

Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 03:29 AM EDT

PDB ID	:	4FM4
Title	:	Wild Type Fe-type Nitrile Hydratase from Comamonas testosteroni Ni1
Authors	:	Kuhn, M.L.; Martinez, S.; Gumataotao, N.; Bornscheuer, U.; Liu, D.; Holz,
		R.C.
Deposited on	:	2012-06-15
Resolution	:	2.38 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	:	2.35
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)	:	2.35

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 2.38 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	$\begin{array}{c} {\rm Whole \ archive} \\ (\#{\rm Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973(2.40-2.36)
Sidechain outliers	138945	5975(2.40-2.36)
RSRZ outliers	127900	5397(2.40-2.36)

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	209	71%	21%	7% •
1	С	209	68%	24%	6% ·
1	Е	209	72%	21%	6% •
1	G	209	72%	22%	5%•
1	Ι	209	71%	22%	5%•



Conti	nued fron	n previous	page		
Mol	Chain	Length	Quality of chain		
1	K	209	72%	21%	5%•
1	М	209	71%	22%	5%•
1	О	209	73%	19%	7% •
2	В	206	79%	18%	•
2	D	206	75%	20%	·
2	F	206	76%	19%	·
2	Н	206	81%	14%	·
2	J	206	75%	20%	·
2	L	206	76%	20%	•
2	Ν	206	77%	19%	·
2	Р	206	75%	21%	•

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
1	CSD	Е	104	-	-	Х	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 27326 atoms, of which 8 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	Δ	206	Total	С	Η	Ν	0	S	0	0	0
1	A	200	1610	1026	1	268	306	9	0	0	0
1	С	206	Total	С	Η	Ν	0	S	0	0	0
1		200	1610	1026	1	268	306	9	0	0	0
1	F	206	Total	С	Η	Ν	0	S	0	0	0
1		200	1610	1026	1	268	306	9		0	0
1	C	206	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
1	G		1610	1026	1	268	306	9	0	0	0
1	Т	206	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
1	L	200	1610	1026	1	268	306	9	0	0	0
1	K	206	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
1	Γ	200	1610	1026	1	268	306	9	0	0	0
1	М	206	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
1	I IVI	200	1610	1026	1	268	306	9	0	0	0
1	0	206	Total	С	Η	Ν	0	S	0	0	0
1			1610	1026	1	268	306	9		0	U

• Molecule 1 is a protein called Nitrile hydratase alpha subunit.

• Molecule 2 is a protein called Nitrile hydratase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	206	Total	С	Ν	Ο	S	0	0	0
	D	200	1589	1017	271	293	8	0	0	0
9	Л	206	Total	С	Ν	0	S	0	0	0
	D	200	1589	1017	271	293	8	0		0
0	Б	206	Total	С	Ν	0	S	0	0	0
	Г		1589	1017	271	293	8			
0	ц	206	Total	С	Ν	0	S	0	0	0
	11		1589	1017	271	293	8			0
0	т	206	Total	С	Ν	0	S	0	0	0
	200	1589	1017	271	293	8	0	0	0	
2 L	206	Total	С	Ν	0	S	0	0	0	
		1589	1017	271	293	8	0	0	0	



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	2 N	206	Total	С	Ν	Ο	S	0	0	0
			1589	1017	271	293	8			
2	9 D	206	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	200	1589	1017	271	293	8	0	0	0	

• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	Total O P 5 4 1	0	0
3	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	Ι	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	K	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	М	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	О	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Fe 1 1	0	0
4	С	1	Total Fe 1 1	0	0
4	Ε	1	Total Fe 1 1	0	0
4	G	1	Total Fe 1 1	0	0
4	Ι	1	Total Fe 1 1	0	0
4	K	1	Total Fe 1 1	0	0
4	М	1	Total Fe 1 1	0	0
4	О	1	Total Fe 1 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	98	Total O 98 98	0	0
5	В	113	Total O 113 113	0	0
5	С	91	Total O 91 91	0	0
5	D	106	Total O 106 106	0	0
5	Е	107	Total O 107 107	0	0
5	F	112	Total O 112 112	0	0
5	G	93	Total O 93 93	0	0
5	Н	110	Total O 110 110	0	0
5	Ι	108	Total O 108 108	0	0
5	J	92	Total O 92 92	0	0
5	К	113	Total O 113 113	0	0
5	L	122	$\begin{array}{ccc} Total & O \\ 122 & 122 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	М	99	Total O 99 99	0	0
5	Ν	104	Total O 104 104	0	0
5	О	115	Total O 115 115	0	0
5	Р	103	Total O 103 103	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: Nitrile hydratase alpha subunit



• Molecule 1: Nitrile hydratase alpha subunit







• Molecule 2: Nitrile hydratase beta subunit



• Molecule 2: Nitrile hydratase beta subunit

C	nai	n	F:														7(6%															19	1%			•					
M1	H5	89	G9 K10		K18 T19	H20	N21	K23		E27	K30	M33	N34	A35	136	L40		H53	E56	R57	M58		H62	Y63	L64	T65	A66 S67	2	F73	1/0 L79	18.L	E90	L91	E92	TO7	191 898	S102	L103 P104	S105	S106	LOL A	•
P111	E116	L121	R124			H135	T136 B137		I142		V150	Y158	P159	D160	E160	COT J	L183	1071	V 197	L202		E206																				
•	Mo	ole	cu	le	2:	ľ	Vi	tr	ile	ł	ıy	dı	ra	ta	se	e l	be	eta	เร	u	bι	ın	it																			





• Molecule 2: Nitrile hydratase beta subunit



• Molecule 2: Nitrile hydratase beta subunit



Chain L:	76%	20% •
M1 H5 H5 G8 G8 G9 K10 C11 C12 C12 C12 C12 C12 C12 C12 C12 C12	Y 46 H153 E56 E56 E56 Y 63 Y 63 Y 63 F 7 E 90 E 90 E 90 E 91 E 92	L95 G96 197 197 197 8102 1103 1103 8105 8105 8105 8105 8105
P111 K113 K113 E116 E116 H135 H137 K145 Y156 P157 P157 P158 P156 P166	C177 L188 P186	
• Molecule 2: Nitrile hydratase	beta subunit	
Chain N:	77%	19% •
M1 G8 C9 C10 M21 M21 M21 M21 M27 M23 M27 M27 M27 M27 M27 M27 M27 M27	G54 155 155 155 155 155 155 155 164 164 166 178 166 178 178 178 178 178 178 178 178 178 178	K94 195 196 197 197 100 1103 100 1103 106 106 106 106 106
V127 V127 F131 H135 H135 V156 V156 P159 P159 V163 V163 V163 V163 V163 V183 V183 V183 V183 V183 V183 V183 V18		
• Molecule 2: Nitrile hydratase	beta subunit	
Chain P:	75%	21% •
M1 L7 K10 K10 K18 K18 N21 N21 N21 N22 N22 N22 N22 N22	R57 M58 E59 F50 R61 F53 F73 F73 F73 F73 F73 F73 F73 F73 F73 F7	T97 598 799 8102 8103 8104 8104 8106 8106 8116



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants	111.40Å 111.40Å 475.31Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	36.16 - 2.38	Depositor
Resolution (A)	36.16 - 2.38	EDS
% Data completeness	99.3 (36.16-2.38)	Depositor
(in resolution range)	87.0 (36.16-2.38)	EDS
R _{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.30 (at 2.39 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
B B.	0.188 , 0.227	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.184 , 0.223	DCC
R_{free} test set	13171 reflections (5.03%)	wwPDB-VP
Wilson B-factor $(Å^2)$	31.9	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , 36.2	EDS
L-test for $twinning^2$	$< L >=0.50, < L^2>=0.34$	Xtriage
	0.487 for -h,-k,l	
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtriage
	0.487 for -k,-h,-l	
F_o, F_c correlation	0.96	EDS
Total number of atoms	27326	wwPDB-VP
Average B, all atoms $(Å^2)$	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.33% 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: CSD, PO4, FE $\,$

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	Bo	ond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.54	0/1630	0.66	0/2227
1	С	0.57	0/1630	0.71	0/2227
1	Е	0.57	0/1630	0.69	0/2227
1	G	0.57	0/1630	0.70	0/2227
1	Ι	0.53	0/1630	0.67	0/2227
1	Κ	0.57	0/1630	0.71	0/2227
1	М	0.55	0/1630	0.68	0/2227
1	0	0.55	0/1630	0.67	0/2227
2	В	0.56	0/1636	0.65	0/2216
2	D	0.58	0/1636	0.65	1/2216~(0.0%)
2	F	0.59	0/1636	0.67	1/2216~(0.0%)
2	Н	0.59	0/1636	0.66	1/2216~(0.0%)
2	J	0.56	0/1636	0.66	0/2216
2	L	0.60	0/1636	0.67	1/2216~(0.0%)
2	N	0.57	0/1636	0.65	0/2216
2	Р	0.58	0/1636	0.66	0/2216
All	All	0.57	0/26128	0.67	4/35544~(0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	1
1	С	0	1
1	Е	0	1
1	G	0	1
1	Ι	0	1
1	Κ	0	1
1	М	0	1



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Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	1
All	All	0	8

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	Н	105	SER	N-CA-C	-6.11	94.51	111.00
2	F	105	SER	N-CA-C	-5.75	95.47	111.00
2	L	105	SER	N-CA-C	-5.52	96.10	111.00
2	D	105	SER	N-CA-C	-5.26	96.79	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	153	THR	Peptide
1	С	153	THR	Peptide
1	Е	153	THR	Peptide
1	G	153	THR	Peptide
1	Ι	153	THR	Peptide
1	Κ	153	THR	Peptide
1	М	153	THR	Peptide
1	0	153	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1609	1	1592	43	0
1	С	1609	1	1590	49	0
1	Е	1609	1	1591	42	0
1	G	1609	1	1591	42	0
1	Ι	1609	1	1591	48	0
1	K	1609	1	1590	48	0
1	М	1609	1	1590	52	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1		1600	1	1590		
$\frac{1}{2}$	B	1580	0	1530	37	0
$\frac{2}{2}$	D	1589	0	1538	43	0
$\frac{2}{2}$	F	1589	0	1538	40	0
2	H	1589	0	1538	38	0
2	I	1589	0	1538	48	0
2	U U	1589	0	1538	46	0
2	N	1589	0	1538	33	0
2	P	1589	0	1538	47	0
3	A	5	0	0	0	0
3	С	5	0	0	1	0
3	E	5	0	0	1	0
3	G	5	0	0	0	0
3	Ι	5	0	0	0	0
3	K	5	0	0	0	0
3	М	5	0	0	0	0
3	0	5	0	0	0	0
4	А	1	0	0	0	0
4	С	1	0	0	0	0
4	Е	1	0	0	0	0
4	G	1	0	0	0	0
4	Ι	1	0	0	0	0
4	Κ	1	0	0	0	0
4	М	1	0	0	0	0
4	0	1	0	0	0	0
5	A	98	0	0	7	0
5	В	113	0	0	4	0
5	С	91	0	0	5	1
5	D	106	0	0	2	0
5	E	107	0	0	6	0
5	F	112	0	0	4	1
5	G	93	0	0	4	0
5	H	110	0	0	8	0
5	l	108	0	0	5	0
5	J	92	0	0	8	0
5	K	113	0	0	8	0
5		122	0	0	5	0
<u>с</u>	IVI	99	0	0		0
С С		104	0	0		U 1
D F		110	0	0	4	
	Г 	103	U	U 25020	<u>ර</u> 640	
All	All	27318	8	25029	040	2



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 13.

