.79	0.65
1:C:195:ASP:O	1:C:196:LYS:HD2	1.97	0.64
1:B:164:GLN:H	1:B:164:GLN:HE21	1.45	0.64
1:F:235:GLU:OE1	1:F:238:LYS:HE3	1.97	0.64
1:D:89:ASP:H	1:D:92:GLN:NE2	1.96	0.64
1:C:4:VAL:HG22	1:C:6:GLU:H	1.61	0.64
1:B:182:VAL:HG13	1:B:186:ALA:HB3	1.80	0.64
1:E:133:CYS:HA	1:E:159:THR:HG21	1.79	0.64
1:D:44:ASN:O	1:D:90:LEU:HD13	1.98	0.63
1:D:164:GLN:HE21	1:D:164:GLN:N	1.92	0.63
1:F:49:TRP:NE1	1:F:53:LYS:HD3	2.12	0.63
1:A:164:GLN:H	1:A:164:GLN:NE2	1.94	0.63
1:A:317:THR:HG22	1:A:318:GLU:H	1.61	0.63
1:B:196:LYS:HD3	1:B:229:TRP:HB3	1.79	0.63
1:E:236:THR:HG23	1:E:292:THR:HG23	1.80	0.63
1:F:256:PRO:HB3	1:F:274:VAL:CG2	2.28	0.63
1:B:247:GLN:NE2	1:B:252:GLU:HB2	2.13	0.63
1:C:6:GLU:HB3	1:C:35:LEU:HD13	1.81	0.63
1:D:6:GLU:HB3	1:D:35:LEU:HD13	1.80	0.63
1:E:160:ARG:CB	1:F:183:VAL:HG21	2.29	0.63
1:F:3:VAL:HG21	1:F:58:ILE:CD1	2.28	0.63
1:A:251:ILE:CG2	1:A:252:GLU:H	2.11	0.63
1:A:52:MET:HB3	1:A:77:MET:HE1	1.79	0.63
1:C:89:ASP:OD1	1:C:92:GLN:HB2	1.99	0.63
1:B:317:THR:HB	1:B:321:GLU:HB2	1.79	0.62
1:A:305:ILE:CD1	1:C:314:LEU:HD12	2.30	0.62
1:F:133:CYS:HA	1:F:159:THR:HG21	1.82	0.62
1:E:44:ASN:HD21	1:E:46:ASP:HB2	1.63	0.62
1:A:70:PRO:HB2	1:A:74:ARG:HH12	1.65	0.62
1:E:41:LYS:HA	1:E:41:LYS:HE2	1.81	0.62
1:F:253:MET:HE2	1:F:277:PRO:HA	1.80	0.62
1:B:5:LYS:HG3	1:B:6:GLU:OE1	2.00	0.62
1:D:4:VAL:HG12	1:D:6:GLU:H	1.63	0.62
1:A:317:THR:HG22	1:A:318:GLU:N	2.15	0.61
1:B:34:GLN:O	1:B:38:GLU:HG3	1.99	0.61
1:D:45:VAL:HG22	1:D:90:LEU:N	2.15	0.61
1:E:214:ILE:HD12	1:E:280:ASP:HB3	1.82	0.61
1:E:318:GLU:HG2	1:E:320:TRP:CZ2	2.35	0.61
1:F:50:LYS:O	1:F:54:GLN:HG3	2.00	0.61
1:D:314:LEU:HD11	1:F:297:ILE:CG2	2.30	0.61
1:E:292:THR:HG22	1:E:294:ARG:N	1.99	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:254:ARG:HG3	1:F:278:ALA:HB2	1.81	0.61
1:A:240:HIS:CD2	1:A:241:PRO:HD2	2.35	0.61
1:D:314:LEU:HD11	1:F:297:ILE:HG21	1.81	0.61
1:A:70:PRO:HB2	1:A:74:ARG:NH1	2.16	0.61
1:E:292:THR:HG21	1:E:294:ARG:HG3	1.83	0.61
1:A:264:GLU:O	1:A:267:THR:HB	2.01	0.61
1:D:144:THR:O	1:D:148:GLN:HG3	2.00	0.61
1:D:269:PRO:HD2	1:D:272:ILE:HD12	1.83	0.61
1:D:79:ARG:HH21	1:D:79:ARG:HG3	1.66	0.61
1:F:105:ILE:O	1:F:109:GLU:HG3	2.00	0.61
1:F:188:ARG:HA	1:F:222:THR:HG21	1.83	0.61
1:A:251:ILE:HG22	1:A:252:GLU:HG2	1.83	0.60
1:B:89:ASP:H	1:B:92:GLN:NE2	1.99	0.60
4:C:604:HOH:O	1:D:182:VAL:HG13	2.02	0.60
1:B:89:ASP:CG	1:B:92:GLN:HE21	2.05	0.60
1:E:144:THR:O	1:E:148:GLN:HG3	2.00	0.59
1:A:5:LYS:HG2	1:A:6:GLU:OE2	2.01	0.59
1:C:10:ILE:HG21	1:C:28:SER:HB3	1.84	0.59
1:C:211:ILE:CD1	1:C:244:MET:HG2	2.32	0.59
1:A:271:ASN:HD22	1:A:271:ASN:N	1.93	0.59
1:B:314:LEU:HB3	1:D:294:ARG:HB3	1.85	0.59
1:C:76:VAL:HG23	1:C:77:MET:H	1.67	0.59
1:F:129:ILE:CD1	1:F:196:LYS:HB2	2.33	0.59
1:F:144:THR:O	1:F:148:GLN:HG3	2.03	0.59
1:B:206:VAL:HG13	1:B:241:PRO:HA	1.84	0.59
1:C:221:LEU:HD11	1:D:221:LEU:HD22	1.83	0.59
1:A:5:LYS:HD3	1:A:5:LYS:H	1.66	0.58
1:B:79:ARG:HG3	1:B:79:ARG:HH11	1.68	0.58
1:B:244:MET:HB2	1:D:122:ARG:NH1	2.18	0.58
1:E:143:LYS:O	1:E:147:GLU:HG3	2.04	0.58
1:B:227:ARG:HG2	1:E:227:ARG:CG	2.34	0.58
1:F:307:ARG:HH21	1:F:307:ARG:HG3	1.68	0.58
1:A:52:MET:HE2	1:A:97:ILE:HD13	1.85	0.58
1:B:143:LYS:HD3	1:B:175:TYR:CE2	2.38	0.58
1:B:182:VAL:CG1	1:B:186:ALA:HB3	2.34	0.58
1:F:120:ALA:HB1	1:F:148:GLN:OE1	2.04	0.58
1:F:313:ALA:HB3	1:F:316:TYR:CD2	2.39	0.58
1:F:251:ILE:HD12	1:F:251:ILE:N	2.19	0.57
1:C:49:TRP:NE1	1:C:53:LYS:HE3	2.19	0.57
1:E:292:THR:CG2	1:E:293:GLU:N	2.67	0.57
1:E:34:GLN:O	1:E:38:GLU:HG3	2.04	0.57



