

# Full wwPDB X-ray Structure Validation Report (i)

#### Apr 21, 2024 – 02:28 am BST

PDB ID	:	2C2L
Title	:	Crystal structure of the CHIP U-box E3 ubiquitin ligase
Authors	:	Zhang, M.; Roe, S.M.; Pearl, L.H.
Deposited on	:	2005-09-29
Resolution	:	3.30  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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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.



Motrie	Whole archive	Similar resolution
WIEUTIC	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
R <sub>free</sub>	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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				
			4%				
1	А	281	44%	49%	7%		
	-		2%				
1	В	281	46%	44%	9% •		
	~		3%				
1	С	281	44%	49%	7%		
	-		2%				
1	D	281	47%	43%	9% •		
_	-		11%				
2	E	9	33%	44%	22%		



Mol	Chain	Length	Quality of chain				
			22%				
2	F	9	44%	33%	22%		
2	G	9	44%	33%	22%		
			33%				
2	Н	9	33%	44%	22%		

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	А	1307	-	-	Х	-
4	NI	В	1307	-	-	-	Х
4	NI	В	1308	-	-	-	Х
4	NI	В	1309	-	-	-	Х



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9521 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called CARBOXY TERMINUS OF HSP70-INTERACTING PRO-TEIN.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	291	Total	С	Ν	0	S	0	0	0
	A	201	2294	1424	417	439	14	0	0	0
1	В	281	Total	С	Ν	Ο	S	0	0	0
	D	201	2294	1424	417	439	14	0		0
1	C	0.01	Total	С	Ν	0	S	0	0	0
	C	201	2294	1424	417	439	14	0	0	0
1	D	991	Total	С	Ν	0	S	0	0	0
	D	201	2294	1424	417	439	14	U	U	0

• Molecule 2 is a protein called HSP90.

Mol	Chain	Residues		At	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
2	F	0	Total	С	Ν	Ο	S	0	0	0
	Ľ	9	74	41	12	20	1	0	0	0
2	F	0	Total	С	Ν	Ο	S	0	0	0
	I.	9	74	41	12	20	1	0		0
0	С	0	Total	С	Ν	Ο	S	0	0	0
	G	я 9	74	41	12	20	1	0	0	0
0	<u>о п</u>	0	Total	С	Ν	Ο	S	0	0	0
	п	9	74	41	12	20	1	0	0	0

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	4	Total Ni 4 4	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	4	Total O 4 4	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	3	Total O 3 3	0	0
5	D	2	Total O 2 2	0	0
5	G	1	Total O 1 1	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: CARBOXY TERMINUS OF HSP70-INTERACTING PROTEIN









44%

22%



 $\bullet$  Molecule 2: HSP90

33%

33%

Chain H:





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	76.04Å 204.41Å 144.71Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.75^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	40.00 - 3.30	Depositor
Resolution (A)	30.05 - 3.31	EDS
% Data completeness	21.5 (40.00-3.30)	Depositor
(in resolution range)	$93.8 \ (30.05 - 3.31)$	EDS
R <sub>merge</sub>	0.07	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.33 (at 3.31 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
P. P.	0.247 , $0.286$	Depositor
$\Lambda, \Lambda_{free}$	0.242 , $0.279$	DCC
$R_{free}$ test set	1606 reflections $(5.03\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	78.0	Xtriage
Anisotropy	0.815	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , $41.8$	EDS
L-test for $twinning^2$	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.327 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9521	wwPDB-VP
Average B, all atoms $(Å^2)$	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: NI,  $\mathrm{SO4}$ 

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).

Mol Chain		Bo	Bond lengths		angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.50	1/2337~(0.0%)	0.60	0/3144
1	В	0.50	0/2337	0.62	0/3144
1	С	0.50	1/2337~(0.0%)	0.60	0/3144
1	D	0.51	0/2337	0.62	0/3144
2	Е	0.60	0/73	0.61	0/95
2	F	0.59	0/73	0.58	0/95
2	G	0.60	0/73	0.60	0/95
2	Н	0.62	0/73	0.58	0/95
All	All	0.51	2/9640~(0.0%)	0.61	0/12956

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	245	CYS	CB-SG	-6.38	1.71	1.82
1	С	245	CYS	CB-SG	-5.95	1.72	1.81

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	2294	0	2234	147	0



n	COL	
4	$O_{2}L$	

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	2294	0	2234	183	0
1	С	2294	0	2234	151	0
1	D	2294	0	2234	175	0
2	Е	74	0	62	10	0
2	F	74	0	62	15	0
2	G	74	0	62	10	0
2	Н	74	0	62	12	0
3	А	15	0	0	2	0
3	В	10	0	0	0	0
3	С	5	0	0	0	0
3	D	5	0	0	0	0
4	В	4	0	0	0	0
5	А	4	0	0	0	0
5	С	3	0	0	0	0
5	D	2	0	0	0	0
5	G	1	0	0	0	0
All	All	9521	0	9184	634	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 34.

All (634) 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 $(\text{\AA})$	overlap (Å)
1:D:74:MET:HG3	1:D:75:GLN:H	1.12	1.05
1:B:74:MET:HG3	1:B:75:GLN:H	1.11	1.05
1:D:96:LYS:HG3	2:H:505:MET:HE2	1.40	1.02
1:D:71:TYR:HB3	1:D:76:GLN:HB3	1.42	1.01
1:B:71:TYR:HB3	1:B:76:GLN:HB3	1.43	0.99
1:B:96:LYS:HG3	2:F:505:MET:HE2	1.43	0.99
1:C:194:ILE:HA	1:C:197:GLN:HB2	1.43	0.96
1:D:138:SER:O	1:D:142:ILE:HD12	1.66	0.96
1:A:194:ILE:HA	1:A:197:GLN:HB2	1.44	0.95
1:B:138:SER:O	1:B:142:ILE:HD12	1.67	0.95
1:A:182:GLN:HE21	1:A:198:GLN:HG3	1.36	0.91
1:B:56:ARG:HH22	1:C:56:ARG:HH21	0.96	0.90
1:A:151:ILE:HD13	1:A:151:ILE:H	1.36	0.88
1:C:182:GLN:HE21	1:C:198:GLN:HG3	1.39	0.88
1:B:258:ILE:HD12	1:B:259:GLU:H	1.37	0.87
1:A:221:GLU:HB3	1:A:223:ARG:HG2	1.57	0.87
1:C:151:ILE:H	1:C:151:ILE:HD13	1.37	0.86