All (640) 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 $(Å)$	overlap (Å)
1:K:207:ALA:CB	2:P:42:SER:HB3	1.71	1.20
2:F:124:ARG:HG3	2:F:124:ARG:HH11	0.99	1.13
1:G:154:ALA:O	5:G:447:HOH:O	1.83	0.96
2:F:97:THR:HG22	2:F:98:SER:H	1.30	0.96
1:K:207:ALA:HB1	2:P:42:SER:HB3	1.46	0.95
1:M:43:GLN:H	1:M:43:GLN:HE21	1.04	0.95
1:I:43:GLN:HE21	1:I:43:GLN:N	1.64	0.94
1:K:204:ALA:O	1:K:205:LEU:HB2	1.68	0.93
2:F:104:PRO:CA	2:F:105:SER:HB2	1.97	0.93
1:O:43:GLN:HE21	1:O:43:GLN:N	1.67	0.93
2:H:10:LYS:HE3	5:H:378:HOH:O	1.66	0.93
2:D:104:PRO:CA	2:D:105:SER:HB2	2.01	0.91
1:K:154:ALA:O	5:K:403:HOH:O	1.88	0.91
2:D:104:PRO:CB	2:D:105:SER:HB2	2.00	0.91
1:I:43:GLN:H	1:I:43:GLN:NE2	1.69	0.90
1:E:204:ALA:O	1:E:205:LEU:HB2	1.69	0.90
2:F:124:ARG:HG3	2:F:124:ARG:NH1	1.78	0.89
1:O:43:GLN:H	1:O:43:GLN:NE2	1.69	0.89
2:P:104:PRO:CA	2:P:105:SER:HB2	2.03	0.89
2:B:163:ALA:O	5:B:349:HOH:O	1.91	0.88
1:E:2:THR:N	5:E:460:HOH:O	2.06	0.88
1:O:43:GLN:HE21	1:O:43:GLN:H	0.87	0.86
1:E:154:ALA:O	5:E:473:HOH:O	1.93	0.85
2:P:104:PRO:CB	2:P:105:SER:HB2	2.06	0.85
2:D:1:MET:HE3	2:D:56:GLU:HB3	1.58	0.85
2:H:104:PRO:CA	2:H:105:SER:HB2	2.05	0.84
2:N:104:PRO:CA	2:N:105:SER:HB2	2.07	0.84
1:M:167:GLY:N	1:M:169:GLU:OE1	2.10	0.84
2:J:163:ALA:O	5:J:344:HOH:O	1.94	0.84
2:P:59:GLU:OE1	5:P:333:HOH:O	1.96	0.83
2:N:104:PRO:CB	2:N:105:SER:HB2	2.08	0.83
2:L:10:LYS:HE3	2:L:10:LYS:HA	1.59	0.83
1:M:43:GLN:HE21	1:M:43:GLN:N	1.77	0.83
1:A:167:GLY:N	1:A:169:GLU:OE1	2.12	0.82
1:K:154:ALA:HB3	5:K:507:HOH:O	1.78	0.82
1:0:76:SER:O	1:O:108:THR:HG21	1.78	0.82
2:B:104:PRO:CB	2:B:105:SER:HB2	2.10	0.82



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:J:10:LYS:HE3	2:J:10:LYS:HA	1.61	0.82
2:F:104:PRO:HA	2:F:105:SER:CB	2.09	0.82
2:J:97:THR:HG22	2:J:98:SER:N	1.94	0.82
1:C:175:GLN:O	1:C:178:THR:HB	1.80	0.81
1:O:167:GLY:N	1:O:169:GLU:OE1	2.12	0.81
1:C:154:ALA:O	5:C:402:HOH:O	1.98	0.80
1:G:108:THR:HG22	1:G:109:ILE:HG12	1.64	0.80
1:G:2:THR:HG21	1:G:7:MET:SD	2.21	0.80
2:F:104:PRO:HA	2:F:105:SER:HB2	1.63	0.79
2:F:104:PRO:CB	2:F:105:SER:HB2	2.12	0.79
2:N:92:GLU:OE1	2:N:98:SER:HA	1.83	0.79
1:C:2:THR:HG21	1:C:7:MET:SD	2.22	0.79
1:K:205:LEU:O	1:K:207:ALA:N	2.16	0.79
1:A:154:ALA:O	5:A:412:HOH:O	1.99	0.79
1:E:175:GLN:O	1:E:178:THR:HB	1.83	0.79
1:O:205:LEU:C	1:O:205:LEU:HD23	2.04	0.78
1:K:207:ALA:HA	2:P:42:SER:CB	2.14	0.78
2:H:104:PRO:CB	2:H:105:SER:HB2	2.15	0.77
2:H:78:THR:HG21	2:H:102:SER:HB2	1.66	0.77
1:G:175:GLN:O	1:G:178:THR:HB	1.85	0.77
1:E:76:SER:O	1:E:108:THR:HG21	1.84	0.77
2:L:92:GLU:HG2	2:L:98:SER:HA	1.66	0.77
1:K:175:GLN:O	1:K:178:THR:HB	1.84	0.76
1:I:43:GLN:HE21	1:I:43:GLN:H	0.83	0.76
1:I:154:ALA:O	5:I:461:HOH:O	2.03	0.76
2:P:61:ARG:O	2:P:65:THR:HB	1.86	0.76
2:H:113:LYS:HA	2:H:113:LYS:HE3	1.68	0.76
1:G:102:CSD:O	1:G:103:SER:HB3	1.86	0.76
1:K:207:ALA:HB2	2:P:42:SER:HB3	1.67	0.76
2:N:104:PRO:HA	2:N:105:SER:CB	2.15	0.76
2:J:61:ARG:O	2:J:65:THR:HB	1.86	0.76
1:K:207:ALA:CA	2:P:42:SER:HB3	2.17	0.76
2:B:104:PRO:CA	2:B:105:SER:HB2	2.15	0.75
1:G:105:THR:HG21	1:G:113:ALA:HB2	1.66	0.75
1:0:154:ALA:O	5:O:412:HOH:O	2.02	0.75
1:C:104:CSD:HA	3:C:301:PO4:O4	1.87	0.75
1:M:17:LEU:HD23	1:M:21:LEU:CD2	2.15	0.75
2:J:92:GLU:OE1	2:J:98:SER:HA	1.86	0.75
1:M:105:THR:HG21	1:M:113:ALA:HB2	1.68	0.75
2:F:97:THR:HG22	2:F:98:SER:N	2.02	0.74
2:F:58:MET:O	5:F:397:HOH:O	2.03	0.74



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:105:THR:HG21	1:E:113:ALA:HB2	1.68	0.73
2:F:10:LYS:NZ	5:F:345:HOH:O	2.20	0.73
1:C:167:GLY:N	1:C:169:GLU:OE1	2.20	0.73
1:M:43:GLN:H	1:M:43:GLN:NE2	1.84	0.73
1:E:2:THR:HG21	1:E:7:MET:SD	2.29	0.73
1:I:82:LYS:HE2	1:I:155:ASP:OD2	1.89	0.73
2:B:59:GLU:OE1	5:B:408:HOH:O	2.07	0.73
2:B:61:ARG:O	2:B:65:THR:HB	1.89	0.73
2:F:22:ALA:O	2:F:23:LYS:HB2	1.87	0.73
2:N:61:ARG:O	2:N:65:THR:HB	1.89	0.73
1:K:207:ALA:HA	2:P:42:SER:HB2	1.70	0.72
2:D:104:PRO:HA	2:D:105:SER:CB	2.18	0.72
1:I:37:MET:HE2	1:I:37:MET:HA	1.71	0.72
2:P:104:PRO:HA	2:P:105:SER:CB	2.18	0.72
1:I:167:GLY:N	1:I:169:GLU:OE1	2.22	0.72
1:O:82:LYS:HE2	1:0:155:ASP:OD2	1.88	0.72
1:M:154:ALA:O	5:M:447:HOH:O	2.08	0.71
1:K:154:ALA:N	5:K:403:HOH:O	2.22	0.71
2:H:104:PRO:HA	2:H:105:SER:HB2	1.72	0.71
1:A:205:LEU:HD23	1:A:205:LEU:C	2.10	0.71
1:G:191:LEU:O	5:G:420:HOH:O	2.09	0.70
2:D:97:THR:HG22	2:D:98:SER:N	2.07	0.70
2:H:104:PRO:HA	2:H:105:SER:CB	2.22	0.70
2:P:104:PRO:CA	2:P:105:SER:CB	2.71	0.69
2:J:97:THR:CG2	2:J:98:SER:N	2.56	0.69
1:G:3:ASP:OD1	1:G:5:ALA:N	2.26	0.69
2:D:61:ARG:O	2:D:65:THR:HB	1.93	0.68
1:C:154:ALA:N	5:C:402:HOH:O	2.25	0.68
2:F:87:THR:OG1	2:F:90:GLU:HG3	1.94	0.68
2:P:67:SER:HB3	5:P:373:HOH:O	1.93	0.68
1:M:154:ALA:N	5:M:447:HOH:O	2.27	0.68
1:K:207:ALA:CB	2:P:42:SER:CB	2.63	0.68
1:K:2:THR:HG21	1:K:7:MET:SD	2.33	0.68
1:I:137:ILE:CD1	1:I:188:VAL:CG2	2.72	0.67
2:J:104:PRO:CA	2:J:105:SER:HB2	2.25	0.67
1:E:154:ALA:N	5:E:473:HOH:O	2.28	0.67
2:F:61:ARG:O	2:F:65:THR:HB	1.95	0.67
2:N:104:PRO:CA	2:N:105:SER:CB	2.69	0.67
1:0:76:SER:O	1:0:108:THR:CG2	2.43	0.67
2:B:97:THR:HG22	2:B:98:SER:O	1.95	0.67
1:E:102:CSD:O	1:E:103:SER:HB3	1.93	0.67