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:206:VAL:CG1	1:E:243:THR:HG22	2.34	0.57
1:F:235:GLU:HG2	1:F:237:TYR:CZ	2.39	0.57
1:E:236:THR:HG23	1:E:292:THR:CG2	2.34	0.57
1:F:240:HIS:HD2	1:F:241:PRO:HD2	1.68	0.57
1:B:67:VAL:HG23	1:B:240:HIS:CE1	2.40	0.57
1:E:183:VAL:HG12	1:E:185:SER:H	1.69	0.57
1:A:70:PRO:O	1:A:74:ARG:HG3	2.04	0.57
1:A:294:ARG:NH2	1:C:315:LYS:HD2	2.19	0.57
1:B:164:GLN:H	1:B:164:GLN:NE2	2.01	0.57
1:E:171:GLU:O	1:E:174:SER:HB3	2.05	0.57
1:A:31:TYR:CE2	1:A:35:LEU:HD11	2.39	0.57
1:A:251:ILE:CG2	1:A:252:GLU:N	2.66	0.57
1:C:54:GLN:O	1:C:58:ILE:HG13	2.05	0.57
1:F:199:MET:HE1	1:F:216:THR:HA	1.87	0.57
1:E:211:ILE:HD11	1:E:244:MET:CG	2.30	0.57
1:B:143:LYS:HD3	1:B:175:TYR:CZ	2.40	0.56
1:B:285:GLU:CD	1:B:285:GLU:H	2.08	0.56
1:C:222:THR:O	1:C:226:HIS:HD2	1.87	0.56
1:F:242:GLU:HG2	1:F:243:THR:N	2.20	0.56
1:D:6:GLU:HG3	1:D:39:LYS:HD2	1.86	0.56
1:E:292:THR:CG2	1:E:294:ARG:HG3	2.35	0.56
1:F:70:PRO:O	1:F:74:ARG:HG3	2.04	0.56
1:F:143:LYS:HZ3	1:F:143:LYS:HB2	1.69	0.56
1:A:34:GLN:O	1:A:38:GLU:HG3	2.05	0.56
1:B:17:MET:HE2	1:B:63:ARG:HD2	1.86	0.56
1:C:3:VAL:CG1	1:C:8:LEU:HD11	2.35	0.56
4:D:636:HOH:O	1:F:296:ILE:HD13	2.06	0.56
1:F:235:GLU:HA	1:F:293:GLU:OE1	2.06	0.56
1:A:271:ASN:H	1:A:271:ASN:ND2	2.03	0.56
1:F:114:ARG:HG3	1:F:114:ARG:NH1	2.21	0.56
1:B:70:PRO:HB2	1:B:74:ARG:NH1	2.20	0.56
1:E:138:ALA:HB1	1:E:198:VAL:HG12	1.87	0.56
1:F:260:ILE:HD12	1:F:274:VAL:HG11	1.88	0.55
1:C:82:ILE:HG23	1:C:83:ALA:N	2.21	0.55
1:D:40:SER:HB3	1:D:94:ARG:NH2	2.22	0.55
1:E:224:LYS:HE2	1:E:227:ARG:NH1	2.21	0.55
1:F:271:ASN:N	1:F:271:ASN:HD22	2.04	0.55
1:A:3:VAL:HG11	1:A:55:ALA:HA	1.88	0.55
1:E:195:ASP:O	1:E:196:LYS:HG3	2.06	0.55
1:A:218:LEU:HD22	1:B:218:LEU:HD22	1.89	0.55
1:D:297:ILE:HD13	1:D:305:ILE:CD1	2.37	0.55