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:221:GLU:HB3	1:C:223:ARG:HG2	1.58	0.86
1:D:258:ILE:HD12	1:D:259:GLU:H	1.38	0.86
1:B:74:MET:HG3	1:B:75:GLN:N	1.91	0.85
1:C:160:SER:HB3	1:C:163:HIS:HB2	1.57	0.84
1:D:74:MET:HG3	1:D:75:GLN:N	1.92	0.84
1:A:160:SER:HB3	1:A:163:HIS:HB2	1.58	0.83
1:B:56:ARG:NH2	1:C:56:ARG:HH21	1.76	0.83
1:C:164:SER:O	1:C:167:THR:HG22	1.79	0.82
1:B:75:GLN:C	1:B:77:PRO:HD2	1.98	0.82
1:A:164:SER:O	1:A:167:THR:HG22	1.79	0.82
1:D:75:GLN:C	1:D:77:PRO:HD2	1.98	0.82
1:D:26:SER:HA	1:D:56:ARG:HH12	1.45	0.81
1:B:26:SER:HA	1:B:56:ARG:HH12	1.45	0.81
1:B:131:ASN:HD22	1:B:131:ASN:H	1.28	0.81
1:B:258:ILE:HD12	1:B:259:GLU:N	1.96	0.80
1:D:258:ILE:HD12	1:D:259:GLU:N	1.96	0.80
1:D:37:LEU:HB2	1:D:46:ALA:HB2	1.63	0.79
1:D:71:TYR:HB3	1:D:76:GLN:CB	2.12	0.79
1:D:131:ASN:H	1:D:131:ASN:HD22	1.29	0.79
1:B:71:TYR:HB3	1:B:76:GLN:CB	2.12	0.79
1:B:174:ARG:HG2	1:B:175:GLU:OE1	1.82	0.78
1:D:174:ARG:HG2	1:D:175:GLU:OE1	1.82	0.78
1:B:37:LEU:HB2	1:B:46:ALA:HB2	1.64	0.78
1:B:181:CYS:HA	1:B:184:ASN:HD22	1.49	0.78
1:D:181:CYS:HA	1:D:184:ASN:HD22	1.49	0.78
1:D:149:ASN:O	1:D:153:GLU:HG3	1.84	0.77
1:C:248:PRO:HA	1:D:282:ILE:HD13	1.66	0.77
1:B:149:ASN:O	1:B:153:GLU:HG3	1.85	0.77
1:B:93:GLN:HE21	1:C:93:GLN:HG3	1.50	0.77
1:D:43:TYR:N	1:D:44:PRO:HD2	1.99	0.77
1:B:43:TYR:N	1:B:44:PRO:HD2	1.99	0.76
1:C:301:VAL:C	1:C:303:ASP:H	1.87	0.76
1:C:255:ARG:O	1:C:259:GLU:HB2	1.86	0.76
1:A:301:VAL:C	1:A:303:ASP:H	1.88	0.75
1:A:284:ASN:HD21	1:B:284:ASN:HD21	1.32	0.74
1:A:255:ARG:O	1:A:259:GLU:HB2	1.88	0.74
1:B:72:LEU:HD23	1:B:76:GLN:HG2	1.71	0.73
1:D:66:ASN:CG	2:H:508:VAL:HG13	2.09	0.73
1:B:76:GLN:N	1:B:77:PRO:HD2	2.04	0.73
1:B:56:ARG:HH22	1:C:56:ARG:NH2	1.80	0.72
1:C:78:GLU:HB2	1:C:79:GLN:NE2	2.04	0.72



		Interatomic Clash			
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:D:72:LEU:HD23	1:D:76:GLN:HG2	1.71	0.72		
1:D:76:GLN:N	1:D:77:PRO:HD2	2.05	0.72		
1:A:78:GLU:HB2	1:A:79:GLN:NE2	2.05	0.71		
1:A:182:GLN:NE2	1:A:198:GLN:HG3	2.04	0.71		
1:B:194:ILE:HA	1:B:197:GLN:HB3	1.73	0.70		
1:A:248:PRO:HA	1:B:282:ILE:HD13	1.73	0.70		
1:D:194:ILE:HA	1:D:197:GLN:HB3	1.74	0.70		
1:D:194:ILE:O	1:D:198:GLN:HB2	1.91	0.69		
1:C:66:ASN:CG	2:G:508:VAL:HG13	2.13	0.69		
1:C:284:ASN:HD21	1:D:284:ASN:HD21	1.38	0.68		
1:D:50:TYR:OH	2:H:508:VAL:HG11	1.92	0.68		
1:A:66:ASN:CG	2:E:508:VAL:HG13	2.13	0.68		
1:B:182:GLN:HG3	1:B:198:GLN:NE2	2.09	0.68		
1:A:284:ASN:HD21	1:B:284:ASN:ND2	1.92	0.68		
1:B:110:SER:HB3	1:B:113:GLU:OE1	1.94	0.68		
1:B:194:ILE:O	1:B:198:GLN:HB2	1.92	0.68		
1:D:37:LEU:CB	1:D:46:ALA:HB2	2.24	0.68		
1:C:182:GLN:NE2	1:C:198:GLN:HG3	2.08	0.68		
1:C:212:MET:O	1:C:215:LEU:HB2	1.93	0.68		
1:B:264:ARG:O	1:B:264:ARG:HD3	1.94	0.68		
1:A:134:ASP:O	1:A:138:SER:HB3	1.94	0.67		
1:C:134:ASP:O	1:C:138:SER:HB3	1.94	0.67		
1:D:110:SER:HB3	1:D:113:GLU:OE1	1.94	0.67		
1:B:103:GLN:OE1	1:B:103:GLN:HA	1.93	0.67		
1:B:37:LEU:CB	1:B:46:ALA:HB2	2.25	0.67		
1:B:94:SER:HB3	1:B:97:ALA:HB3	1.76	0.67		
1:C:251:ILE:HD12	1:C:251:ILE:N	2.09	0.67		
1:D:145:LYS:HD3	1:D:304:TYR:CD2	2.29	0.67		
1:A:284:ASN:ND2	1:B:284:ASN:HD21	1.91	0.67		
1:B:145:LYS:HD3	1:B:304:TYR:CD2	2.30	0.67		
1:D:264:ARG:O	1:D:264:ARG:HD3	1.94	0.67		
1:A:212:MET:O	1:A:215:LEU:HB2	1.95	0.67		
1:D:94:SER:HB3	1:D:97:ALA:HB3	1.77	0.66		
1:A:251:ILE:N	1:A:251:ILE:HD12	2.10	0.66		
1:B:255:ARG:O	1:B:259:GLU:HB2	1.95	0.66		
1:D:182:GLN:HG3	1:D:198:GLN:NE2	2.11	0.66		
1:C:103:GLN:O	1:C:106:LEU:HB2	1.97	0.65		
1:D:103:GLN:OE1	1:D:103:GLN:HA	1.95	0.65		
1:A:103:GLN:O	1:A:106:LEU:HB2	1.97	0.65		
1:A:182:GLN:HG2	1:A:198:GLN:HE21	1.61	0.65		
2:E:508:VAL:HG12	2:E:508:VAL:O	1.96	0.65		