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:N:124:ARG:HD2	2:N:206:GLU:OE1	1.95	0.67
1:G:204:ALA:O	1:G:205:LEU:CB	2.43	0.67
2:H:185:PRO:HD2	2:N:131:PHE:CE2	2.30	0.67
2:L:10:LYS:HE3	2:L:10:LYS:CA	2.24	0.67
1:A:154:ALA:HB3	5:B:410:HOH:O	1.94	0.67
1:I:41:LEU:HB3	1:I:43:GLN:NE2	2.09	0.67
2:L:177:CYS:O	5:L:337:HOH:O	2.11	0.67
1:E:167:GLY:N	1:E:169:GLU:OE1	2.27	0.66
2:F:53:HIS:O	2:F:57:ARG:HG3	1.95	0.66
2:H:58:MET:O	5:H:358:HOH:O	2.12	0.66
1:M:82:LYS:HE2	1:M:155:ASP:OD2	1.93	0.66
2:N:52:ARG:O	2:N:56:GLU:HG3	1.96	0.66
2:P:19:THR:HG22	2:P:20:HIS:N	2.11	0.66
1:K:207:ALA:HB1	2:P:42:SER:CB	2.24	0.66
1:A:137:ILE:CD1	1:A:188:VAL:CG2	2.74	0.66
2:P:97:THR:HG22	2:P:98:SER:O	1.96	0.66
1:A:28:THR:O	5:A:428:HOH:O	2.15	0.65
1:A:31:ASP:O	5:A:477:HOH:O	2.13	0.65
2:P:104:PRO:HA	2:P:105:SER:HB2	1.77	0.65
1:G:76:SER:O	1:G:108:THR:HG21	1.97	0.65
2:D:92:GLU:HG2	2:D:98:SER:HA	1.78	0.65
1:A:61:GLN:NE2	5:A:451:HOH:O	2.20	0.65
1:M:17:LEU:HD23	1:M:21:LEU:HD22	1.78	0.65
2:J:52:ARG:O	2:J:56:GLU:HG3	1.96	0.64
2:J:104:PRO:CB	2:J:105:SER:HB2	2.27	0.64
1:K:198:LEU:HD12	1:M:198:LEU:HD12	1.79	0.64
1:M:205:LEU:C	1:M:205:LEU:HD23	2.16	0.64
1:E:166:GLN:HG3	1:I:193:ALA:CB	2.27	0.64
2:F:124:ARG:HH11	2:F:124:ARG:CG	1.91	0.64
1:I:61:GLN:NE2	5:I:478:HOH:O	1.86	0.64
1:K:116:TRP:CD1	2:L:18:LYS:HG2	2.33	0.64
1:G:14:LEU:HD13	2:H:36:ILE:HG21	1.81	0.63
1:K:112:MET:HE3	5:K:464:HOH:O	1.98	0.63
1:K:207:ALA:CA	2:P:42:SER:CB	2.76	0.63
2:H:10:LYS:CE	5:H:378:HOH:O	2.36	0.63
2:J:22:ALA:O	2:J:23:LYS:HB2	1.97	0.63
1:I:105:THR:HG21	1:I:113:ALA:HB2	1.79	0.63
1:G:4:ASN:OD1	2:H:29:TRP:NE1	2.23	0.63
2:D:22:ALA:O	2:D:23:LYS:HB2	1.96	0.63
1:M:137:ILE:CD1	1:M:188:VAL:CG2	2.77	0.62
1:K:82:LYS:HE2	1:K:155:ASP:OD2	1.99	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:165:PRO:HG3	1:A:191:LEU:HB3	1.80	0.62
1:E:76:SER:O	1:E:108:THR:CG2	2.47	0.62
1:M:137:ILE:HD12	1:M:188:VAL:HG21	1.81	0.62
2:L:10:LYS:HA	2:L:10:LYS:CE	2.30	0.62
2:P:143:ARG:HD2	5:P:360:HOH:O	2.00	0.62
1:A:108:THR:HG22	1:A:109:ILE:HG12	1.80	0.62
2:P:92:GLU:OE1	2:P:98:SER:HA	1.99	0.62
2:B:19:THR:HG22	2:B:20:HIS:O	2.00	0.62
1:M:175:GLN:O	1:M:178:THR:HB	1.98	0.62
1:0:175:GLN:O	1:0:178:THR:HB	2.00	0.62
2:D:78:THR:HG21	2:D:102:SER:HB2	1.81	0.61
1:G:132:THR:O	1:G:136:GLU:HG3	2.00	0.61
2:J:10:LYS:NZ	5:J:386:HOH:O	2.14	0.61
2:B:87:THR:OG1	2:B:90:GLU:HG3	2.00	0.61
2:B:97:THR:HG22	2:B:98:SER:N	2.14	0.61
1:C:105:THR:HG21	1:C:113:ALA:HB2	1.82	0.61
2:L:22:ALA:O	2:L:23:LYS:HB2	1.99	0.61
2:N:22:ALA:O	2:N:23:LYS:HB2	1.99	0.61
1:A:76:SER:O	1:A:108:THR:HG21	2.00	0.61
2:B:1:MET:HE3	2:L:12:GLY:CA	2.30	0.61
2:D:1:MET:CE	2:D:56:GLU:HB3	2.28	0.61
2:L:97:THR:HG22	2:L:98:SER:N	2.16	0.61
2:F:158:TYR:CE2	2:F:160:ASP:HB2	2.36	0.61
1:I:137:ILE:HD12	1:I:188:VAL:CG2	2.30	0.61
2:J:97:THR:CG2	2:J:98:SER:H	2.12	0.61
2:L:104:PRO:CB	2:L:105:SER:HB2	2.30	0.61
2:B:104:PRO:HA	2:B:105:SER:CB	2.30	0.61
2:J:92:GLU:HG3	2:J:97:THR:O	2.01	0.60
2:P:104:PRO:HB2	2:P:105:SER:HB2	1.81	0.60
1:K:76:SER:O	1:K:108:THR:OG1	2.19	0.60
2:D:5:HIS:CG	2:D:56:GLU:HG2	2.36	0.60
2:P:90:GLU:O	2:P:93:ALA:HB3	2.01	0.60
2:P:10:LYS:HA	2:P:10:LYS:HE3	1.84	0.60
1:E:3:ASP:HB2	1:E:6:VAL:HG23	1.82	0.60
1:A:175:GLN:O	1:A:178:THR:HB	2.02	0.60
2:B:104:PRO:HB2	2:B:105:SER:HB2	1.82	0.60
1:C:204:ALA:O	1:C:205:LEU:CB	2.50	0.60
2:J:104:PRO:HA	2:J:105:SER:CB	2.32	0.60
1:K:205:LEU:HD22	1:0:78:PRO:HB3	1.83	0.60
2:B:104:PRO:CA	2:B:105:SER:CB	2.79	0.60
2:B:131:PHE:CE2	2:L:185:PRO:HD2	2.37	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:M:165:PRO:HG3	1:M:191:LEU:HB3	1.83	0.60
1:C:137:ILE:CD1	1:C:188:VAL:CG2	2.80	0.59
1:G:116:TRP:CD1	2:H:18:LYS:HG2	2.37	0.59
1:K:106:ALA:HB2	1:K:157:ARG:HB3	1.83	0.59
1:A:119:GLU:HB3	5:A:437:HOH:O	2.01	0.59
2:B:97:THR:CG2	2:B:98:SER:N	2.64	0.59
1:C:112:MET:HE3	5:C:486:HOH:O	2.02	0.59
1:O:108:THR:HG22	1:O:109:ILE:HG12	1.84	0.59
1:E:108:THR:HG22	1:E:109:ILE:HG12	1.85	0.59
1:M:76:SER:O	1:M:108:THR:HG21	2.03	0.59
1:E:28:THR:O	5:E:453:HOH:O	2.17	0.59
2:J:10:LYS:HD3	5:J:386:HOH:O	2.01	0.59
2:N:163:ALA:O	5:N:345:HOH:O	2.17	0.59
1:K:204:ALA:O	1:K:205:LEU:CB	2.43	0.59
2:P:10:LYS:HA	2:P:10:LYS:CE	2.32	0.59
2:L:10:LYS:NZ	5:L:392:HOH:O	2.36	0.59
2:P:52:ARG:O	2:P:56:GLU:HG3	2.03	0.59
2:L:158:TYR:CE2	2:L:160:ASP:HB2	2.38	0.59
1:E:204:ALA:O	1:E:205:LEU:CB	2.47	0.58
2:F:106:SER:HB3	5:F:382:HOH:O	2.02	0.58
2:B:92:GLU:OE1	2:B:98:SER:HA	2.04	0.58
1:K:137:ILE:CD1	1:K:188:VAL:HG22	2.33	0.58
1:A:82:LYS:HE2	1:A:155:ASP:OD2	2.03	0.58
2:B:88:ALA:O	2:B:92:GLU:HG3	2.03	0.58
1:E:198:LEU:HD12	1:I:198:LEU:HD12	1.84	0.58
1:K:37:MET:HG2	1:K:38:HIS:CE1	2.37	0.58
1:O:41:LEU:HB3	1:O:43:GLN:NE2	2.19	0.58
2:L:78:THR:HG21	2:L:102:SER:HB2	1.84	0.58
1:G:137:ILE:CD1	1:G:188:VAL:HG22	2.34	0.58
2:J:97:THR:HG22	2:J:98:SER:H	1.66	0.58
2:N:97:THR:HG22	2:N:98:SER:N	2.18	0.58
1:O:3:ASP:HB3	1:O:6:VAL:H	1.68	0.57
2:J:158:TYR:CE2	2:J:160:ASP:HB2	2.39	0.57
2:L:97:THR:CG2	2:L:98:SER:N	2.67	0.57
1:M:29:VAL:HG21	2:N:32:LYS:HD3	1.86	0.57
1:E:14:LEU:HD13	2:F:36:ILE:HG21	1.86	0.57
1:G:76:SER:O	1:G:108:THR:CG2	2.52	0.57
2:L:104:PRO:HA	2:L:105:SER:CB	2.34	0.57
1:M:17:LEU:CD2	1:M:21:LEU:CD2	2.82	0.57
1:O:198:LEU:HB3	1:O:199:PRO:HD2	1.86	0.57
1:A:137:ILE:HD11	1:A:188:VAL:CG2	2.35	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:I:137:ILE:HD12	1:I:188:VAL:HG21	1.86	0.57
2:H:106:SER:HB3	5:H:368:HOH:O	2.03	0.57
2:B:75:THR:O	2:B:79:LEU:HB2	2.05	0.57
1:C:14:LEU:HD13	2:D:36:ILE:HG21	1.86	0.56
1:A:154:ALA:N	5:A:412:HOH:O	2.38	0.56
2:D:5:HIS:CD2	2:D:56:GLU:HG2	2.40	0.56
1:I:165:PRO:HG3	1:I:191:LEU:HB3	1.88	0.56
1:C:137:ILE:HD11	1:C:188:VAL:CG2	2.35	0.56
2:D:104:PRO:HB2	2:D:105:SER:HB2	1.88	0.56
1:I:119:GLU:HB3	5:I:408:HOH:O	2.04	0.56
1:C:76:SER:O	1:C:108:THR:OG1	2.22	0.56
2:L:104:PRO:CA	2:L:105:SER:HB2	2.36	0.56
2:D:171:GLU:OE1	5:D:379:HOH:O	2.18	0.56
1:M:137:ILE:HD12	1:M:188:VAL:CG2	2.34	0.56
1:C:106:ALA:HB2	1:C:157:ARG:HB3	1.88	0.56
1:E:167:GLY:CA	1:E:169:GLU:OE1	2.53	0.56
2:P:19:THR:CG2	2:P:20:HIS:N	2.69	0.56
1:A:49:VAL:HG13	1:A:161:LEU:HD12	1.88	0.55
2:B:1:MET:CE	2:L:12:GLY:CA	2.84	0.55
1:M:119:GLU:HB3	5:M:410:HOH:O	2.06	0.55
2:L:10:LYS:NZ	5:L:347:HOH:O	2.39	0.55
2:B:52:ARG:O	2:B:56:GLU:HG3	2.06	0.55
2:D:106:SER:HB3	5:D:391:HOH:O	2.05	0.55
2:L:5:HIS:CG	2:L:56:GLU:HG2	2.42	0.55
1:M:108:THR:HG22	1:M:109:ILE:HG12	1.87	0.55
2:F:92:GLU:HG2	2:F:98:SER:HA	1.88	0.55
2:J:10:LYS:CD	5:J:386:HOH:O	2.55	0.55
1:M:3:ASP:HB3	1:M:6:VAL:H	1.71	0.55
1:A:137:ILE:HD12	1:A:188:VAL:CG2	2.37	0.55
2:H:5:HIS:CG	2:H:56:GLU:HG2	2.42	0.55
1:I:175:GLN:O	1:I:178:THR:HB	2.07	0.55
1:A:45:GLY:O	1:A:49:VAL:HG23	2.07	0.55
2:L:92:GLU:CG	2:L:98:SER:HA	2.34	0.55
2:H:23:LYS:N	5:H:402:HOH:O	2.15	0.55
2:L:104:PRO:CA	2:L:105:SER:CB	2.85	0.55
2:N:92:GLU:HG3	2:N:97:THR:O	2.06	0.55
2:N:158:TYR:CE2	2:N:160:ASP:HB2	2.42	0.55
2:D:97:THR:HG22	2:D:98:SER:H	1.71	0.55
1:C:101:LEU:HB2	5:C:406:HOH:O	2.06	0.55
1:I:37:MET:HE2	1:I:37:MET:CA	2.37	0.54
1:K:207:ALA:N	5:K:428:HOH:O	2.39	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:L:46:TYR:CG	2:L:79:LEU:HD23	2.42	0.54
1:E:104:CSD:C	1:E:105:THR:CG2	2.85	0.54
1:I:3:ASP:OD2	1:I:3:ASP:N	2.25	0.54
2:L:145:LYS:HG3	2:L:183:LEU:HD12	1.88	0.54
1:M:41:LEU:HB3	1:M:43:GLN:NE2	2.23	0.54
2:N:79:LEU:O	2:N:83:LYS:HG3	2.08	0.54
1:0:142:PRO:HD2	1:O:145:ILE:HD12	1.89	0.54
1:A:16:VAL:O	1:A:20:GLU:HG3	2.08	0.54
1:G:137:ILE:HD11	1:G:188:VAL:HG22	1.89	0.54
1:M:102:CSD:O	1:M:123:ARG:HD2	2.08	0.54
1:M:105:THR:CG2	1:M:113:ALA:HB2	2.35	0.54
1:E:166:GLN:HG3	1:I:193:ALA:HB3	1.88	0.54
2:H:113:LYS:HE3	2:H:113:LYS:CA	2.32	0.54
1:A:49:VAL:HG13	1:A:161:LEU:CD1	2.38	0.54
2:H:158:TYR:CE2	2:H:160:ASP:HB2	2.43	0.54
1:M:60:ALA:O	5:M:484:HOH:O	2.18	0.54
1:O:153:THR:HG21	2:P:195:VAL:HG13	1.90	0.54
1:E:165:PRO:HB3	1:E:192:GLU:HA	1.90	0.54
2:J:19:THR:HG22	2:J:20:HIS:N	2.23	0.54
2:H:104:PRO:CA	2:H:105:SER:CB	2.77	0.53
2:N:19:THR:HG22	2:N:20:HIS:N	2.23	0.53
1:O:200:ALA:HB1	1:O:201:PRO:HD2	1.90	0.53
2:P:22:ALA:O	2:P:23:LYS:HB2	2.08	0.53
1:C:3:ASP:OD1	1:C:5:ALA:N	2.42	0.53
1:K:137:ILE:HD11	1:K:188:VAL:HG22	1.90	0.53
1:I:103:SER:O	1:I:103:SER:OG	2.24	0.52
1:C:37:MET:HB3	1:C:38:HIS:CD2	2.43	0.52
1:I:143:GLU:N	2:L:116:GLU:OE2	2.27	0.52
2:J:20:HIS:ND1	5:J:392:HOH:O	2.29	0.52
2:F:78:THR:HG21	2:F:102:SER:HB2	1.91	0.52
1:I:106:ALA:HB2	1:I:157:ARG:HB3	1.91	0.52
1:I:156:THR:HB	5:I:407:HOH:O	2.08	0.52
2:J:19:THR:CG2	2:J:20:HIS:N	2.72	0.52
2:P:53:HIS:CG	2:P:135:HIS:HB2	2.45	0.52
2:B:53:HIS:CG	2:B:135:HIS:HB2	2.45	0.52
2:J:53:HIS:CG	2:J:135:HIS:HB2	2.44	0.52
1:O:137:ILE:CD1	1:O:188:VAL:HG22	2.39	0.52
1:A:137:ILE:CD1	1:A:188:VAL:HG22	2.39	0.52
1:K:3:ASP:OD1	1:K:5:ALA:N	2.43	0.52
2:B:19:THR:HG22	2:B:20:HIS:N	2.24	0.52
2:H:53:HIS:CG	2:H:135:HIS:HB2	2.45	0.52