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:F:44:ASN:C	1:F:44:ASN:HD22	2.08	0.55	
1:C:4:VAL:HG12	1:C:36:GLN:OE1	2.07	0.55	
1:D:133:CYS:HA	1:D:159:THR:HG21	1.88	0.55	
1:C:270:LYS:H	1:C:270:LYS:CD	2.19	0.55	
1:B:183:VAL:HG22	4:B:611:HOH:O	2.07	0.54	
1:A:21:GLY:O	1:A:25:ILE:HG23	2.08	0.54	
1:B:17:MET:HE1	1:B:63:ARG:HD2	1.89	0.54	
1:B:17:MET:O	1:B:20:ARG:NH2	2.40	0.54	
1:D:145:ALA:O	1:D:150:LYS:HB2	2.07	0.54	
1:F:222:THR:O	1:F:226:HIS:HD2	1.89	0.54	
1:A:107:ASN:HD21	1:C:315:LYS:HE2	1.72	0.54	
1:D:313:ALA:HB3	1:D:315:LYS:HE3	1.90	0.54	
1:F:99:ASN:O	1:F:103:GLU:HG3	2.07	0.54	
1:A:67:VAL:HG13	1:A:240:HIS:CD2	2.42	0.54	
1:A:243:THR:HG22	1:A:244:MET:N	2.23	0.54	
1:E:4:VAL:HG22	1:E:36:GLN:OE1	2.07	0.54	
1:F:20:ARG:O	1:F:24:LYS:HE3	2.08	0.54	
1:A:49:TRP:CE3	1:A:49:TRP:HA	2.43	0.54	
1:B:192:LYS:NZ	1:B:192:LYS:HB3	2.23	0.54	
1:F:305:ILE:O	1:F:309:GLU:HB2	2.07	0.54	
1:D:42:ALA:HB2	1:D:51:GLU:OE2	2.08	0.53	
1:C:221:LEU:CD1	1:D:221:LEU:HD22	2.37	0.53	
1:A:3:VAL:HG11	1:A:58:ILE:HD12	1.90	0.53	
1:B:314:LEU:O	1:D:294:ARG:HD3	2.07	0.53	
1:D:77:MET:HB3	1:D:319:PRO:HB2	1.90	0.53	
1:A:158:GLU:HG3	1:A:181:TYR:OH	2.09	0.53	
1:E:16:ASN:OD1	1:E:18:GLU:HG3	2.08	0.53	
1:C:213:LYS:HD3	1:C:214:ILE:H	1.74	0.53	
1:D:247:GLN:HG3	1:F:122:ARG:HE	1.74	0.53	
1:C:8:LEU:HD12	1:C:8:LEU:N	2.21	0.53	
1:F:6:GLU:O	1:F:9:GLU:HB3	2.08	0.53	
1:A:15:LYS:C	1:A:17:MET:H	2.12	0.53	
1:A:52:MET:CE	1:A:97:ILE:HD13	2.39	0.53	
1:B:153:LYS:HD3	1:B:180:ILE:HD11	1.90	0.53	
1:C:4:VAL:CG1	1:C:7:VAL:HG23	2.39	0.53	
1:E:143:LYS:NZ	1:E:175:TYR:HB3	2.23	0.53	
1:E:162:LYS:HZ3	1:E:258:GLU:HB3	1.74	0.53	
1:F:146:TRP:CG	1:F:177:ILE:HG12	2.44	0.53	
1:F:254:ARG:HB2	1:F:276:ASN:ND2	2.23	0.53	
1:B:292:THR:HG22	1:B:293:GLU:N	2.24	0.52	
1:C:242:GLU:HG2	1:C:243:THR:N	2.24	0.52	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:F:132:HIS:CB	1:F:199:MET:HE3	2.38	0.52	
1:B:133:CYS:HA	1:B:159:THR:HG21	1.90	0.52	
1:D:143:LYS:HD2	1:D:175:TYR:CZ	2.45	0.52	
1:D:318:GLU:CG	1:D:320:TRP:CZ2	2.93	0.52	
1:E:158:GLU:HG3	1:E:181:TYR:OH	2.09	0.52	
1:F:307:ARG:HG3	1:F:307:ARG:NH2	2.25	0.52	
1:A:160:ARG:HB3	1:B:183:VAL:HG21	1.90	0.52	
1:D:79:ARG:HG3	1:D:79:ARG:NH2	2.25	0.52	
1:F:4:VAL:HG12	1:F:5:LYS:N	2.25	0.52	
1:B:67:VAL:HG23	1:B:240:HIS:ND1	2.25	0.52	
1:D:254:ARG:HB2	1:D:276:ASN:ND2	2.25	0.52	
1:B:50:LYS:O	1:B:54:GLN:HG3	2.10	0.52	
1:E:254:ARG:HH11	1:E:254:ARG:HG3	1.75	0.52	
1:A:294:ARG:HB2	1:C:314:LEU:HD13	1.92	0.52	
1:C:164:GLN:NE2	1:C:164:GLN:N	2.51	0.52	
1:D:227:ARG:HH11	1:D:227:ARG:HB3	1.75	0.52	
1:E:196:LYS:HG2	1:E:229:TRP:HB3	1.92	0.52	
1:A:54:GLN:O	1:A:58:ILE:HG13	2.10	0.52	
1:D:222:THR:O	1:D:226:HIS:HD2	1.92	0.52	
1:C:161:PRO:HB3	1:C:259:VAL:HG22	1.92	0.52	
1:F:236:THR:N	1:F:293:GLU:OE1	2.34	0.52	
1:A:183:VAL:HG21	1:B:160:ARG:CB	2.38	0.52	
1:D:105:ILE:O	1:D:109:GLU:HG3	2.09	0.52	
1:A:45:VAL:HG22	1:A:90:LEU:H	1.75	0.51	
1:C:79:ARG:HG3	1:C:79:ARG:HH11	1.74	0.51	
1:A:69:LEU:HB3	1:A:70:PRO:CD	2.41	0.51	
1:A:205:THR:HG21	1:A:244:MET:HG2	1.91	0.51	
1:C:287:VAL:HG13	1:C:299:PRO:HG2	1.93	0.51	
1:C:235:GLU:HG3	1:C:237:TYR:CZ	2.46	0.51	
1:A:6:GLU:HA	1:A:9:GLU:HG2	1.91	0.51	
1:A:123:ILE:HD12	1:A:129:ILE:HD11	1.92	0.51	
1:B:224:LYS:HE3	1:B:227:ARG:HH12	1.76	0.51	
1:E:297:ILE:HD13	1:E:305:ILE:CD1	2.40	0.51	
1:F:257:THR:HG23	1:F:261:PRO:HA	1.92	0.51	
1:B:236:THR:HG23	1:B:292:THR:CG2	2.40	0.51	
1:D:262:GLU:O	1:D:266:LYS:HG3	2.10	0.51	
1:F:171:GLU:HG2	1:F:175:TYR:CE2	2.42	0.51	
1:F:61:GLU:HA	1:F:64:PRO:HG3	1.92	0.51	
1:A:44:ASN:HB3	1:A:47:GLU:HB3	1.93	0.51	
1:A:49:TRP:HA	1:A:49:TRP:HE3	1.74	0.51	
1:C:8:LEU:H	1:C:8:LEU:CD1	2.20	0.51	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:E:79:ARG:HH11	1:E:79:ARG:HG3	1.76	0.51	
1:D:27:ARG:HD3	1:D:108:SER:OG	2.11	0.51	
1:E:67:VAL:O	1:E:70:PRO:HD2	2.11	0.51	
1:B:214:ILE:HD12	1:B:280:ASP:HB3	1.94	0.50	
1:C:48:PHE:O	1:C:51:GLU:HB3	2.10	0.50	
1:C:319:PRO:HG2	1:C:320:TRP:CE3	2.47	0.50	
1:D:182:VAL:HG12	1:D:186:ALA:HB3	1.94	0.50	
1:E:206:VAL:HG12	1:E:243:THR:HG22	1.92	0.50	
1:F:44:ASN:ND2	1:F:47:GLU:H	2.09	0.50	
1:E:186:ALA:HB2	1:F:214:ILE:CD1	2.34	0.50	
1:E:213:LYS:HD3	1:E:278:ALA:O	2.10	0.50	
1:E:292:THR:HG22	1:E:293:GLU:N	2.27	0.50	
1:C:69:LEU:HB3	1:C:70:PRO:CD	2.42	0.50	
1:F:45:VAL:HG22	1:F:90:LEU:N	2.27	0.50	
1:C:49:TRP:CD1	1:C:53:LYS:HE3	2.47	0.50	
1:F:45:VAL:HG11	1:F:88:ALA:O	2.12	0.50	
1:A:44:ASN:HB3	1:A:47:GLU:CB	2.41	0.50	
1:F:207:ASN:ND2	1:F:245:LEU:HD22	2.26	0.50	
1:B:316:TYR:OH	1:D:107:ASN:ND2	2.44	0.50	
1:C:69:LEU:HB3	1:C:70:PRO:HD3	1.93	0.50	
1:D:20:ARG:O	1:D:24:LYS:HE2	2.12	0.50	
1:C:13:LYS:CB	1:C:19:ILE:HG12	2.42	0.50	
1:A:6:GLU:HA	1:A:9:GLU:OE2	2.12	0.49	
1:A:164:GLN:N	1:A:164:GLN:NE2	2.54	0.49	
1:A:181:TYR:CE2	1:B:260:ILE:HD11	2.47	0.49	
1:B:314:LEU:HD11	1:D:297:ILE:CG2	2.42	0.49	
1:C:4:VAL:HG13	1:C:7:VAL:HG23	1.93	0.49	
1:C:76:VAL:CG2	1:C:77:MET:N	2.74	0.49	
1:C:270:LYS:HD2	1:C:270:LYS:N	2.27	0.49	
1:E:251:ILE:HD13	1:E:251:ILE:N	2.27	0.49	
1:E:260:ILE:HG13	1:E:268:TRP:CH2	2.47	0.49	
1:A:17:MET:HG2	1:A:20:ARG:HD2	1.93	0.49	
1:E:143:LYS:HZ2	1:E:175:TYR:HB3	1.76	0.49	
1:F:63:ARG:N	1:F:64:PRO:HD3	2.27	0.49	
1:F:222:THR:HG22	1:F:226:HIS:CD2	2.47	0.49	
1:F:293:GLU:CD	1:F:293:GLU:H	2.15	0.49	
1:E:152:ILE:HD13	1:E:152:ILE:H	1.77	0.49	
1:A:243:THR:HG22	1:A:244:MET:H	1.77	0.49	
1:B:292:THR:CG2	1:B:293:GLU:N	2.75	0.49	
1:D:45:VAL:HG11	1:D:88:ALA:O	2.13	0.49	
1:B:285:GLU:HG3	4:D:604:HOH:O	2.12	0.49	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:251:ILE:HG12	1:E:252:GLU:N	2.27	0.49	
1:F:196:LYS:HD3	1:F:229:TRP:HB3	1.94	0.49	
1:A:9:GLU:O	1:A:13:LYS:HG3	2.13	0.49	
1:C:10:ILE:CG2	1:C:28:SER:HB3	2.43	0.49	
1:E:25:ILE:HD11	1:E:63:ARG:HH11	1.77	0.49	
1:F:313:ALA:HB3	1:F:316:TYR:HD2	1.76	0.49	
1:C:212:ASN:O	1:C:279:PHE:HB3	2.12	0.49	
1:E:135:SER:OG	1:E:200:GLY:HA3	2.13	0.49	
1:A:4:VAL:HG13	1:A:36:GLN:OE1	2.12	0.48	
1:F:242:GLU:HG2	1:F:243:THR:H	1.77	0.48	
1:A:10:ILE:O	1:A:14:ILE:HG13	2.13	0.48	
1:A:267:THR:HG22	1:A:268:TRP:HD1	1.78	0.48	
1:C:255:ASP:O	1:C:258:GLU:HB2	2.12	0.48	
1:D:182:VAL:HG11	1:D:186:ALA:HB3	1.95	0.48	
1:F:69:LEU:HB3	1:F:70:PRO:CD	2.43	0.48	
1:B:314:LEU:HD22	1:D:294:ARG:O	2.13	0.48	
1:C:5:LYS:O	1:C:9:GLU:HB2	2.14	0.48	
1:C:76:VAL:CG2	1:C:77:MET:H	2.26	0.48	
1:D:40:SER:HB3	1:D:94:ARG:HH21	1.79	0.48	
1:F:23:GLY:HA3	1:F:27:ARG:HH12	1.78	0.48	
1:B:162:LYS:HE2	1:B:164:GLN:OE1	2.13	0.48	
1:A:211:ILE:HD13	1:A:251:ILE:HD11	1.95	0.48	
1:A:145:ALA:O	1:A:150:LYS:HB2	2.13	0.48	
1:B:78:HIS:CE1	1:B:311:GLY:HA3	2.48	0.48	
1:C:133:CYS:HA	1:C:159:THR:HG21	1.95	0.48	
1:D:4:VAL:HG12	1:D:6:GLU:HG2	1.96	0.48	
1:F:162:LYS:HE2	1:F:164:GLN:OE1	2.13	0.48	
1:C:102:LYS:HD3	1:C:102:LYS:O	2.14	0.48	
1:C:101:ALA:O	1:C:105:ILE:HG13	2.14	0.48	
1:C:314:LEU:O	1:C:316:TYR:N	2.46	0.48	
1:E:314:LEU:H	1:E:314:LEU:HD23	1.77	0.48	
1:C:269:PRO:HD2	1:C:272:ILE:HD12	1.95	0.47	
1:D:4:VAL:CG1	1:D:6:GLU:HG2	2.43	0.47	
1:A:159:THR:O	1:A:159:THR:HG22	2.12	0.47	
1:C:307:ARG:HG2	1:C:312:TRP:O	2.13	0.47	
1:E:156:VAL:HG23	1:E:179:VAL:HG13	1.96	0.47	
1:B:105:ILE:O	1:B:109:GLU:HG3	2.14	0.47	
1:C:3:VAL:HG13	1:C:8:LEU:HD11	1.96	0.47	
1:F:253:MET:CE	1:F:277:PRO:HA	2.44	0.47	
1:A:186:ALA:HA	1:B:214:ILE:HD11	1.96	0.47	
1:B:291:ILE:HD13	1:B:296:ILE:HG12	1.94	0.47	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:C:270:LYS:CD	1:C:270:LYS:N	2.77	0.47	
1:F:9:GLU:O	1:F:12:GLU:HB2	2.14	0.47	
1:A:17:MET:C	1:A:19:ILE:H	2.16	0.47	
1:D:52:MET:CE	1:D:97:ILE:HG21	2.45	0.47	
1:D:182:VAL:HG12	1:D:183:VAL:N	2.29	0.47	
1:A:257:THR:HA	1:A:260:ILE:O	2.14	0.47	
1:B:79:ARG:HG3	1:B:79:ARG:NH1	2.30	0.47	
1:B:278:ALA:HA	4:B:668:HOH:O	2.14	0.47	
1:F:20:ARG:HA	1:F:25:ILE:HD11	1.97	0.47	
1:A:45:VAL:HG11	1:A:88:ALA:O	2.15	0.47	
1:B:70:PRO:HB2	1:B:74:ARG:HH12	1.80	0.47	
1:F:199:MET:HE1	1:F:216:THR:CG2	2.39	0.47	
1:A:122:ARG:CZ	1:C:243:THR:HG22	2.45	0.46	
1:C:49:TRP:HA	1:C:49:TRP:CE3	2.50	0.46	
1:C:65:THR:HG23	1:C:66:ALA:N	2.30	0.46	
1:D:45:VAL:HG22	1:D:90:LEU:HB2	1.96	0.46	
1:F:271:ASN:N	1:F:271:ASN:ND2	2.62	0.46	
1:E:3:VAL:HG21	1:E:58:ILE:HD12	1.98	0.46	
1:B:78:HIS:CG	1:B:311:GLY:HA3	2.50	0.46	
1:B:247:GLN:HG3	1:B:247:GLN:O	2.15	0.46	
4:E:619:HOH:O	1:F:182:VAL:HG23	2.15	0.46	
1:F:132:HIS:HB2	1:F:199:MET:HE3	1.97	0.46	
1:B:206:VAL:CG1	1:B:241:PRO:HA	2.44	0.46	
1:C:16:ASN:O	1:C:17:MET:HB2	2.16	0.46	
1:E:294:ARG:HE	1:E:294:ARG:C	2.19	0.46	
1:C:318:GLU:HG3	1:C:319:PRO:HD2	1.97	0.46	
1:C:241:PRO:HA	1:C:306:LEU:CD1	2.46	0.46	
1:F:31:TYR:CZ	1:F:35:LEU:HD21	2.51	0.46	
1:F:129:ILE:HD12	1:F:196:LYS:HB2	1.98	0.46	
1:D:84:TYR:C	1:D:86:SER:H	2.19	0.46	
1:F:4:VAL:CG1	1:F:5:LYS:N	2.78	0.46	
1:C:262:GLU:O	1:C:266:LYS:HG2	2.16	0.46	
1:F:162:LYS:HB2	1:F:164:GLN:HE22	1.81	0.46	
1:A:211:ILE:HG21	1:A:251:ILE:HD12	1.97	0.46	
1:F:260:ILE:HD13	1:F:268:TRP:CZ3	2.51	0.46	
1:C:263:ASP:OD2	1:C:264:GLU:N	2.49	0.45	
1:D:42:ALA:HA	1:D:47:GLU:OE2	2.16	0.45	
1:D:52:MET:HE1	1:D:97:ILE:HG21	1.98	0.45	
1:C:40:SER:HB2	1:C:51:GLU:OE2	2.16	0.45	
1:D:36:GLN:O	1:D:40:SER:HB2	2.16	0.45	
1:D:236:THR:N	1:D:293:GLU:OE2	2.47	0.45	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:254:ARG:HG3	1:E:254:ARG:NH1	2.31	0.45	
1:E:318:GLU:CG	1:E:319:PRO:HD2	2.36	0.45	
1:F:170:LYS:O	1:F:173:ALA:HB3	2.17	0.45	
1:B:0:HIS:HE1	1:B:51:GLU:OE2	2.00	0.45	
1:B:289:VAL:HB	1:B:296:ILE:HG23	1.98	0.45	
1:C:8:LEU:O	1:C:12:GLU:HG3	2.16	0.45	
1:D:16:ASN:O	1:D:17:MET:HB2	2.17	0.45	
2:E:401:PEG:H21	2:E:401:PEG:H42	1.73	0.45	
1:F:253:MET:HE2	1:F:277:PRO:CA	2.46	0.45	
1:D:77:MET:CB	1:D:319:PRO:HB2	2.46	0.45	
1:E:271:ASN:HD21	1:F:173:ALA:CA	2.30	0.45	
1:A:95:PHE:O	1:A:99:ASN:HB2	2.17	0.45	
1:E:195:ASP:C	1:E:196:LYS:HG3	2.37	0.45	
1:A:25:ILE:HG13	1:A:26:ALA:N	2.27	0.45	
1:A:25:ILE:HD11	1:A:69:LEU:HB2	1.99	0.45	
1:C:45:VAL:HG11	1:C:88:ALA:O	2.16	0.45	
1:F:57:LYS:O	1:F:61:GLU:HG3	2.17	0.45	
1:A:11:ALA:HB1	1:A:62:THR:HG21	1.99	0.45	
1:B:89:ASP:H	1:B:92:GLN:HE21	1.63	0.45	
1:C:49:TRP:HA	1:C:49:TRP:HE3	1.82	0.45	
1:D:34:GLN:O	1:D:38:GLU:HG3	2.17	0.45	
1:F:206:VAL:CG1	1:F:241:PRO:HA	2.46	0.45	
1:B:224:LYS:HD2	2:B:401:PEG:H31	1.98	0.45	
1:C:214:ILE:HD11	1:D:186:ALA:HA	1.99	0.45	
1:D:317:THR:O	1:D:317:THR:HG22	2.17	0.45	
1:A:107:ASN:HD21	1:C:315:LYS:CE	2.30	0.45	
1:D:307:ARG:HD2	1:D:308:GLU:OE1	2.17	0.45	
1:E:262:GLU:O	1:E:266:LYS:HG3	2.17	0.45	
1:F:6:GLU:N	1:F:6:GLU:OE1	2.49	0.45	
1:F:91:GLU:OE1	1:F:94:ARG:NH1	2.50	0.45	
1:B:144:THR:O	1:B:148:GLN:HG3	2.17	0.44	
1:C:26:ALA:HB2	1:C:68:SER:HB2	1.98	0.44	
1:C:35:LEU:C	1:C:37:ALA:N	2.71	0.44	
1:C:221:LEU:HD13	1:D:221:LEU:CD1	2.43	0.44	
1:E:143:LYS:HE2	1:E:147:GLU:CG	2.46	0.44	
1:F:210:VAL:HG21	1:F:232:ILE:HG13	1.99	0.44	
1:B:207:ASN:OD1	1:D:298:PRO:HB3	2.16	0.44	
1:F:23:GLY:O	1:F:26:ALA:HB3	2.17	0.44	
1:B:70:PRO:O	1:B:74:ARG:HG3	2.18	0.44	
1:B:78:HIS:CD2	1:B:311:GLY:HA3	2.53	0.44	
1:C:33:LEU:HD11	1:C:73:LEU:HG	1.98	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:206:VAL:HG13	1:D:241:PRO:HA	1.98	0.44	
1:B:206:VAL:HG13	1:B:241:PRO:C	2.36	0.44	
1:C:79:ARG:C	1:C:82:ILE:HG22	2.37	0.44	
1:D:26:ALA:HB2	1:D:68:SER:HB2	1.99	0.44	
1:E:314:LEU:H	1:E:314:LEU:CD2	2.29	0.44	
1:F:239:PHE:N	1:F:239:PHE:CD2	2.84	0.44	
1:B:26:ALA:HB2	1:B:68:SER:HB2	2.00	0.44	
1:B:153:LYS:HD3	1:B:180:ILE:CD1	2.47	0.44	
1:D:1:MET:HA	1:D:54:GLN:HE21	1.82	0.44	
1:E:164:GLN:HE21	1:E:164:GLN:N	2.05	0.44	
1:A:15:LYS:C	1:A:17:MET:N	2.71	0.44	
1:A:59:LEU:O	1:A:69:LEU:HD21	2.18	0.44	
1:E:177:ILE:O	1:E:179:VAL:HG23	2.18	0.44	
1:E:181:TYR:CE2	1:F:260:ILE:HD11	2.52	0.44	
1:F:15:LYS:HB2	1:F:62:THR:HB	1.99	0.44	
1:D:45:VAL:HG12	1:D:45:VAL:O	2.18	0.44	
1:F:182:VAL:HG22	1:F:186:ALA:HB3	1.98	0.44	
1:C:241:PRO:HA	1:C:306:LEU:HD13	2.00	0.44	
1:E:159:THR:O	1:E:159:THR:HG22	2.18	0.44	
1:E:204:ILE:HD12	1:E:210:VAL:HG22	2.00	0.44	
1:F:297:ILE:HD13	1:F:305:ILE:CD1	2.48	0.44	
1:A:133:CYS:HA	1:A:159:THR:HG21	2.00	0.43	
1:C:114:ARG:O	1:C:117:GLU:HB3	2.18	0.43	
1:D:89:ASP:CG	1:D:90:LEU:N	2.72	0.43	
1:B:50:LYS:HE3	1:B:50:LYS:HB2	1.86	0.43	
1:C:135:SER:O	1:C:139:ILE:HG13	2.18	0.43	
1:E:160:ARG:HB2	1:F:183:VAL:HG21	2.01	0.43	
1:F:125:ASP:OD1	1:F:151:ASP:N	2.48	0.43	
1:E:268:TRP:HD1	1:E:268:TRP:H	1.64	0.43	
1:B:52:MET:HG2	1:B:97:ILE:CD1	2.48	0.43	
1:B:88:ALA:HB1	1:B:92:GLN:HB2	2.00	0.43	
1:C:158:GLU:HG3	1:C:181:TYR:OH	2.17	0.43	
1:C:160:ARG:HB3	1:C:161:PRO:HA	2.00	0.43	
1:E:221:LEU:HD13	1:F:221:LEU:HD13	2.01	0.43	
1:E:297:ILE:HD13	1:E:305:ILE:HD11	2.00	0.43	
1:A:6:GLU:HA	1:A:9:GLU:CG	2.48	0.43	
1:A:16:ASN:HB2	1:A:18:GLU:HG3	2.00	0.43	
1:A:224:LYS:HG3	1:A:286:TYR:CD1	2.54	0.43	
1:C:35:LEU:C	1:C:37:ALA:H	2.22	0.43	
1:C:153:LYS:HE2	1:C:180:ILE:HD11	1.99	0.43	
1:E:313:ALA:HB3	1:E:315:LYS:HG2	2.00	0.43	