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:255:ARG:O	1:D:259:GLU:HB2	1.96	0.65
1:B:182:GLN:HG3	1:B:198:GLN:HE22	1.59	0.64
2:G:508:VAL:HG12	2:G:508:VAL:O	1.96	0.64
1:B:50:TYR:OH	2:F:508:VAL:HG11	1.97	0.64
2:F:508:VAL:HG12	2:F:508:VAL:O	1.97	0.64
2:H:508:VAL:HG12	2:H:508:VAL:O	1.97	0.64
1:B:66:ASN:CG	2:F:508:VAL:HG13	2.18	0.64
1:C:182:GLN:HG2	1:C:198:GLN:HE21	1.62	0.63
1:B:154:ARG:O	1:B:154:ARG:HD3	1.99	0.63
1:A:148:TRP:HA	1:A:151:ILE:HD11	1.80	0.63
1:B:284:ASN:OD1	1:B:287:MET:HB2	1.98	0.63
1:A:201:ILE:HD12	1:A:204:LYS:HB3	1.80	0.63
1:C:183:ARG:HG3	1:C:186:GLU:HG3	1.81	0.63
1:D:154:ARG:O	1:D:154:ARG:HD3	1.99	0.63
1:A:78:GLU:HB2	1:A:79:GLN:HE21	1.62	0.63
1:C:78:GLU:HB2	1:C:79:GLN:HE21	1.62	0.63
1:A:183:ARG:HG3	1:A:186:GLU:HG3	1.81	0.62
1:D:131:ASN:HB2	2:H:502:THR:HG23	1.81	0.62
1:A:85:ARG:HG3	1:A:85:ARG:HH11	1.64	0.62
1:B:131:ASN:HD22	1:B:131:ASN:N	1.95	0.62
1:C:284:ASN:ND2	1:D:284:ASN:HD21	1.96	0.62
1:D:182:GLN:HG3	1:D:198:GLN:HE22	1.62	0.62
1:C:148:TRP:HA	1:C:151:ILE:HD11	1.82	0.62
1:D:85:ARG:HG3	1:D:85:ARG:HH11	1.64	0.62
1:D:284:ASN:OD1	1:D:287:MET:HB2	2.00	0.61
1:C:85:ARG:HG3	1:C:85:ARG:HH11	1.65	0.61
1:C:185:HIS:HB3	1:C:188:HIS:HB2	1.82	0.61
1:A:185:HIS:HB3	1:A:188:HIS:HB2	1.82	0.61
1:A:189:GLU:HG2	1:A:193:HIS:ND1	2.16	0.61
1:C:156:ILE:N	1:C:156:ILE:HD12	2.16	0.61
1:A:166:LEU:HD23	1:A:169:LEU:HD12	1.83	0.61
1:B:85:ARG:HG3	1:B:85:ARG:HH11	1.65	0.61
1:A:156:ILE:HD12	1:A:156:ILE:N	2.16	0.60
1:B:291:ILE:O	1:B:295:ILE:HD12	2.00	0.60
1:C:151:ILE:HD13	1:C:151:ILE:N	2.15	0.60
1:C:201:ILE:HD12	1:C:204:LYS:HB3	1.83	0.60
1:C:111:TYR:O	1:C:115:ILE:HG23	2.01	0.60
1:C:96:LYS:HG3	2:G:505:MET:HE1	1.84	0.60
1:C:142:ILE:O	1:C:146:LYS:HG3	2.02	0.60
1:C:189:GLU:HG2	1:C:193:HIS:ND1	2.17	0.60
1:B:71:TYR:CE2	1:B:79:GLN:HB3	2.37	0.60