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:N:104:PRO:HB2	2:N:105:SER:HB2	1.89	0.52
1:C:108:THR:HG23	1:C:109:ILE:HG12	1.92	0.52
2:F:124:ARG:NH1	2:F:124:ARG:CG	2.59	0.52
2:F:97:THR:CG2	2:F:98:SER:H	2.10	0.51
1:C:37:MET:C	1:C:38:HIS:HD2	2.13	0.51
2:J:10:LYS:CE	5:J:386:HOH:O	2.58	0.51
2:H:22:ALA:N	5:H:402:HOH:O	2.44	0.51
1:E:104:CSD:O	1:E:105:THR:HG22	2.10	0.51
1:K:103:SER:HB3	2:L:68:TYR:HE1	1.75	0.51
2:B:10:LYS:HA	2:B:10:LYS:CE	2.40	0.51
2:F:19:THR:CG2	2:F:20:HIS:N	2.74	0.51
2:N:19:THR:HG22	2:N:20:HIS:O	2.10	0.51
2:F:197:VAL:HG11	2:F:202:LEU:HD21	1.92	0.51
1:G:101:LEU:HB2	5:G:403:HOH:O	2.09	0.51
1:I:137:ILE:HD11	1:I:188:VAL:CG2	2.39	0.51
1:K:155:ASP:HB2	2:L:156:TYR:CD2	2.46	0.51
2:D:64:LEU:HD21	2:J:4:MET:CE	2.41	0.51
1:E:104:CSD:C	1:E:105:THR:HG22	2.41	0.51
1:G:106:ALA:HB2	1:G:157:ARG:HB3	1.92	0.51
1:K:2:THR:N	5:K:455:HOH:O	2.43	0.51
2:F:19:THR:HG22	2:F:20:HIS:O	2.10	0.51
2:B:92:GLU:CD	2:B:98:SER:HA	2.31	0.51
1:C:90:THR:HB	1:C:91:PRO:CD	2.41	0.51
1:E:174:ALA:HB1	1:I:203:VAL:HG11	1.92	0.51
1:M:45:GLY:O	1:M:49:VAL:HG23	2.11	0.51
1:E:29:VAL:HG21	2:F:32:LYS:HG3	1.92	0.50
1:E:116:TRP:CD1	2:F:18:LYS:HG2	2.46	0.50
1:A:3:ASP:HB3	1:A:6:VAL:HG23	1.92	0.50
2:L:59:GLU:OE1	5:L:408:HOH:O	2.20	0.50
2:N:19:THR:CG2	2:N:20:HIS:N	2.74	0.50
2:F:5:HIS:CG	2:F:56:GLU:HG2	2.46	0.50
1:I:16:VAL:O	1:I:20:GLU:HG3	2.11	0.50
2:J:10:LYS:HE3	2:J:10:LYS:CA	2.37	0.50
2:J:90:GLU:O	2:J:93:ALA:HB3	2.11	0.50
1:G:155:ASP:H	1:G:157:ARG:HH12	1.59	0.50
2:P:97:THR:CG2	2:P:98:SER:N	2.74	0.50
1:C:37:MET:C	1:C:38:HIS:CD2	2.85	0.50
1:I:37:MET:CA	1:I:37:MET:CE	2.89	0.50
1:I:105:THR:HG22	1:I:117:TYR:CE2	2.47	0.50
1:G:3:ASP:OD1	1:G:3:ASP:C	2.50	0.50
1:M:49:VAL:HG13	1:M:161:LEU:CD1	2.42	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:127:VAL:O	2:H:144:GLY:HA2	2.11	0.50
1:A:137:ILE:HD12	1:A:188:VAL:HG21	1.94	0.50
2:D:97:THR:CG2	2:D:98:SER:N	2.74	0.50
2:H:113:LYS:HA	2:H:113:LYS:CE	2.38	0.50
2:L:63:TYR:C	2:L:63:TYR:CD2	2.84	0.50
2:D:64:LEU:HD21	2:J:4:MET:HE2	1.93	0.50
2:L:104:PRO:HB2	2:L:105:SER:HB2	1.92	0.50
1:K:167:GLY:N	1:K:169:GLU:OE1	2.42	0.49
1:K:167:GLY:CA	1:K:169:GLU:OE1	2.61	0.49
2:L:97:THR:HG22	2:L:98:SER:O	2.11	0.49
1:A:135:LYS:NZ	5:A:494:HOH:O	2.29	0.49
1:A:155:ASP:HB2	2:B:156:TYR:CD2	2.47	0.49
1:C:137:ILE:HD12	1:C:188:VAL:HG21	1.94	0.49
2:B:1:MET:CE	2:L:12:GLY:HA3	2.42	0.49
1:G:99:CYS:HB3	1:G:103:SER:HA	1.93	0.49
2:J:104:PRO:CA	2:J:105:SER:CB	2.86	0.49
2:N:97:THR:CG2	2:N:98:SER:N	2.76	0.49
2:D:63:TYR:C	2:D:63:TYR:CD2	2.85	0.49
1:E:201:PRO:HG3	1:I:178:THR:HG21	1.94	0.49
2:F:53:HIS:CG	2:F:135:HIS:HB2	2.47	0.49
2:D:185:PRO:HD2	2:J:131:PHE:CE2	2.48	0.49
1:I:80:HIS:O	1:I:155:ASP:HA	2.12	0.49
2:J:19:THR:HG22	2:J:20:HIS:O	2.13	0.49
1:O:155:ASP:H	1:O:157:ARG:HH12	1.60	0.49
2:P:97:THR:HG22	2:P:98:SER:N	2.27	0.49
1:E:104:CSD:HA	3:E:301:PO4:O3	2.13	0.49
2:B:19:THR:CG2	2:B:20:HIS:N	2.75	0.48
1:C:37:MET:CE	1:C:37:MET:HA	2.43	0.48
1:A:167:GLY:CA	1:A:169:GLU:OE1	2.61	0.48
2:H:55:ILE:HG23	2:H:71:ARG:HB3	1.95	0.48
1:O:106:ALA:HB2	1:O:157:ARG:HB3	1.93	0.48
1:A:76:SER:O	1:A:108:THR:CG2	2.61	0.48
1:O:137:ILE:CD1	1:O:188:VAL:CG2	2.91	0.48
1:C:104:CSD:C	1:C:105:THR:CG2	2.91	0.48
2:H:5:HIS:ND1	2:H:56:GLU:HG2	2.28	0.48
1:I:205:LEU:C	1:I:205:LEU:HD23	2.34	0.48
1:K:10:ARG:HA	2:L:95:LEU:HD11	1.94	0.48
2:L:160:ASP:OD2	2:L:160:ASP:N	2.47	0.48
1:G:167:GLY:CA	1:G:169:GLU:OE1	2.62	0.48
1:I:29:VAL:HB	1:I:30:PRO:HD3	1.96	0.48
1:I:59:LYS:NZ	1:I:88:GLU:OE2	2.39	0.48



	• • • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:M:3:ASP:HB3	1:M:6:VAL:HG23	1.95	0.48
2:B:10:LYS:HA	2:B:10:LYS:HE3	1.93	0.48
1:C:14:LEU:HD22	1:C:14:LEU:O	2.14	0.48
1:K:14:LEU:HD13	2:L:36:ILE:HG21	1.94	0.47
1:E:137:ILE:CD1	1:E:188:VAL:CG2	2.92	0.47
2:N:127:VAL:HG21	2:N:142:ILE:HD12	1.95	0.47
1:C:154:ALA:CA	5:C:402:HOH:O	2.63	0.47
1:C:206:GLY:HA2	1:C:207:ALA:HA	1.70	0.47
1:E:78:PRO:HG2	1:E:81:HIS:CG	2.49	0.47
2:H:10:LYS:NZ	5:H:385:HOH:O	2.20	0.47
1:M:106:ALA:HB2	1:M:157:ARG:HB3	1.95	0.47
1:G:204:ALA:O	1:G:205:LEU:HB2	2.15	0.47
2:J:10:LYS:HA	2:J:10:LYS:CE	2.41	0.47
2:L:53:HIS:CG	2:L:135:HIS:HB2	2.50	0.47
2:N:78:THR:HG21	2:N:102:SER:HB2	1.95	0.47
2:P:160:ASP:OD2	2:P:160:ASP:N	2.48	0.47
1:G:154:ALA:N	5:G:447:HOH:O	2.47	0.47
2:D:92:GLU:CG	2:D:98:SER:HA	2.42	0.47
1:M:137:ILE:HD11	1:M:188:VAL:CG2	2.44	0.47
2:P:10:LYS:HE3	2:P:10:LYS:CA	2.44	0.47
1:C:155:ASP:HB2	2:D:156:TYR:CD2	2.50	0.47
1:K:90:THR:HB	1:K:91:PRO:CD	2.45	0.47
1:E:106:ALA:HB2	1:E:157:ARG:HB3	1.96	0.46
2:H:145:LYS:HG3	2:H:183:LEU:HD12	1.97	0.46
2:P:64:LEU:HD12	2:P:64:LEU:HA	1.58	0.46
1:C:37:MET:HA	1:C:37:MET:HE2	1.97	0.46
1:I:137:ILE:HD11	1:I:188:VAL:HG23	1.96	0.46
1:O:155:ASP:N	1:O:157:ARG:HH12	2.13	0.46
2:F:116:GLU:OE2	1:M:143:GLU:N	2.39	0.46
1:K:156:THR:OG1	5:K:422:HOH:O	2.19	0.46
2:D:46:TYR:CG	2:D:79:LEU:HD23	2.50	0.46
2:J:113:LYS:HA	2:J:113:LYS:HD3	1.80	0.46
2:D:158:TYR:CE2	2:D:160:ASP:HB2	2.51	0.46
1:M:53:TRP:CE2	1:M:164:ARG:HB2	2.51	0.46
1:C:132:THR:O	1:C:136:GLU:HG3	2.16	0.46
2:D:104:PRO:HA	2:D:105:SER:HB2	1.77	0.46
1:G:14:LEU:CD1	2:H:36:ILE:HG21	2.46	0.46
1:K:3:ASP:OD1	1:K:3:ASP:C	2.54	0.46
1:K:3:ASP:OD1	1:K:4:ASN:N	2.49	0.46
1:0:154:ALA:O	1:O:155:ASP:HB2	2.16	0.46
1:C:204:ALA:O	1:C:205:LEU:HB3	2.15	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:166:GLN:CG	1:I:193:ALA:HB3	2.46	0.46
2:P:54:GLY:HA3	2:P:75:THR:OG1	2.16	0.46
1:A:15:PHE:HB2	2:B:36:ILE:HD11	1.98	0.46
1:I:198:LEU:HB3	1:I:199:PRO:HD2	1.97	0.46
2:J:99:VAL:HA	2:J:100:PRO:HD3	1.83	0.46
1:O:156:THR:OG1	5:O:467:HOH:O	2.21	0.45
2:H:121:LEU:HD12	2:H:121:LEU:HA	1.79	0.45
1:A:164:ARG:HA	1:A:165:PRO:HD3	1.88	0.45
1:E:102:CSD:O	1:E:103:SER:CB	2.64	0.45
2:D:33:MET:SD	2:D:73:PHE:HA	2.56	0.45
2:J:55:ILE:HG13	2:J:75:THR:HB	1.97	0.45
2:D:54:GLY:HA3	2:D:75:THR:OG1	2.17	0.45
1:G:37:MET:HG2	1:G:38:HIS:NE2	2.32	0.45
1:G:40:TRP:HB3	1:G:107:PHE:O	2.17	0.45
2:N:90:GLU:O	2:N:93:ALA:HB3	2.16	0.45
1:O:167:GLY:CA	1:O:169:GLU:OE1	2.64	0.45
1:A:14:LEU:HD22	1:A:18:THR:HG23	1.99	0.45
1:A:48:LEU:CD1	1:A:73:LEU:HD12	2.46	0.45
1:G:204:ALA:O	1:G:205:LEU:HB3	2.17	0.45
2:H:64:LEU:HA	2:H:64:LEU:HD12	1.58	0.45
2:L:87:THR:OG1	2:L:90:GLU:HG3	2.16	0.45
1:O:105:THR:HG21	1:O:113:ALA:HB2	1.98	0.45
1:C:132:THR:OG1	2:D:189:GLU:OE1	2.25	0.45
2:D:127:VAL:HG21	2:D:142:ILE:HD12	1.98	0.45
2:J:55:ILE:O	2:J:58:MET:HG3	2.17	0.45
2:J:97:THR:HG22	2:J:98:SER:O	2.16	0.45
2:P:158:TYR:CE2	2:P:160:ASP:HB2	2.52	0.45
1:E:90:THR:HB	1:E:91:PRO:CD	2.46	0.45
1:C:14:LEU:HD22	1:C:18:THR:HG23	1.99	0.44
1:C:66:GLY:HA3	1:C:84:PHE:O	2.17	0.44
1:I:37:MET:HE3	1:I:37:MET:HB2	1.73	0.44
1:O:137:ILE:HD11	1:O:188:VAL:CG2	2.47	0.44
1:G:77:PHE:HB3	1:G:78:PRO:HD2	1.99	0.44
1:C:49:VAL:HB	1:C:180:ILE:HD13	1.99	0.44
2:F:64:LEU:HD12	2:F:64:LEU:HA	1.64	0.44
2:L:19:THR:HB	5:L:314:HOH:O	2.17	0.44
1:O:80:HIS:O	1:0:155:ASP:HA	2.17	0.44
2:B:12:GLY:HA3	2:L:1:MET:CE	2.48	0.44
2:B:126:HIS:HB2	2:B:205:ALA:HB2	1.99	0.44
1:M:27:GLN:HB2	5:M:462:HOH:O	2.18	0.44
2:D:53:HIS:O	2:D:57:ARG:HG2	2.17	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:M:82:LYS:HD2	2:N:156:TYR:CD1	2.52	0.44
2:N:53:HIS:CG	2:N:135:HIS:HB2	2.52	0.44
2:N:55:ILE:O	2:N:58:MET:HG3	2.16	0.44
1:O:3:ASP:HB2	1:O:6:VAL:HG23	2.00	0.44
2:P:157:PRO:O	2:P:159:PRO:HD3	2.18	0.44
2:B:64:LEU:HD12	2:B:64:LEU:HA	1.55	0.44
2:F:111:PRO:HG2	2:F:169:PHE:CD1	2.53	0.44
1:I:155:ASP:HB2	2:J:156:TYR:CD2	2.53	0.44
1:M:17:LEU:CD2	1:M:21:LEU:HD21	2.47	0.44
2:B:40:LEU:HD12	2:B:40:LEU:HA	1.86	0.44
2:F:127:VAL:HG21	2:F:142:ILE:HD12	1.99	0.44
2:D:87:THR:OG1	2:D:90:GLU:HG3	2.17	0.43
1:I:200:ALA:HB1	1:I:201:PRO:HD2	2.00	0.43
2:J:20:HIS:HB3	5:J:392:HOH:O	2.17	0.43
1:E:132:THR:O	1:E:136:GLU:HG3	2.18	0.43
1:O:205:LEU:HD23	1:O:205:LEU:O	2.17	0.43
2:J:104:PRO:HB2	2:J:105:SER:HB2	1.99	0.43
2:L:111:PRO:HG2	2:L:169:PHE:CD1	2.53	0.43
1:M:29:VAL:HB	1:M:30:PRO:HD3	2.00	0.43
1:G:104:CSD:C	1:G:105:THR:CG2	2.96	0.43
1:I:37:MET:HA	1:I:37:MET:CE	2.45	0.43
1:I:154:ALA:N	5:I:461:HOH:O	2.51	0.43
2:L:110:GLN:HB3	2:L:111:PRO:HD2	2.01	0.43
1:M:49:VAL:HG13	1:M:161:LEU:HD12	2.00	0.43
2:N:47:ASN:OD1	2:N:50:GLU:HG3	2.18	0.43
1:K:11:VAL:HG12	2:L:32:LYS:HG2	2.01	0.43
1:M:105:THR:HG22	1:M:117:TYR:CE2	2.54	0.43
1:C:178:THR:HG22	1:C:179:LEU:HD13	2.01	0.43
2:F:137:ARG:HD2	2:F:137:ARG:HA	1.82	0.43
1:M:77:PHE:HB3	1:M:78:PRO:HD2	2.00	0.43
1:A:41:LEU:HB3	1:A:43:GLN:OE1	2.18	0.43
1:E:154:ALA:CA	5:E:473:HOH:O	2.67	0.43
1:C:198:LEU:HD23	1:C:198:LEU:HA	1.75	0.43
1:A:105:THR:CG2	1:A:117:TYR:CE2	3.01	0.43
1:C:116:TRP:CD1	2:D:18:LYS:HG2	2.54	0.43
2:D:64:LEU:HD12	2:D:64:LEU:HA	1.80	0.43
2:F:92:GLU:CG	2:F:98:SER:HA	2.48	0.43
2:H:104:PRO:HB2	2:H:105:SER:HB2	1.99	0.43
1:A:48:LEU:HD12	1:A:73:LEU:HD12	2.00	0.43
1:I:120:LEU:HB3	2:J:13:PHE:CE1	2.54	0.43
1:C:49:VAL:HG22	1:C:161:LEU:CD1	2.49	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:137:ILE:HD12	1:E:188:VAL:HG21	2.01	0.42
1:G:103:SER:HB2	1:G:118:LYS:HG3	2.00	0.42
2:J:127:VAL:HG21	2:J:142:ILE:HD12	1.99	0.42
2:J:160:ASP:OD2	2:J:160:ASP:N	2.52	0.42
1:K:101:LEU:HB2	5:K:404:HOH:O	2.18	0.42
1:O:137:ILE:HG22	2:P:18:LYS:HB2	2.01	0.42
1:M:17:LEU:O	1:M:21:LEU:HD22	2.18	0.42
2:P:19:THR:HG22	2:P:20:HIS:O	2.19	0.42
2:D:10:LYS:HE3	5:J:381:HOH:O	2.19	0.42
1:G:105:THR:CG2	1:G:113:ALA:HB2	2.44	0.42
2:L:19:THR:CG2	2:L:20:HIS:N	2.83	0.42
1:C:137:ILE:CD1	1:C:188:VAL:HG22	2.48	0.42
1:O:154:ALA:N	5:O:412:HOH:O	2.51	0.42
1:O:165:PRO:HB3	1:O:192:GLU:HA	2.01	0.42
2:P:78:THR:HG21	2:P:102:SER:HB2	2.01	0.42
2:N:40:LEU:HD12	2:N:40:LEU:HA	1.93	0.42
1:O:185:LEU:HD12	1:O:185:LEU:HA	1.88	0.42
1:G:10:ARG:HA	2:H:95:LEU:CD1	2.50	0.42
2:J:165:GLY:HA2	2:J:167:TYR:CZ	2.55	0.42
1:K:48:LEU:HD11	1:K:70:SER:HA	2.01	0.42
1:0:122:TYR:0	1:O:126:ILE:HG22	2.18	0.42
1:A:170:ASP:OD1	1:A:170:ASP:N	2.49	0.42
1:G:17:LEU:HD23	1:G:17:LEU:HA	1.83	0.42
1:K:193:ALA:HB1	1:K:194:PRO:HA	2.01	0.42
2:L:110:GLN:HB3	2:L:111:PRO:CD	2.50	0.42
1:O:137:ILE:HD11	1:O:188:VAL:HG22	2.02	0.42
1:C:183:ASP:OD1	2:D:18:LYS:HE2	2.19	0.42
1:G:49:VAL:HG22	1:G:161:LEU:HD13	2.01	0.42
2:H:13:PHE:CD1	2:N:60:PRO:HG2	2.55	0.42
2:J:64:LEU:HA	2:J:64:LEU:HD12	1.67	0.42
1:M:156:THR:HB	5:M:404:HOH:O	2.20	0.42
2:N:103:LEU:N	2:N:103:LEU:HD12	2.35	0.42
1:O:155:ASP:HB2	2:P:156:TYR:CD2	2.55	0.42
1:C:17:LEU:HD23	1:C:17:LEU:HA	1.88	0.42
1:C:137:ILE:CD1	1:C:188:VAL:HG21	2.50	0.42
1:C:169:GLU:H	1:C:169:GLU:HG2	1.47	0.42
2:D:113:LYS:HD3	2:D:113:LYS:HA	1.81	0.42
2:D:127:VAL:O	2:D:144:GLY:HA2	2.19	0.42
1:E:48:LEU:HD13	1:E:75:PHE:HE2	1.85	0.42
1:E:155:ASP:N	$1:\overline{E:157:ARG:HH12}$	2.18	0.42
2:J:54:GLY:HA3	2:J:75:THR:OG1	2.20	0.42