	A + O	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:F:52:MET:CE	1:F:97:ILE:HG21	2.49	0.43	
1:F:263:ASP:HA	1:F:266:LYS:CD	2.48	0.43	
1:F:283:PRO:HB3	1:F:285:GLU:OE2	2.19	0.43	
1:B:307:ARG:HG3	1:B:307:ARG:HH11	1.83	0.43	
1:C:40:SER:H	1:C:94:ARG:NH2	2.16	0.43	
1:E:131:THR:OG1	1:E:132:HIS:N	2.52	0.43	
1:A:271:ASN:N	1:A:271:ASN:ND2	2.64	0.43	
1:B:292:THR:HG23	1:B:293:GLU:OE1	2.19	0.43	
1:E:119:GLY:CA	1:E:291:ILE:HD13	2.48	0.43	
1:A:288:ASP:OD1	2:A:401:PEG:H31	2.19	0.43	
1:B:153:LYS:HA	1:B:178:PRO:HG2	1.99	0.43	
1:D:46:ASP:O	1:D:50:LYS:HB2	2.18	0.43	
1:F:204:ILE:HD12	1:F:210:VAL:HG22	2.01	0.43	
1:A:69:LEU:O	1:A:73:LEU:HD22	2.19	0.43	
1:B:134:HIS:HE1	1:B:171:GLU:OE1	2.02	0.43	
1:C:319:PRO:HG2	1:C:320:TRP:HE3	1.84	0.43	
1:D:65:THR:O	1:D:66:ALA:C	2.56	0.43	
1:A:4:VAL:HG22	1:A:7:VAL:HG23	2.01	0.42	
1:C:314:LEU:HD23	1:C:314:LEU:HA	1.82	0.42	
1:D:318:GLU:HG3	1:D:320:TRP:CH2	2.54	0.42	
1:E:146:TRP:HB2	1:E:152:ILE:HD11	2.01	0.42	
1:A:48:PHE:HB2	1:A:90:LEU:CD1	2.49	0.42	
1:C:318:GLU:HG2	1:C:320:TRP:CZ2	2.53	0.42	
1:D:4:VAL:HG12	1:D:5:LYS:N	2.33	0.42	
1:D:139:ILE:HA	1:D:142:MET:HE3	2.01	0.42	
1:A:17:MET:C	1:A:19:ILE:N	2.73	0.42	
1:A:160:ARG:CB	1:B:183:VAL:HG21	2.49	0.42	
1:E:275:TRP:CH2	1:F:180:ILE:HD13	2.55	0.42	
1:A:78:HIS:CG	1:A:311:GLY:HA3	2.54	0.42	
1:C:4:VAL:CG2	1:C:6:GLU:HG2	2.50	0.42	
1:E:268:TRP:CD1	1:E:268:TRP:N	2.88	0.42	
1:F:143:LYS:HD3	1:F:175:TYR:CE1	2.54	0.42	
1:C:268:TRP:HA	1:C:269:PRO:HD3	1.88	0.42	
1:C:313:ALA:O	1:C:316:TYR:HB2	2.18	0.42	
1:D:245:LEU:HA	1:D:281:VAL:HG11	2.02	0.42	
1:A:49:TRP:NE1	1:A:53:LYS:HE3	2.34	0.42	
1:C:211:ILE:HD11	1:C:244:MET:CG	2.48	0.42	
1:C:270:LYS:H	1:C:270:LYS:HD2	1.85	0.42	
1:E:152:ILE:HD13	1:E:152:ILE:N	2.34	0.42	
1:A:36:GLN:O	1:A:40:SER:HB2	2.20	0.42	
1:B:257:THR:HA	1:B:260:ILE:O	2.20	0.42	