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:111:TYR:HE2	1:B:146:LYS:HB3	1.67	0.60
1:D:71:TYR:CE2	1:D:79:GLN:HB3	2.37	0.60
1:C:166:LEU:HD23	1:C:169:LEU:HD12	1.84	0.59
1:D:74:MET:CG	1:D:75:GLN:H	1.99	0.59
1:C:131:ASN:ND2	2:G:502:THR:HG23	2.17	0.59
1:C:228:ILE:HD12	1:C:229:PRO:O	2.02	0.59
1:C:284:ASN:HD21	1:D:284:ASN:ND2	2.00	0.59
1:D:111:TYR:HE2	1:D:146:LYS:HB3	1.68	0.59
1:A:142:ILE:O	1:A:146:LYS:HG3	2.03	0.59
1:B:74:MET:CG	1:B:75:GLN:H	1.98	0.59
1:A:165:TYR:O	1:A:168:ARG:HG2	2.02	0.59
1:D:164:SER:O	1:D:167:THR:HG22	2.03	0.59
1:A:228:ILE:HD12	1:A:229:PRO:O	2.02	0.59
1:B:182:GLN:HE21	1:B:198:GLN:NE2	2.01	0.58
1:B:145:LYS:CE	1:B:304:TYR:HB3	2.33	0.58
1:B:54:ILE:HD13	1:B:64:TYR:CE1	2.38	0.58
1:A:111:TYR:O	1:A:115:ILE:HG23	2.03	0.58
1:B:134:ASP:HA	1:B:137:PRO:HG2	1.86	0.58
1:A:212:MET:HA	1:A:215:LEU:HD12	1.85	0.58
1:B:164:SER:O	1:B:167:THR:HG22	2.04	0.58
1:C:154:ARG:HH11	1:C:154:ARG:HG2	1.69	0.58
1:C:212:MET:HA	1:C:215:LEU:HD12	1.85	0.58
1:D:211:ASP:O	1:D:214:GLU:HB3	2.03	0.58
1:D:57:ASN:C	1:D:57:ASN:HD22	2.07	0.58
1:D:134:ASP:HA	1:D:137:PRO:HG2	1.86	0.58
1:B:57:ASN:C	1:B:57:ASN:HD22	2.07	0.57
1:B:72:LEU:HA	1:B:76:GLN:HG3	1.85	0.57
1:D:145:LYS:HD3	1:D:304:TYR:HD2	1.67	0.57
1:B:132:PHE:HB3	1:B:135:ASP:HB2	1.86	0.57
1:D:145:LYS:CE	1:D:304:TYR:HB3	2.34	0.57
1:C:98:HIS:HB3	1:C:121:ALA:HB2	1.87	0.57
1:D:54:ILE:HD13	1:D:64:TYR:CE1	2.39	0.57
1:C:165:TYR:O	1:C:168:ARG:HG2	2.04	0.57
1:A:154:ARG:HG2	1:A:154:ARG:HH11	1.70	0.57
1:B:237:SER:O	1:B:238:PHE:HB2	2.04	0.57
1:C:160:SER:HB3	1:C:163:HIS:CB	2.33	0.57
1:C:174:ARG:HH21	1:C:205:HIS:CB	2.17	0.57
1:A:160:SER:HB3	1:A:163:HIS:CB	2.33	0.57
1:B:145:LYS:HD3	1:B:304:TYR:HD2	1.68	0.57
1:B:211:ASP:O	1:B:214:GLU:HB3	2.04	0.57
1:A:174:ARG:HH21	1:A:205:HIS:CB	2.18	0.57



	A	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:140:LEU:O	1:B:144:LYS:HG2	2.05	0.57
1:D:140:LEU:O	1:D:144:LYS:HG2	2.05	0.57
1:D:291:ILE:O	1:D:295:ILE:HD12	2.04	0.57
1:A:98:HIS:HB3	1:A:121:ALA:HB2	1.87	0.56
1:A:189:GLU:HG2	1:A:193:HIS:CE1	2.41	0.56
1:A:196:ALA:O	1:A:200:CYS:HB2	2.05	0.56
1:C:299:GLY:O	1:C:300:TRP:O	2.23	0.56
1:D:72:LEU:HA	1:D:76:GLN:HG3	1.86	0.56
1:D:131:ASN:CG	2:H:502:THR:HG23	2.26	0.56
1:C:28:GLN:O	1:C:32:GLU:HG3	2.04	0.56
1:A:28:GLN:O	1:A:32:GLU:HG3	2.04	0.56
1:A:151:ILE:H	1:A:151:ILE:CD1	2.12	0.56
1:C:139:ALA:HA	1:C:142:ILE:HD12	1.88	0.56
1:D:29:GLU:O	1:D:31:LYS:N	2.39	0.56
1:D:132:PHE:HB3	1:D:135:ASP:HB2	1.87	0.56
1:B:85:ARG:O	1:B:89:GLU:HG3	2.05	0.56
1:A:139:ALA:HA	1:A:142:ILE:HD12	1.88	0.56
1:D:66:ASN:OD1	2:H:508:VAL:HG13	2.06	0.56
1:D:237:SER:O	1:D:238:PHE:HB2	2.05	0.56
1:B:180:GLU:HG3	1:B:181:CYS:N	2.21	0.56
1:D:180:GLU:HG3	1:D:181:CYS:N	2.21	0.56
1:A:282:ILE:HD12	1:B:282:ILE:HD12	1.88	0.55
1:B:298:ASN:O	1:B:301:VAL:HG23	2.06	0.55
1:D:85:ARG:O	1:D:89:GLU:HG3	2.06	0.55
1:A:131:ASN:ND2	2:E:502:THR:HG23	2.20	0.55
1:A:174:ARG:HH21	1:A:205:HIS:HB2	1.71	0.55
1:A:294:PHE:O	1:A:298:ASN:ND2	2.39	0.55
1:A:36:ARG:HD2	3:A:1307:SO4:O1	2.06	0.55
1:D:43:TYR:N	1:D:44:PRO:CD	2.67	0.55
1:A:164:SER:C	1:A:167:THR:HG22	2.26	0.55
1:B:60:VAL:HG22	1:C:59:LEU:O	2.07	0.55
1:C:255:ARG:HA	1:C:258:ILE:HD11	1.89	0.55
1:B:43:TYR:N	1:B:44:PRO:CD	2.67	0.55
1:C:294:PHE:O	1:C:298:ASN:ND2	2.39	0.55
1:A:255:ARG:HA	1:A:258:ILE:HD11	1.89	0.55
1:C:164:SER:C	1:C:167:THR:HG22	2.27	0.55
1:C:189:GLU:HG2	1:C:193:HIS:CE1	2.42	0.55
1:C:174:ARG:HH21	1:C:205:HIS:HB2	1.72	0.55
1:A:42:LYS:HE2	1:C:283:PRO:CD	2.37	0.54
1:A:176:ARG:HH12	1:B:173:GLU:HG2	1.72	0.54
1:C:301:VAL:O	1:C:302:GLU:HB3	2.06	0.54