	A	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:N:64:LEU:HD12	2:N:64:LEU:HA	1.80	0.42
1:A:155:ASP:N	1:A:157:ARG:HH12	2.17	0.41
1:E:10:ARG:HB3	2:F:73:PHE:CZ	2.55	0.41
1:G:137:ILE:HD12	1:G:188:VAL:HG22	2.01	0.41
1:I:102:CSD:O	1:I:123:ARG:HD2	2.19	0.41
1:A:102:CSD:O	1:A:103:SER:HB3	2.19	0.41
2:D:145:LYS:HA	2:D:145:LYS:HD3	1.77	0.41
2:H:19:THR:CG2	2:H:20:HIS:N	2.82	0.41
1:O:156:THR:HB	5:O:410:HOH:O	2.20	0.41
1:O:205:LEU:C	1:O:205:LEU:CD2	2.78	0.41
2:B:99:VAL:HA	2:B:100:PRO:HD3	1.86	0.41
2:B:158:TYR:CE2	2:B:160:ASP:HB2	2.56	0.41
1:C:80:HIS:O	1:C:155:ASP:HA	2.20	0.41
2:H:137:ARG:HA	2:H:137:ARG:HD2	1.93	0.41
1:M:76:SER:O	1:M:108:THR:CG2	2.67	0.41
1:0:17:LEU:O	1:O:21:LEU:HD22	2.20	0.41
2:B:160:ASP:OD2	2:B:160:ASP:N	2.53	0.41
1:G:104:CSD:C	1:G:105:THR:HG22	2.51	0.41
1:K:77:PHE:HB3	1:K:78:PRO:HD2	2.02	0.41
1:K:137:ILE:CD1	1:K:188:VAL:CG2	2.98	0.41
1:K:185:LEU:HD12	1:K:185:LEU:HA	1.86	0.41
1:M:85:VAL:HG12	1:M:87:LEU:HD13	2.02	0.41
1:A:80:HIS:O	1:A:155:ASP:HA	2.20	0.41
1:K:165:PRO:HB3	1:K:192:GLU:HA	2.03	0.41
2:D:121:LEU:HD12	2:D:121:LEU:HA	1.82	0.41
1:C:137:ILE:HD12	1:C:188:VAL:CG2	2.51	0.41
1:G:37:MET:C	1:G:38:HIS:CD2	2.94	0.41
2:L:5:HIS:ND1	2:L:56:GLU:HG2	2.36	0.41
1:M:64:SER:HB3	5:M:484:HOH:O	2.21	0.41
1:0:10:ARG:HB3	2:P:73:PHE:CZ	2.56	0.41
2:P:55:ILE:O	2:P:58:MET:HG3	2.20	0.41
2:P:179:LYS:HD3	2:P:181:LYS:HE3	2.03	0.41
1:A:198:LEU:HB3	1:A:199:PRO:HD2	2.02	0.41
1:C:165:PRO:HB3	1:C:192:GLU:HA	2.03	0.41
2:F:121:LEU:HD12	2:F:121:LEU:HA	1.91	0.41
1:M:3:ASP:CB	1:M:6:VAL:HG23	2.51	0.41
2:F:106:SER:OG	2:F:107:PRO:HD2	2.21	0.41
2:J:92:GLU:O	2:J:95:LEU:O	2.39	0.41
2:L:137:ARG:HD2	2:L:137:ARG:HA	1.90	0.41
1:M:90:THR:HB	1:M:91:PRO:CD	2.51	0.41
1:M:180:ILE:N	1:M:180:ILE:HD12	2.36	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:N:45:ILE:O	2:N:83:LYS:HD2	2.21	0.41
1:O:66:GLY:HA3	1:O:84:PHE:O	2.21	0.41
2:H:19:THR:HB	5:H:326:HOH:O	2.21	0.41
2:J:66:ALA:HB1	2:J:70:GLU:HB3	2.02	0.41
1:M:198:LEU:HD23	1:M:198:LEU:HA	1.81	0.41
2:P:7:LEU:O	2:P:10:LYS:HB2	2.20	0.41
2:D:97:THR:CG2	2:D:98:SER:H	2.33	0.40
1:C:105:THR:HG22	1:C:117:TYR:CE2	2.56	0.40
2:F:27:GLU:HA	5:F:400:HOH:O	2.21	0.40
1:G:90:THR:HB	1:G:91:PRO:CD	2.51	0.40
1:I:205:LEU:HD23	1:I:206:GLY:N	2.37	0.40
1:M:108:THR:CG2	1:M:109:ILE:HG12	2.50	0.40
1:A:55:ASP:OD1	1:A:55:ASP:C	2.60	0.40
1:A:79:LYS:HE2	5:B:407:HOH:O	2.22	0.40
1:A:185:LEU:HD12	1:A:185:LEU:HA	1.88	0.40
2:B:55:ILE:HG23	2:B:71:ARG:HB3	2.04	0.40
1:E:119:GLU:HB3	5:E:407:HOH:O	2.21	0.40
2:H:22:ALA:O	2:H:23:LYS:HB2	2.22	0.40
1:M:155:ASP:H	1:M:157:ARG:HH12	1.68	0.40
1:C:10:ARG:HB3	2:D:73:PHE:CZ	2.56	0.40
2:P:113:LYS:HA	2:P:113:LYS:HD3	1.84	0.40
2:F:63:TYR:CD2	2:F:63:TYR:C	2.94	0.40
2:F:183:LEU:HD12	2:F:183:LEU:HA	1.83	0.40
1:G:155:ASP:HB2	2:H:156:TYR:CD2	2.56	0.40
1:G:155:ASP:N	1:G:157:ARG:HH12	2.18	0.40
1:I:90:THR:HB	1:I:91:PRO:CD	2.52	0.40
1:I:164:ARG:HA	1:I:165:PRO:HD3	1.88	0.40
2:J:174:TYR:HE2	2:J:199:GLN:HG3	1.86	0.40
1:O:43:GLN:N	1:0:43:GLN:NE2	2.46	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:490:HOH:O	5:O:511:HOH:O[2_555]	1.77	0.43
5:F:376:HOH:O	5:P:374:HOH:O[1_565]	2.12	0.08