	i agein	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:182:VAL:CG1	1:D:183:VAL:N	2.83	0.42	
1:A:267:THR:O	1:A:267:THR:CG2	2.67	0.42	
1:B:222:THR:O	1:B:226:HIS:HD2	2.01	0.42	
1:E:69:LEU:HB3	1:E:70:PRO:CD	2.46	0.42	
1:F:303:ILE:O	1:F:307:ARG:HG2	2.19	0.42	
1:A:52:MET:HG3	1:A:97:ILE:CD1	2.50	0.42	
1:D:11:ALA:HB1	1:D:62:THR:CG2	2.50	0.42	
1:D:44:ASN:C	1:D:90:LEU:HD13	2.40	0.42	
1:D:164:GLN:NE2	1:D:164:GLN:N	2.61	0.42	
1:F:132:HIS:HA	1:F:157:THR:OG1	2.19	0.42	
1:F:162:LYS:HD3	1:F:258:GLU:OE2	2.20	0.42	
1:B:206:VAL:HG22	1:B:242:GLU:O	2.19	0.41	
1:E:143:LYS:HZ2	1:E:175:TYR:CB	2.33	0.41	
1:F:129:ILE:HD13	1:F:196:LYS:HB2	2.02	0.41	
1:A:49:TRP:CZ2	1:A:81:LYS:HA	2.56	0.41	
1:A:283:PRO:HD2	1:A:286:TYR:CD2	2.55	0.41	
1:C:199:MET:CE	1:C:216:THR:HG23	2.51	0.41	
1:E:146:TRP:HE3	1:E:152:ILE:HD13	1.84	0.41	
1:E:288:ASP:O	1:E:299:PRO:HD3	2.20	0.41	
1:F:44:ASN:C	1:F:44:ASN:ND2	2.74	0.41	
1:A:222:THR:O	1:A:226:HIS:HD2	2.04	0.41	
1:B:8:LEU:O	1:B:12:GLU:HG2	2.20	0.41	
1:B:314:LEU:HB3	1:D:294:ARG:CB	2.48	0.41	
1:D:67:VAL:O	1:D:70:PRO:HD2	2.20	0.41	
1:D:318:GLU:HA	1:D:319:PRO:HD3	1.96	0.41	
1:A:49:TRP:CE2	1:A:53:LYS:HE3	2.56	0.41	
1:B:224:LYS:HA	2:B:401:PEG:H31	2.02	0.41	
1:C:33:LEU:HD13	1:C:76:VAL:HG21	2.02	0.41	
1:F:239:PHE:N	1:F:239:PHE:HD2	2.18	0.41	
1:F:31:TYR:CE2	1:F:35:LEU:HD11	2.56	0.41	
1:F:132:HIS:HB3	1:F:199:MET:CE	2.51	0.41	
1:A:16:ASN:CB	1:A:18:GLU:HG3	2.50	0.41	
1:A:183:VAL:HG22	4:A:603:HOH:O	2.21	0.41	
1:B:4:VAL:HG12	1:B:6:GLU:HG2	2.03	0.41	
1:B:227:ARG:HG2	1:E:227:ARG:HG2	2.02	0.41	
1:B:269:PRO:C	1:B:271:ASN:N	2.74	0.41	
1:C:90:LEU:O	1:C:94:ARG:HB2	2.21	0.41	
1:C:210:VAL:HG21	1:C:232:ILE:HG13	2.03	0.41	
1:F:31:TYR:O	1:F:34:GLN:N	2.54	0.41	
1:F:206:VAL:HG22	1:F:242:GLU:O	2.21	0.41	
1:B:106:HIS:O	1:B:110:LYS:HG2	2.20	0.40	