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:219:VAL:O	1:A:219:VAL:HG13	2.07	0.54	
1:A:301:VAL:O	1:A:302:GLU:HB3	2.06	0.54	
1:B:131:ASN:HB2	2:F:502:THR:HG23	1.89	0.54	
1:D:182:GLN:HE21	1:D:198:GLN:NE2	2.06	0.54	
1:A:301:VAL:C	1:A:303:ASP:N	2.57	0.54	
1:C:196:ALA:O	1:C:200:CYS:HB2	2.08	0.54	
1:D:131:ASN:CB	2:H:502:THR:HG23	2.37	0.54	
1:A:151:ILE:HD13	1:A:151:ILE:N	2.14	0.54	
1:D:201:ILE:HD12	1:D:204:LYS:HZ2	1.72	0.54	
1:C:219:VAL:HG22	1:C:219:VAL:O	2.07	0.54	
1:C:301:VAL:C	1:C:303:ASP:N	2.56	0.54	
2:H:505:MET:C	2:H:507:GLU:H	2.11	0.54	
1:B:69:LEU:HD23	2:F:508:VAL:CG2	2.37	0.54	
1:B:93:GLN:NE2	1:C:93:GLN:HG3	2.21	0.54	
1:B:181:CYS:O	1:B:184:ASN:HB2	2.07	0.54	
1:D:298:ASN:O	1:D:301:VAL:HG23	2.07	0.54	
1:C:151:ILE:H	1:C:151:ILE:CD1	2.13	0.54	
1:A:189:GLU:HB3	1:A:194:ILE:HG23	1.89	0.54	
1:A:24:SER:N	1:A:25:PRO:HD2	2.23	0.54	
1:B:111:TYR:CE2	1:B:146:LYS:HB3	2.43	0.54	
1:D:42:LYS:C	1:D:44:PRO:HD2	2.28	0.54	
1:D:181:CYS:O	1:D:184:ASN:HB2	2.08	0.54	
2:E:505:MET:C	2:E:507:GLU:H	2.11	0.54	
1:D:68:ALA:HB2	1:D:83:ASP:HB3	1.90	0.54	
1:B:26:SER:HB3	1:B:29:GLU:CD	2.28	0.53	
1:B:42:LYS:C	1:B:44:PRO:HD2	2.28	0.53	
1:B:273:ARG:HG2	1:B:273:ARG:HH11	1.73	0.53	
1:C:25:PRO:CG	1:C:30:LEU:HD21	2.38	0.53	
1:B:136:ILE:N	1:B:137:PRO:HD2	2.23	0.53	
1:C:219:VAL:O	1:C:219:VAL:HG13	2.09	0.53	
1:A:299:GLY:O	1:A:300:TRP:O	2.26	0.53	
1:D:29:GLU:C	1:D:31:LYS:H	2.12	0.53	
1:C:212:MET:O	1:C:215:LEU:N	2.38	0.53	
1:A:25:PRO:CG	1:A:30:LEU:HD21	2.38	0.53	
1:D:76:GLN:H	1:D:76:GLN:CD	2.10	0.53	
1:D:111:TYR:CE2	1:D:146:LYS:HB3	2.44	0.53	
1:C:24:SER:N	1:C:25:PRO:HD2	2.24	0.53	
1:B:68:ALA:HB2	1:B:83:ASP:HB3	1.91	0.53	
2:F:505:MET:C	2:F:507:GLU:H	2.12	0.53	
2:G:505:MET:C	2:G:507:GLU:H	2.12	0.53	
1:A:176:ARG:NH1	1:B:173:GLU:HG2	2.24	0.52	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:96:LYS:HG3	2:E:505:MET:HE1	1.91	0.52	
1:B:24:SER:HB2	1:B:25:PRO:HD3	1.90	0.52	
1:B:29:GLU:O	1:B:31:LYS:N	2.42	0.52	
1:B:178:LEU:O	1:B:182:GLN:HB3	2.09	0.52	
1:B:241:MET:HE1	1:B:253:TYR:HA	1.90	0.52	
1:D:241:MET:HE1	1:D:253:TYR:HA	1.90	0.52	
1:C:167:THR:HG23	1:C:168:ARG:N	2.25	0.52	
1:B:76:GLN:CD	1:B:76:GLN:H	2.11	0.52	
1:D:136:ILE:N	1:D:137:PRO:HD2	2.24	0.52	
1:D:178:LEU:O	1:D:182:GLN:HB3	2.10	0.52	
1:B:72:LEU:HD23	1:B:76:GLN:CG	2.40	0.52	
1:C:282:ILE:HD12	1:D:282:ILE:HD12	1.92	0.52	
1:B:66:ASN:OD1	2:F:508:VAL:HG13	2.10	0.52	
1:A:212:MET:O	1:A:215:LEU:N	2.40	0.52	
1:A:284:ASN:ND2	1:B:284:ASN:ND2	2.55	0.52	
1:B:201:ILE:O	1:B:201:ILE:HG23	2.10	0.52	
1:A:167:THR:HG23	1:A:168:ARG:N	2.25	0.52	
1:A:180:GLU:O	1:A:181:CYS:HB2	2.09	0.52	
1:D:101:LEU:O	1:D:101:LEU:HD23	2.10	0.51	
1:C:133:GLY:O	1:C:135:ASP:N	2.36	0.51	
1:A:219:VAL:O	1:A:219:VAL:HG22	2.10	0.51	
1:B:204:LYS:HZ3	1:B:205:HIS:CE1	2.28	0.51	
1:D:201:ILE:HG23	1:D:201:ILE:O	2.10	0.51	
1:B:251:ILE:N	1:B:251:ILE:HD12	2.25	0.51	
1:C:189:GLU:HB3	1:C:194:ILE:HG23	1.92	0.51	
1:A:230:ASP:C	1:A:232:LEU:H	2.13	0.51	
1:B:93:GLN:HG3	1:C:93:GLN:HE21	1.76	0.51	
1:A:133:GLY:O	1:A:135:ASP:N	2.35	0.51	
1:B:76:GLN:N	1:B:77:PRO:CD	2.73	0.51	
1:C:101:LEU:HG	1:C:105:GLN:NE2	2.25	0.51	
1:B:29:GLU:C	1:B:31:LYS:H	2.14	0.51	
1:D:76:GLN:N	1:D:77:PRO:CD	2.73	0.51	
1:A:207:LYS:HB2	1:A:207:LYS:NZ	2.26	0.51	
1:D:72:LEU:HD23	1:D:76:GLN:CG	2.41	0.51	
1:A:209:MET:O	1:A:212:MET:HB3	2.11	0.51	
1:C:180:GLU:O	1:C:181:CYS:HB2	2.10	0.51	
1:A:37:LEU:HD23	1:C:285:LEU:HD11	1.94	0.50	
1:C:44:PRO:HG2	1:C:45:GLU:OE1	2.11	0.50	
1:C:260:GLU:HG3	1:C:261:HIS:N	2.27	0.50	
1:D:235:LYS:N	1:D:235:LYS:HE2	2.26	0.50	
1:A:24:SER:N	1:A:25:PRO:CD	2.74	0.50	