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	202/209~(97%)	192 (95%)	8 (4%)	2(1%)	15 21
1	С	202/209~(97%)	195 (96%)	6 (3%)	1 (0%)	29 39
1	Е	202/209~(97%)	195 (96%)	4 (2%)	3~(2%)	10 12
1	G	202/209~(97%)	193 (96%)	6 (3%)	3~(2%)	10 12
1	Ι	202/209~(97%)	196 (97%)	4 (2%)	2(1%)	15 21
1	К	202/209~(97%)	194 (96%)	5 (2%)	3~(2%)	10 12
1	М	202/209~(97%)	194 (96%)	7 (4%)	1 (0%)	29 39
1	Ο	202/209~(97%)	194 (96%)	6 (3%)	2(1%)	15 21
2	В	204/206~(99%)	196 (96%)	6 (3%)	2(1%)	15 21
2	D	204/206~(99%)	196 (96%)	4 (2%)	4(2%)	7 8
2	F	204/206~(99%)	194 (95%)	6 (3%)	4(2%)	7 8
2	Н	204/206~(99%)	194 (95%)	6 (3%)	4(2%)	7 8
2	J	204/206~(99%)	190 (93%)	11 (5%)	3~(2%)	10 12
2	L	204/206~(99%)	195~(96%)	6 (3%)	3~(2%)	10 12
2	N	204/206~(99%)	192 (94%)	7 (3%)	5 (2%)	5 5
2	Р	204/206~(99%)	191 (94%)	11 (5%)	2(1%)	15 21
All	All	3248/3320 (98%)	3101 (96%)	103 (3%)	44 (1%)	11 14

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	103	SER
1	А	154	ALA
2	В	106	SER
1	С	154	ALA
2	D	105	SER
1	Е	103	SER



Mol	Chain	Res	
1	E	154	
1	E	205	LEU
2	F	105	SEB
2	F	106	SER
1	G	100	SER
1	G	154	ALA
2	н Н	104	SER
2	H	106	SER
1	I	154	
1	K	154	ALA
1	K	205	LEU
$\frac{1}{2}$	IX L	$\frac{205}{105}$	SEB
$\frac{2}{2}$	L	100	SER
1	M	154	
$\frac{1}{2}$	N	104	SER
1	0	154	
2	P	101	SER
2	B	105	SER
2	J	105	SER
1	K K	206	GLY
1	0	103	SER
2	D	8	GLY
2	D	106	SER
1	G	205	LEU
2	H	96	GLY
2	D	21	ASN
2	J	106	SER
2	N	8	GLY
2	F	23	LYS
2	Н	23	LYS
1	I	103	SER
2	J	23	LYS
2	N	23	LYS
2	Р	106	SER
2	L	8	GLY
2	F	8	GLY
2	N	106	SER
2	N	185	PRO

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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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	172/175~(98%)	151 (88%)	21 (12%)	5 5
1	С	172/175~(98%)	149~(87%)	23~(13%)	4 4
1	Ε	172/175~(98%)	152 (88%)	20 (12%)	5 6
1	G	172/175~(98%)	155~(90%)	17 (10%)	8 10
1	Ι	172/175~(98%)	152 (88%)	20 (12%)	5 6
1	Κ	172/175~(98%)	153 (89%)	19 (11%)	6 7
1	М	172/175~(98%)	156 (91%)	16 (9%)	9 11
1	Ο	172/175~(98%)	149~(87%)	23~(13%)	4 4
2	В	164/164~(100%)	152~(93%)	12~(7%)	14 20
2	D	164/164~(100%)	149 (91%)	15~(9%)	9 12
2	F	164/164~(100%)	151 (92%)	13~(8%)	12 17
2	Η	164/164~(100%)	152~(93%)	12~(7%)	14 20
2	J	164/164~(100%)	148 (90%)	16 (10%)	8 10
2	L	164/164~(100%)	149 (91%)	15~(9%)	9 12
2	Ν	164/164~(100%)	153~(93%)	11 (7%)	16 23
2	Р	164/164~(100%)	147 (90%)	17 (10%)	7 9
All	All	2688/2712 (99%)	2418 (90%)	270 (10%)	7 10

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	14	LEU
1	А	17	LEU
1	А	21	LEU
1	А	48	LEU
1	А	65	GLU
1	А	76	SER
1	А	79	LYS
1	А	87	LEU



Mol	Chain	Res	Type
1	А	101	LEU
1	А	108	THR
1	А	120	LEU
1	А	134	LEU
1	А	137	ILE
1	А	155	ASP
1	А	166	GLN
1	А	169	GLU
1	А	178	THR
1	А	179	LEU
1	А	185	LEU
1	А	191	LEU
1	А	205	LEU
2	В	10	LYS
2	В	18	LYS
2	В	34	ASN
2	В	40	LEU
2	В	42	SER
2	В	65	THR
2	В	67	SER
2	В	79	LEU
2	В	105	SER
2	В	121	LEU
2	В	160	ASP
2	В	183	LEU
1	С	3	ASP
1	С	14	LEU
1	С	19	LYS
1	С	21	LEU
1	С	27	GLN
1	С	37	MET
1	C	48	LEU
1	С	65	GLU
1	С	79	LYS
1	С	87	LEU
1	C	101	LEU
1	С	105	THR
1	С	108	THR
1	C	120	LEU
1	С	134	LEU
1	С	137	ILE
1	С	169	GLU



Mol	Chain	Res	Type
1	С	178	THR
1	С	179	LEU
1	С	185	LEU
1	С	188	VAL
1	С	191	LEU
1	С	203	VAL
2	D	1	MET
2	D	18	LYS
2	D	19	THR
2	D	34	ASN
2	D	40	LEU
2	D	65	THR
2	D	79	LEU
2	D	99	VAL
2	D	105	SER
2	D	113	LYS
2	D	121	LEU
2	D	160	ASP
2	D	166	GLU
2	D	183	LEU
2	D	186	ASP
1	Е	12	ASP
1	Е	14	LEU
1	Е	21	LEU
1	Е	37	MET
1	Е	48	LEU
1	Е	79	LYS
1	Е	87	LEU
1	Е	101	LEU
1	Е	105	THR
1	Е	108	THR
1	E	120	LEU
1	Е	134	LEU
1	E	137	ILE
1	E	166	GLN
1	E	169	GLU
1	Е	178	THR
1	E	179	LEU
1	E	185	LEU
1	E	191	LEU
1	Е	205	LEU
2	F	10	LYS



Mol	Chain	Res	Type		
2	F	18	LYS		
2	F	34	ASN		
2	F	40	LEU		
2	F	65	THR		
2	F	67	SER		
2	F	79	LEU		
2	F	105	SER		
2	F	121	LEU		
2	F	124	ARG		
2	F	150	VAL		
2	F	160	ASP		
2	F	183	LEU		
1	G	3	ASP		
1	G	12	ASP		
1	G	14	LEU		
1	G	21	LEU		
1	G	48	LEU		
1	G	87	LEU		
1	G	101	LEU		
1	G	105	THR		
1	G	108	THR		
1	G	120	LEU		
1	G	134	LEU		
1	G	166	GLN		
1	G	179	LEU		
1	G	185	LEU		
1	G	188	VAL		
1	G	191	LEU		
1	G	203	VAL		
2	H	10	LYS		
2	Н	18	LYS		
2	Н	19	THR		
2	Н	32	LYS		
2	Η	34	ASN		
2	Н	40	LEU		
2	H	79	LEU		
2	Н	95	LEU		
2	Н	105	SER		
2	Н	113	LYS		
2	Η	160	ASP		
2	Н	183	LEU		
1	Ι	2	THR		



Mol	Chain	Res	Type
1	Ι	3	ASP
1	Ι	14	LEU
1	Ι	17	LEU
1	Ι	21	LEU
1	Ι	27	GLN
1	Ι	43	GLN
1	Ι	48	LEU
1	Ι	87	LEU
1	Ι	101	LEU
1	Ι	103	SER
1	Ι	120	LEU
1	Ι	134	LEU
1	Ι	155	ASP
1	Ι	169	GLU
1	Ι	178	THR
1	Ι	179	LEU
1	Ι	185	LEU
1	Ι	191	LEU
1	Ι	205	LEU
2	J	4	MET
2	J	10	LYS
2	J	32	LYS
2	J	40	LEU
2	J	65	THR
2	J	79	LEU
2	J	92	GLU
2	J	99	VAL
2	J	105	SER
2	J	113	LYS
2	J	124	ARG
2	J	150	VAL
2	J	160	ASP
2	J	181	LYS
2	J	183	LEU
2	J	206	GLU
1	K	3	ASP
1	K	14	LEU
1	K	21	LEU
1	K	37	MET
1	K	48	LEU
1	K	61	GLN
1	K	87	LEU



Mol	Chain	Res	Type	
1	K	101	LEU	
1	K	108	THR	
1	K	120	LEU	
1	K	134	LEU	
1	K	137	ILE	
1	K	178	THR	
1	K	179	LEU	
1	K	185	LEU	
1	K	188	VAL	
1	K	191	LEU	
1	K	203	VAL	
1	K	205	LEU	
2	L	10	LYS	
2	L	18	LYS	
2	L	19	THR	
2	L	32	LYS	
2	L	34	ASN	
2	L	40	LEU	
2	L	67	SER	
2	L	79	LEU	
2	L	99	VAL	
2	L	105	SER	
2	L	113	LYS	
2	L	121	LEU	
2	L	160	ASP	
2	L	166	GLU	
2	L	183	LEU	
1	М	14	LEU	
1	М	21	LEU	
1	М	43	GLN	
1	М	48	LEU	
1	М	87	LEU	
1	М	101	LEU	
1	М	105	THR	
1	М	108	THR	
1	М	120	LEU	
1	М	134	LEU	
1	М	169	GLU	
1	М	178	THR	
1	М	179	LEU	
1	М	185	LEU	
1	М	191	LEU	



Mol	Chain	Res	Type		
1	М	205	LEU		
2	N	10	LYS		
2	N	40	LEU		
2	N	65	THR		
2	N	67	SER		
2	N	79	LEU		
2	Ν	92	GLU		
2	N	98	SER		
2	N	105	SER		
2	N	160	ASP		
2	N	181	LYS		
2	N	183	LEU		
1	0	3	ASP		
1	0	14	LEU		
1	0	17	LEU		
1	0	21	LEU		
1	0	43	GLN		
1	0	48	LEU		
1	0	87	LEU		
1	0	101	LEU		
1	0	103	SER		
1	0	108	THR		
1	0	119	GLU		
1	0	120	LEU		
1	0	134	LEU		
1	0	137	ILE		
1	0	143	GLU		
1	0	155	ASP		
1	0	169	GLU		
1	0	178	THR		
1	0	179	LEU		
1	Ο	185	LEU		
1	Ο	188	VAL		
1	Ο	191	LEU		
1	Ο	205	LEU		
2	P	10	LYS		
2	Р	18	LYS		
2	Р	34	ASN		
2	P	40	LEU		
2	Р	65	THR		
2	Р	67	SER		
2	Р	79	LEU		