Atom-1	Atom-2	Interatomic	Clash
	1100111-2	distance (Å)	overlap (Å)
1:F:145:ALA:O	1:F:148:GLN:HB2	2.20	0.40
1:F:235:GLU:HG2	1:F:237:TYR:OH	2.21	0.40
1:B:227:ARG:HE	1:E:227:ARG:CG	2.28	0.40
1:B:291:ILE:CD1	1:B:296:ILE:HG12	2.52	0.40
1:C:7:VAL:C	1:C:9:GLU:N	2.75	0.40
1:C:65:THR:HG23	1:C:66:ALA:H	1.85	0.40
1:D:160:ARG:HD2	1:D:161:PRO:HA	2.02	0.40
1:C:22:ALA:HB2	4:C:625:HOH:O	2.20	0.40
1:C:90:LEU:HD21	1:C:94:ARG:HH11	1.87	0.40
1:E:101:ALA:O	1:E:105:ILE:HG13	2.22	0.40
1:F:45:VAL:HG13	1:F:90:LEU:HA	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	318/338~(94%)	302 (95%)	14 (4%)	2(1%)	25	43
1	В	318/338~(94%)	307~(96%)	11 (4%)	0	100	100
1	С	313/338~(93%)	287~(92%)	24 (8%)	2(1%)	25	43
1	D	316/338~(94%)	296 (94%)	18 (6%)	2(1%)	25	43
1	Е	313/338~(93%)	301 (96%)	12 (4%)	0	100	100
1	F	315/338~(93%)	289 (92%)	23 (7%)	3 (1%)	15	28
All	All	1893/2028~(93%)	1782 (94%)	102 (5%)	9 (0%)	29	48