	ti a	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:C:173:GLU:O	1:C:177:GLU:HG2	2.11	0.50	
1:D:24:SER:HB2	1:D:25:PRO:HD3	1.92	0.50	
1:D:76:GLN:O	1:D:77:PRO:C	2.49	0.50	
1:D:251:ILE:N	1:D:251:ILE:HD12	2.26	0.50	
1:D:273:ARG:HG2	1:D:273:ARG:HH11	1.76	0.50	
1:B:56:ARG:HG2	1:B:56:ARG:HH11	1.77	0.50	
1:A:173:GLU:O	1:A:177:GLU:HG2	2.11	0.50	
1:B:37:LEU:HD23	1:B:42:LYS:HE2	1.94	0.50	
1:A:30:LEU:HD13	1:A:52:ARG:HB2	1.94	0.50	
1:D:26:SER:HB3	1:D:29:GLU:CD	2.32	0.50	
1:A:42:LYS:HE3	1:D:249:SER:O	2.11	0.50	
1:A:162:LEU:HD21	1:B:212:MET:HA	1.93	0.50	
1:C:209:MET:O	1:C:212:MET:HB3	2.12	0.50	
1:B:76:GLN:O	1:B:77:PRO:C	2.50	0.49	
1:C:253:TYR:CD1	1:C:258:ILE:HG21	2.47	0.49	
1:D:29:GLU:C	1:D:31:LYS:N	2.65	0.49	
1:D:131:ASN:HD22	1:D:131:ASN:N	1.97	0.49	
1:B:101:LEU:O	1:B:101:LEU:HD23	2.12	0.49	
1:C:207:LYS:HB2	1:C:207:LYS:NZ	2.27	0.49	
1:C:230:ASP:C	1:C:232:LEU:H	2.15	0.49	
1:C:301:VAL:O	1:C:303:ASP:N	2.44	0.49	
1:D:37:LEU:HD13	1:D:45:GLU:HB3	1.93	0.49	
1:A:260:GLU:HG3	1:A:261:HIS:N	2.28	0.49	
1:C:245:CYS:HA	1:C:284:ASN:H	1.77	0.49	
1:A:215:LEU:CD2	1:B:219:VAL:HG21	2.42	0.49	
1:B:235:LYS:HE2	1:B:235:LYS:N	2.28	0.49	
1:D:145:LYS:HD3	1:D:304:TYR:HB3	1.94	0.49	
1:B:129:ARG:HG2	1:B:129:ARG:HH11	1.78	0.49	
1:D:37:LEU:HD23	1:D:42:LYS:HE2	1.95	0.49	
1:A:259:GLU:HA	1:A:259:GLU:OE2	2.13	0.49	
1:A:301:VAL:O	1:A:303:ASP:N	2.45	0.49	
1:C:24:SER:N	1:C:25:PRO:CD	2.76	0.49	
1:B:164:SER:O	1:B:168:ARG:HG3	2.13	0.49	
1:B:255:ARG:HA	1:B:258:ILE:HD11	1.95	0.49	
1:C:235:LYS:HB2	1:C:253:TYR:CD2	2.48	0.49	
1:D:56:ARG:HG2	1:D:56:ARG:HH11	1.78	0.49	
1:A:212:MET:HE2	1:B:166:LEU:HD21	1.95	0.48	
1:D:164:SER:O	1:D:168:ARG:HG3	2.13	0.48	
1:A:253:TYR:CD1	1:A:258:ILE:HG21	2.48	0.48	
1:A:36:ARG:NH1	3:A:1307:SO4:S	2.86	0.48	
1:A:294:PHE:CD1	1:A:298:ASN:ND2	2.81	0.48	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:37:LEU:HD13	1:B:45:GLU:HB3	1.94	0.48	
1:A:182:GLN:CG	1:A:198:GLN:HE21	2.27	0.48	
1:B:76:GLN:HB2	1:B:80:ALA:HB2	1.95	0.48	
1:C:50:TYR:OH	2:G:508:VAL:HG11	2.14	0.48	
1:C:286:ALA:C	1:D:287:MET:HE1	2.33	0.48	
1:D:26:SER:HA	1:D:56:ARG:NH1	2.22	0.48	
1:D:76:GLN:HB2	1:D:80:ALA:HB2	1.95	0.48	
1:A:245:CYS:HA	1:A:284:ASN:H	1.77	0.48	
1:D:286:ALA:O	1:D:290:VAL:HG23	2.13	0.48	
1:B:131:ASN:H	1:B:131:ASN:ND2	2.04	0.48	
1:B:182:GLN:CG	1:B:198:GLN:HE22	2.26	0.48	
1:C:30:LEU:HD13	1:C:52:ARG:HB2	1.96	0.48	
1:D:148:TRP:CE2	1:D:300:TRP:HA	2.49	0.48	
1:D:164:SER:HA	1:D:167:THR:HG22	1.96	0.48	
1:D:242:ARG:HG2	1:D:242:ARG:HH11	1.79	0.48	
1:D:255:ARG:HA	1:D:258:ILE:HD11	1.95	0.48	
1:B:145:LYS:HD3	1:B:304:TYR:HB3	1.94	0.48	
1:B:286:ALA:O	1:B:290:VAL:HG23	2.13	0.48	
1:D:30:LEU:HB2	1:D:53:ALA:HB2	1.96	0.48	
1:A:235:LYS:HB2	1:A:253:TYR:CD2	2.49	0.48	
1:B:241:MET:HE2	1:B:254:ASP:N	2.28	0.48	
1:D:94:SER:HB3	1:D:97:ALA:CB	2.43	0.48	
1:A:101:LEU:HG	1:A:105:GLN:NE2	2.29	0.48	
1:B:94:SER:HB3	1:B:97:ALA:CB	2.43	0.48	
1:B:201:ILE:HD12	1:B:204:LYS:HZ2	1.79	0.48	
1:B:242:ARG:HG2	1:B:242:ARG:HH11	1.79	0.48	
1:B:263:GLN:O	1:B:264:ARG:HB2	2.13	0.48	
1:C:248:PRO:HA	1:D:282:ILE:CD1	2.40	0.48	
1:C:258:ILE:HD13	1:C:281:LEU:HD11	1.96	0.47	
1:B:278:GLN:HG3	1:B:279:GLU:N	2.29	0.47	
1:D:129:ARG:HG2	1:D:129:ARG:HH11	1.79	0.47	
1:D:132:PHE:CE1	2:H:505:MET:HG2	2.49	0.47	
1:A:84:CYS:C	1:A:86:ARG:H	2.17	0.47	
1:C:259:GLU:OE2	1:C:259:GLU:HA	2.14	0.47	
1:B:29:GLU:C	1:B:31:LYS:N	2.68	0.47	
1:A:138:SER:HA	1:A:238:PHE:CD1	2.50	0.47	
1:C:38:PHE:CZ	1:C:69:LEU:HG	2.50	0.47	
1:D:263:GLN:O	1:D:264:ARG:HB2	2.13	0.47	
1:B:26:SER:HA	1:B:56:ARG:NH1	2.23	0.47	
1:D:131:ASN:H	1:D:131:ASN:ND2	2.05	0.47	
1:A:44:PRO:HG2	1:A:45:GLU:OE1	2.14	0.47	