Mol	Chain	Res	Type
2	Р	92	GLU
2	Р	99	VAL
2	Р	105	SER
2	Р	113	LYS
2	Р	121	LEU
2	Р	124	ARG
2	Р	150	VAL
2	Р	160	ASP
2	Р	183	LEU
2	Р	206	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	38	HIS
2	D	5	HIS
1	G	38	HIS
1	Ι	43	GLN
1	М	38	HIS
1	М	43	GLN
1	0	38	HIS
1	0	43	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues 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	B	ond leng	gths	Bond angles			
IVIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
1	CSD	А	102	1,4	3,7,8	1.43	0	1,8,10	3.61	1 (100%)	
1	CSD	Ι	102	1,4	3,7,8	1.45	0	1,8,10	4.05	1 (100%)	
1	CSD	М	104	1,4	3,7,8	1.61	1 (33%)	1,8,10	1.29	0	
1	CSD	Е	104	1,4	3,7,8	1.51	1 (33%)	1,8,10	1.21	0	
1	CSD	G	104	1,4	3,7,8	1.55	0	1,8,10	0.93	0	
1	CSD	М	102	1,4	3,7,8	1.38	0	1,8,10	4.65	1 (100%)	
1	CSD	Ο	104	1,4	3,7,8	1.61	1 (33%)	1,8,10	1.57	0	
1	CSD	А	104	1,4	3,7,8	1.52	1 (33%)	1,8,10	1.94	0	
1	CSD	K	102	1,4	3,7,8	1.42	1 (33%)	1,8,10	4.64	1 (100%)	
1	CSD	С	104	1,4	3,7,8	1.68	1 (33%)	1,8,10	1.08	0	
1	CSD	G	102	1,4	3,7,8	1.46	1 (33%)	1,8,10	4.26	1 (100%)	
1	CSD	С	102	1,4	3,7,8	1.52	0	1,8,10	5.00	1 (100%)	
1	CSD	К	104	1,4	3,7,8	1.69	1 (33%)	1,8,10	1.48	0	
1	CSD	Ο	102	1,4	3,7,8	1.38	0	1,8,10	4.61	1 (100%)	
1	CSD	Ι	104	1,4	3,7,8	1.52	0	1,8,10	1.56	0	
1	CSD	Е	102	1,4	3,7,8	1.45	1 (33%)	1,8,10	4.93	1 (100%)	

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
1	CSD	А	102	1,4	-	0/2/6/8	-
1	CSD	Ι	102	1,4	-	0/2/6/8	-
1	CSD	М	104	1,4	-	0/2/6/8	-
1	CSD	Е	104	1,4	-	0/2/6/8	-
1	CSD	G	104	1,4	-	0/2/6/8	-
1	CSD	М	102	1,4	-	0/2/6/8	-
1	CSD	0	104	1,4	-	0/2/6/8	-
1	CSD	А	104	1,4	-	0/2/6/8	-
1	CSD	K	102	1,4	-	0/2/6/8	-
1	CSD	С	104	1,4	-	0/2/6/8	-
1	CSD	G	102	1,4	-	0/2/6/8	-
1	CSD	С	102	1,4	-	0/2/6/8	-
1	CSD	K	104	1,4	-	0/2/6/8	-
1	CSD	0	102	1,4	-	0/2/6/8	-
1	CSD	Ι	104	1,4	-	0/2/6/8	-
1	CSD	Е	102	1,4	-	0/2/6/8	-



Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
1	Κ	104	CSD	CB-SG	-2.24	1.66	1.79
1	С	104	CSD	CB-SG	-2.21	1.66	1.79
1	Е	104	CSD	CB-SG	-2.08	1.67	1.79
1	G	102	CSD	CB-SG	-2.08	1.67	1.79
1	М	104	CSD	CB-SG	-2.05	1.67	1.79
1	Κ	102	CSD	CB-SG	-2.05	1.67	1.79
1	0	104	CSD	CB-SG	-2.04	1.67	1.79
1	А	104	CSD	CB-SG	-2.03	1.67	1.79
1	Е	102	CSD	CB-SG	-2.03	1.67	1.79

All (9) bond length outliers are listed below:

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	102	CSD	OD1-SG-CB	5.00	115.05	105.54
1	Е	102	CSD	OD1-SG-CB	4.93	114.93	105.54
1	М	102	CSD	OD1-SG-CB	4.65	114.39	105.54
1	Κ	102	CSD	OD1-SG-CB	4.64	114.36	105.54
1	0	102	CSD	OD1-SG-CB	4.61	114.32	105.54
1	G	102	CSD	OD1-SG-CB	4.26	113.65	105.54
1	Ι	102	CSD	OD1-SG-CB	4.05	113.24	105.54
1	А	102	CSD	OD1-SG-CB	3.61	112.41	105.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	102	CSD	1	0
1	Ι	102	CSD	1	0
1	Е	104	CSD	4	0
1	G	104	CSD	2	0
1	М	102	CSD	1	0
1	С	104	CSD	2	0
1	G	102	CSD	1	0
1	Е	102	CSD	2	0



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	Dec	Tink	B	ond leng	gths	E	Bond ang	gles
	туре	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	PO4	K	301	-	4,4,4	0.83	0	$6,\!6,\!6$	0.46	0
3	PO4	Ι	301	-	4,4,4	0.87	0	$6,\!6,\!6$	0.53	0
3	PO4	G	301	-	4,4,4	0.78	0	6,6,6	1.06	0
3	PO4	М	301	-	4,4,4	0.92	0	6,6,6	0.45	0
3	PO4	С	301	-	4,4,4	0.81	0	6,6,6	0.48	0
3	PO4	А	301	-	4,4,4	0.90	0	6,6,6	0.46	0
3	PO4	Е	301	-	4,4,4	0.71	0	6,6,6	0.93	0
3	PO4	0	301	-	4,4,4	0.80	0	6,6,6	0.54	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	301	PO4	1	0
3	Е	301	PO4	1	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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	204/209~(97%)	0.07	1 (0%) 91 91	32, 45, 70, 131	0
1	С	204/209~(97%)	0.06	1 (0%) 91 91	31, 45, 66, 87	1 (0%)
1	Ε	204/209~(97%)	0.10	1 (0%) 91 91	32, 45, 69, 90	1 (0%)
1	G	204/209~(97%)	0.06	0 100 100	33, 45, 69, 91	1 (0%)
1	Ι	204/209~(97%)	0.06	0 100 100	33, 44, 68, 102	0
1	Κ	204/209~(97%)	0.07	1 (0%) 91 91	33, 45, 68, 110	1 (0%)
1	М	204/209~(97%)	0.07	1 (0%) 91 91	33, 45, 69, 124	1 (0%)
1	Ο	204/209~(97%)	0.09	1 (0%) 91 91	32, 45, 70, 120	0
2	В	206/206~(100%)	0.10	1 (0%) 91 91	31, 44, 77, 100	0
2	D	206/206~(100%)	0.12	0 100 100	30, 43, 75, 98	0
2	F	206/206~(100%)	0.11	1 (0%) 91 91	30, 43, 74, 96	0
2	Η	206/206~(100%)	0.07	0 100 100	33, 43, 77, 96	0
2	J	206/206~(100%)	0.08	1 (0%) 91 91	31, 44, 76, 100	0
2	L	206/206~(100%)	0.04	1 (0%) 91 91	31, 44, 75, 96	0
2	Ν	206/206~(100%)	0.09	1 (0%) 91 91	30, 45, 79, 102	0
2	Р	206/206~(100%)	0.10	1 (0%) 91 91	31, 44, 76, 102	0
All	All	3280/3320~(98%)	0.08	12 (0%) 92 93	30, 44, 75, 131	5 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	207	ALA	5.9
1	М	207	ALA	5.9
1	0	207	ALA	4.4
1	Е	207	ALA	3.0
1	Κ	207	ALA	3.0



Mol	Chain	Res	Type	RSRZ
2	Р	116	GLU	2.7
2	В	167	TYR	2.4
2	F	22	ALA	2.4
2	Ν	95	LEU	2.3
2	J	95	LEU	2.2
2	L	22	ALA	2.2
1	С	207	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CSD	С	102	8/9	0.92	0.19	40,55,64,66	8
1	CSD	E	102	8/9	0.93	0.19	34,49,57,60	8
1	CSD	А	102	8/9	0.94	0.13	39,54,61,64	8
1	CSD	0	102	8/9	0.94	0.14	47,51,61,70	8
1	CSD	М	102	8/9	0.95	0.14	41,49,63,63	8
1	CSD	G	102	8/9	0.95	0.20	37,52,61,66	8
1	CSD	Ι	104	8/9	0.96	0.13	57,60,75,77	8
1	CSD	K	102	8/9	0.96	0.19	34,47,59,60	8
1	CSD	А	104	8/9	0.96	0.13	42,50,72,76	8
1	CSD	Ι	102	8/9	0.96	0.14	50,62,69,69	0
1	CSD	М	104	8/9	0.97	0.12	46,49,73,77	8
1	CSD	0	104	8/9	0.97	0.14	52,55,76,78	8
1	CSD	С	104	8/9	0.98	0.13	51,53,66,69	8
1	CSD	K	104	8/9	0.98	0.13	52,59,71,71	8
1	CSD	G	104	8/9	0.98	0.13	56,58,64,64	8
1	CSD	E	104	8/9	0.99	0.13	42,56,66,67	8

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,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
4	FE	М	302	1/1	0.90	0.10	66,66,66,66	1
4	FE	Ι	302	1/1	0.94	0.11	74,74,74,74	1
4	FE	Е	302	1/1	0.95	0.09	70,70,70,70	1
4	FE	G	302	1/1	0.96	0.10	60,60,60,60	1
4	FE	0	302	1/1	0.96	0.12	68,68,68,68	1
4	FE	С	302	1/1	0.97	0.09	$65,\!65,\!65,\!65$	1
3	PO4	K	301	5/5	0.98	0.12	70,78,85,86	0
4	FE	А	302	1/1	0.98	0.12	$65,\!65,\!65,\!65$	1
4	FE	K	302	1/1	0.98	0.11	$59,\!59,\!59,\!59$	1
3	PO4	А	301	5/5	0.98	0.14	54,67,74,76	0
3	PO4	С	301	5/5	0.98	0.13	68,69,81,82	0
3	PO4	М	301	5/5	0.99	0.15	55,68,72,76	0
3	PO4	0	301	5/5	0.99	0.17	54,63,67,71	0
3	PO4	G	301	5/5	0.99	0.14	64,70,76,81	0
3	PO4	Ι	301	5/5	0.99	0.15	55,64,67,71	0
3	PO4	Е	301	5/5	0.99	0.12	69,76,79,85	0

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.

6.5 Other polymers (i)

There are no such residues in this entry.