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	4	VAL



COntic	naea jion	i prevu	bus puye
Mol	Chain	\mathbf{Res}	Type
1	F	245	LEU
1	А	252	GLU
1	D	42	ALA
1	С	314	LEU
1	С	315	LYS
1	F	4	VAL
1	F	64	PRO
1	D	269	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	268/284~(94%)	253~(94%)	15 (6%)	21	40
1	В	268/284~(94%)	254~(95%)	14 (5%)	23	44
1	С	264/284~(93%)	255~(97%)	9(3%)	37	63
1	D	265/284~(93%)	252~(95%)	13~(5%)	25	47
1	Ε	264/284~(93%)	248~(94%)	16 (6%)	18	36
1	F	266/284~(94%)	253~(95%)	13~(5%)	25	47
All	All	1595/1704~(94%)	1515~(95%)	80 (5%)	24	46

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	5	LYS
1	А	20	ARG
1	А	25	ILE
1	А	49	TRP
1	А	89	ASP
1	А	151	ASP
1	А	164	GLN
1	А	221	LEU
1	А	240	HIS
1	А	242	GLU



1 A 263 ASP 1 A 267 THR 1 A 270 LYS	
1 A 267 THR 1 A 270 LYS	_
1 A 270 LYS	
1 11 110 110	-
$1 \qquad A \qquad 271 \qquad ASN$	_
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1 C 17 MET	
1 C 91 GLU	_
1 C 164 GLN	
1 C 221 LEU	
1 C 240 HIS	
1 C 243 THR	
1 C 270 LYS	
1 C 309 GLU	
1 C 314 LEU	
1 D 50 LYS	
1 D 117 GLU	\neg
1 D 164 GLN	
1 D 206 VAL	
1 D 214 ILE	\neg
1 D 221 LEU	
1 D 227 ARG	
1 D 254 ARG	\neg
1 D 293 GLU	
1 D 308 GLU	\neg
1 D 316 TYR	
1 D 317 THR	
1 D 318 GLU	\neg
1 E 69 LEU	



Mol	Chain	Res	Type
1	Е	73	LEU
1	Е	107	ASN
1	Е	117	GLU
1	Е	122	ARG
1	Е	143	LYS
1	Е	152	ILE
1	Е	164	GLN
1	Е	185	SER
1	Е	218	LEU
1	Е	221	LEU
1	Е	224	LYS
1	Е	251	ILE
1	Е	287	VAL
1	Е	294	ARG
1	Е	316	TYR
1	F	6	GLU
1	F	39	LYS
1	F	44	ASN
1	F	45	VAL
1	F	79	ARG
1	F	164	GLN
1	F	221	LEU
1	F	245	LEU
1	F	262	GLU
1	F	280	ASP
1	F	293	GLU
1	F	296	ILE
1	F	303	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	16	ASN
1	А	107	ASN
1	А	134	HIS
1	А	164	GLN
1	А	207	ASN
1	А	226	HIS
1	А	240	HIS
1	А	271	ASN
1	В	0	HIS
1	В	54	GLN