	lo uo pugom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:148:TRP:CE2	1:B:300:TRP:HA	2.50	0.47	
1:C:129:ARG:NH2	1:C:264:ARG:HH21	2.12	0.47	
1:C:229:PRO:HB3	1:C:231:TYR:CE2	2.49	0.47	
1:C:294:PHE:CD1	1:C:298:ASN:ND2	2.83	0.47	
1:D:223:ARG:NH1	1:D:223:ARG:HG2	2.30	0.47	
1:A:239:GLU:HG2	1:A:240:LEU:N	2.30	0.47	
1:C:84:CYS:C	1:C:86:ARG:H	2.17	0.47	
1:D:133:GLY:O	1:D:135:ASP:N	2.47	0.47	
1:D:223:ARG:HG2	1:D:223:ARG:HH11	1.80	0.47	
1:D:278:GLN:HG3	1:D:279:GLU:N	2.29	0.47	
1:C:176:ARG:HH12	1:D:173:GLU:HG2	1.80	0.47	
1:A:138:SER:O	1:A:142:ILE:HG13	2.15	0.47	
1:A:199:ALA:HA	1:A:202:GLU:HB2	1.97	0.47	
1:A:43:TYR:N	1:A:44:PRO:HD2	2.30	0.46	
1:A:229:PRO:HB3	1:A:231:TYR:CE2	2.50	0.46	
1:C:71:TYR:CD2	1:C:79:GLN:HB2	2.51	0.46	
1:C:111:TYR:HB3	1:C:147:ARG:HG3	1.96	0.46	
1:C:138:SER:O	1:C:142:ILE:HG13	2.15	0.46	
1:C:182:GLN:CG	1:C:198:GLN:HE21	2.28	0.46	
1:D:241:MET:HE2	1:D:254:ASP:N	2.30	0.46	
1:B:223:ARG:NH1	1:B:223:ARG:HG2	2.30	0.46	
1:A:257:ASP:C	1:A:259:GLU:H	2.19	0.46	
1:B:105:GLN:C	1:B:107:GLU:H	2.18	0.46	
1:D:105:GLN:C	1:D:107:GLU:H	2.17	0.46	
1:A:38:PHE:CE1	2:E:508:VAL:HG23	2.50	0.46	
1:C:167:THR:CG2	1:C:168:ARG:N	2.78	0.46	
1:D:154:ARG:HG3	1:D:154:ARG:HH11	1.80	0.46	
1:C:81:LEU:HD13	1:C:81:LEU:O	2.16	0.46	
1:C:172:ALA:O	1:C:176:ARG:HG3	2.16	0.46	
1:A:211:ASP:HA	1:A:214:GLU:OE1	2.16	0.46	
1:B:164:SER:HA	1:B:167:THR:HG22	1.98	0.46	
1:B:223:ARG:HG2	1:B:223:ARG:HH11	1.81	0.46	
1:C:66:ASN:OD1	2:G:508:VAL:HG13	2.15	0.46	
1:C:239:GLU:HG2	1:C:240:LEU:N	2.31	0.46	
1:D:76:GLN:N	1:D:76:GLN:OE1	2.45	0.46	
1:C:257:ASP:C 1:C:259:GLU:J		2.19	0.46	
1:A:26:SER:OG	1:A:29:GLU:HG3	2.15	0.46	
1:B:273:ARG:HG2	1:B:273:ARG:NH1	2.29	0.46	
1:A:38:PHE:CZ	1:A:69:LEU:HG	2.51	0.46	
1:B:294:PHE:CE1	1:B:298:ASN:ND2	2.84	0.46	
1:C:211:ASP:HA	1:C:214:GLU:OE1	2.16	0.46	