Mol	Chain	Res	Type
1	В	92	GLN
1	В	132	HIS
1	В	134	HIS
1	В	164	GLN
1	В	226	HIS
1	В	247	GLN
1	В	271	ASN
1	С	92	GLN
1	С	106	HIS
1	С	164	GLN
1	С	226	HIS
1	D	34	GLN
1	D	92	GLN
1	D	99	ASN
1	D	107	ASN
1	D	134	HIS
1	D	164	GLN
1	D	189	HIS
1	D	226	HIS
1	D	247	GLN
1	Е	44	ASN
1	Е	164	GLN
1	Е	226	HIS
1	F	44	ASN
1	F	54	GLN
1	F	164	GLN
1	F	189	HIS
1	F	207	ASN
1	F	226	HIS
1	F	240	HIS
1	F	271	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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mal	Turne	Chain	Res	Dec	Tink	Bond lengths			Bond angles		
	Type	Unann			Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
2	PEG	E	401	-	6,6,6	0.53	0	$5,\!5,\!5$	0.49	0	
2	PEG	D	401	-	6,6,6	0.54	0	$5,\!5,\!5$	0.37	0	
2	PEG	В	401	-	6,6,6	0.54	0	$5,\!5,\!5$	0.41	0	
2	PEG	С	401	-	6,6,6	0.53	0	$5,\!5,\!5$	0.44	0	
2	PEG	А	401	-	6,6,6	0.53	0	$5,\!5,\!5$	0.42	0	
2	PEG	F	401	-	6,6,6	0.52	0	$5,\!5,\!5$	0.46	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	PEG	Е	401	-	-	1/4/4/4	-
2	PEG	D	401	-	-	1/4/4/4	-
2	PEG	В	401	-	-	0/4/4/4	-
2	PEG	С	401	-	-	0/4/4/4	-
2	PEG	А	401	-	-	0/4/4/4	-
2	PEG	F	401	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	Е	401	PEG	C4-C3-O2-C2
2	D	401	PEG	C4-C3-O2-C2

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Е	401	PEG	1	0
2	D	401	PEG	2	0
2	В	401	PEG	2	0
2	А	401	PEG	2	0
2	F	401	PEG	2	0

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	$OWAB(Å^2)$	$\mathbf{Q}{<}0.9$
1	А	320/338~(94%)	0.13	12 (3%) 40 43	14, 36, 87, 104	0
1	В	322/338~(95%)	-0.17	4 (1%) 79 80	12, 29, 56, 82	0
1	С	317/338~(93%)	0.56	49 (15%) 2 1	20, 51, 109, 122	0
1	D	320/338~(94%)	0.17	12 (3%) 40 43	16, 37, 78, 115	0
1	Ε	317/338~(93%)	-0.00	5 (1%) 72 74	24, 42, 68, 92	0
1	F	319/338~(94%)	0.26	15 (4%) 31 33	25, 48, 79, 111	0
All	All	1915/2028~(94%)	0.16	97 (5%) 28 29	12, 41, 86, 122	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	248	LEU	7.2
1	С	93	LEU	7.0
1	D	249	VAL	6.2
1	С	3	VAL	5.9
1	С	49	TRP	5.6
1	С	94	ARG	4.2
1	А	8	LEU	4.0
1	С	246	GLY	4.0
1	D	92	GLN	4.0
1	С	90	LEU	4.0
1	С	2	ALA	4.0
1	С	31	TYR	3.9
1	D	1	MET	3.9
1	С	14	ILE	3.9
1	А	10	ILE	3.8
1	E	316	TYR	3.8
1	С	322	ASP	3.8
1	F	249	VAL	3.7
1	А	14	ILE	3.7



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Mol	Chain	Res	Type	RSRZ
1	С	33	LEU	3.7
1	F	16	ASN	3.6
1	А	54	GLN	3.6
1	С	91	GLU	3.6
1	D	316	TYR	3.6
1	С	42	ALA	3.5
1	С	48	PHE	3.5
1	Е	251	ILE	3.4
1	С	65	THR	3.4
1	С	92	GLN	3.4
1	С	245	LEU	3.4
1	D	245	LEU	3.3
1	А	248	LEU	3.3
1	С	98	ILE	3.3
1	С	17	MET	3.3
1	С	12	GLU	3.2
1	С	95	PHE	3.1
1	D	89	ASP	3.1
1	С	45	VAL	3.0
1	С	96	VAL	3.0
1	С	56	ALA	3.0
1	С	100	ALA	3.0
1	С	54	GLN	2.9
1	Е	314	LEU	2.9
1	С	58	ILE	2.9
1	F	322	ASP	2.9
1	F	43	THR	2.9
1	D	49	TRP	2.8
1	С	20	ARG	2.8
1	А	322	ASP	2.8
1	С	43	THR	2.8
1	Е	175	TYR	2.7
1	D	322	ASP	2.7
1	D	2	ALA	2.7
1	С	59	LEU	2.7
1	С	40	SER	2.7
1	А	247	GLN	2.7
1	В	322	ASP	2.7
1	С	251	ILE	2.6
1	С	88	ALA	2.6
1	С	15	LYS	2.6
1	С	44	ASN	2.6



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Mol	Chain	Res	Type	RSRZ
1	С	50	LYS	2.6
1	А	249	VAL	2.6
1	F	175	TYR	2.6
1	F	12	GLU	2.6
1	В	316	TYR	2.5
1	F	19	ILE	2.5
1	D	90	LEU	2.5
1	С	7	VAL	2.5
1	В	245	LEU	2.4
1	F	8	LEU	2.4
1	С	82	ILE	2.4
1	F	2	ALA	2.4
1	С	66	ALA	2.4
1	В	-2	GLY	2.4
1	С	51	GLU	2.4
1	А	7	VAL	2.3
1	С	4	VAL	2.3
1	F	54	GLN	2.3
1	А	317	THR	2.3
1	F	11	ALA	2.3
1	F	87	GLY	2.2
1	F	270	LYS	2.2
1	С	84	TYR	2.2
1	С	175	TYR	2.2
1	А	40	SER	2.2
1	С	6	GLU	2.2
1	С	8	LEU	2.2
1	С	314	LEU	2.2
1	A	9	GLU	2.2
1	С	16	ASN	2.1
1	Е	270	LYS	2.1
1	D	84	TYR	2.1
1	С	102	LYS	2.1
1	С	99	ASN	2.1
1	F	3	VAL	2.0
1	F	20	ARG	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	B-factors(Å ²)	Q<0.9
2	PEG	D	401	7/7	0.72	0.41	48,49,62,62	0
2	PEG	С	401	7/7	0.74	0.38	49,59,63,67	0
2	PEG	F	401	7/7	0.79	0.30	45,53,64,64	0
2	PEG	Е	401	7/7	0.80	0.36	$51,\!53,\!55,\!55$	0
2	PEG	В	401	7/7	0.80	0.31	$56,\!58,\!60,\!62$	0
2	PEG	А	401	7/7	0.83	0.35	40,51,58,59	0
3	MG	Е	411	1/1	0.91	0.50	56, 56, 56, 56	0
3	MG	В	411	1/1	0.96	0.51	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.