	lo uo pugom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:157:HIS:O	1:D:161:GLU:HB2	2.15	0.46	
1:D:169:LEU:O	1:D:173:GLU:HG3	2.15	0.45	
1:A:47:ALA:HB2	1:A:70:CYS:HB3	1.98	0.45	
1:A:129:ARG:NH2	1:A:264:ARG:HH21	2.14	0.45	
1:B:182:GLN:NE2	1:B:198:GLN:NE2	2.63	0.45	
1:D:38:PHE:O	1:D:41:ARG:N	2.50	0.45	
1:D:73:LYS:O	1:D:74:MET:HB3	2.17	0.45	
1:D:182:GLN:CG	1:D:198:GLN:HE22	2.29	0.45	
1:A:167:THR:CG2	1:A:168:ARG:N	2.79	0.45	
1:B:154:ARG:HH11	1:B:154:ARG:HG3	1.80	0.45	
1:C:138:SER:HA	1:C:238:PHE:CD1	2.51	0.45	
1:D:254:ASP:O	1:D:256:LYS:N	2.48	0.45	
1:B:76:GLN:N	1:B:76:GLN:OE1	2.46	0.45	
1:C:212:MET:HE2	1:D:166:LEU:HD21	1.99	0.45	
1:D:258:ILE:CD1	1:D:259:GLU:N	2.74	0.45	
1:A:258:ILE:HD13	1:A:281:LEU:HD11	1.99	0.45	
1:B:73:LYS:O	1:B:74:MET:HB3	2.17	0.45	
1:B:258:ILE:CD1	1:B:259:GLU:N	2.74	0.45	
1:A:42:LYS:HD3	1:C:283:PRO:HG3	1.97	0.45	
1:A:110:SER:HB3	1:A:113:GLU:OE1	2.16	0.45	
1:A:172:ALA:O	1:A:176:ARG:HG3	2.17	0.45	
1:B:133:GLY:O	1:B:135:ASP:N	2.49	0.45	
1:C:32:GLU:O	1:C:35:ASN:HB2	2.17	0.45	
2:H:502:THR:HG22	2:H:503:SER:N	2.32	0.45	
1:B:46:ALA:HA	1:B:49:CYS:HB3	1.99	0.45	
1:B:57:ASN:C	1:B:57:ASN:ND2	2.69	0.45	
1:B:254:ASP:O	1:B:256:LYS:N	2.49	0.45	
1:C:176:ARG:NH1	1:D:173:GLU:HG2	2.32	0.45	
1:C:199:ALA:HA	1:C:202:GLU:HB2	1.99	0.45	
1:D:226:ARG:HD3	1:D:300:TRP:CZ3	2.52	0.45	
2:E:502:THR:HG22	2:E:503:SER:N	2.31	0.45	
1:B:169:LEU:O	1:B:173:GLU:HG3	2.16	0.45	
1:D:156:ILE:HD12	1:D:156:ILE:N	2.32	0.45	
1:D:294:PHE:CE1	1:D:298:ASN:ND2	2.85	0.45	
1:A:141:ARG:NH1	1:A:141:ARG:HG3	2.31	0.45	
1:B:69:LEU:HD12	1:B:69:LEU:O	2.17	0.45	
1:A:81:LEU:HD13	1:A:81:LEU:O	2.17	0.45	
1:A:85:ARG:HH11	1:A:85:ARG:CG	2.29	0.45	
1:D:46:ALA:HA	1:D:49:CYS:HB3	1.99	0.45	
1:D:182:GLN:O	1:D:184:ASN:N	2.50	0.45	
1:D:242:ARG:HH11	1:D:242:ARG:CG	2.30	0.45	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:32:GLU:O	1:A:35:ASN:HB2	2.17	0.44	
1:B:26:SER:HB3	1:B:29:GLU:CG	2.48	0.44	
1:B:69:LEU:HD23	2:F:508:VAL:HG22	1.97	0.44	
1:B:115:ILE:HD13	1:B:144:LYS:HD3	1.99	0.44	
1:B:132:PHE:O	1:B:135:ASP:HB2	2.17	0.44	
1:B:156:ILE:N	1:B:156:ILE:HD12	2.32	0.44	
1:B:253:TYR:HB2	1:B:258:ILE:HG12	1.99	0.44	
1:C:110:SER:HB3	1:C:113:GLU:OE1	2.17	0.44	
1:C:141:ARG:NH1	1:C:141:ARG:HG3	2.31	0.44	
1:D:253:TYR:HB2	1:D:258:ILE:HG12	1.99	0.44	
1:A:169:LEU:HD22	1:B:173:GLU:CD	2.37	0.44	
1:D:204:LYS:NZ	1:D:205:HIS:HE1	2.15	0.44	
1:A:30:LEU:HB2	1:A:53:ALA:HB2	1.99	0.44	
1:B:134:ASP:O	1:B:138:SER:CB	2.66	0.44	
1:D:57:ASN:C	1:D:57:ASN:ND2	2.70	0.44	
1:D:132:PHE:O	1:D:135:ASP:HB2	2.17	0.44	
1:D:134:ASP:O	1:D:138:SER:CB	2.65	0.44	
2:F:502:THR:HG22	2:F:503:SER:N	2.33	0.44	
1:D:115:ILE:HD13	1:D:144:LYS:HD3	1.99	0.44	
1:D:226:ARG:HD3	1:D:300:TRP:CE3	2.52	0.44	
1:B:131:ASN:CB	2:F:502:THR:HG23	2.48	0.44	
1:B:132:PHE:CE1	2:F:505:MET:HG2	2.52	0.44	
1:B:242:ARG:HH11	1:B:242:ARG:CG	2.30	0.44	
1:C:47:ALA:HB2	1:C:70:CYS:HB3	1.99	0.44	
1:D:182:GLN:OE1	1:D:183:ARG:HB2	2.17	0.44	
1:A:174:ARG:O	1:A:178:LEU:HD13	2.18	0.44	
1:B:204:LYS:HZ3	1:B:205:HIS:HE1	1.64	0.44	
1:C:105:GLN:OE1	1:C:113:GLU:HB3	2.17	0.44	
1:D:182:GLN:C	1:D:184:ASN:H	2.20	0.44	
1:B:157:HIS:O	1:B:161:GLU:HB2	2.17	0.44	
1:C:85:ARG:HH11	1:C:85:ARG:CG	2.30	0.44	
1:C:95:VAL:HG11	1:C:125:ALA:HB2	2.00	0.44	
1:D:273:ARG:HG2	1:D:273:ARG:NH1	2.31	0.44	
2:G:502:THR:HG22	2:G:503:SER:N	2.32	0.44	
1:A:287:MET:O	1:A:288:LYS:C	2.56	0.43	
1:C:237:SER:O	1:C:238:PHE:HB2	2.18	0.43	
1:D:247:THR:HB	1:D:248:PRO:CD	2.48	0.43	
1:A:71:TYR:CD2	1:A:79:GLN:HB2	2.53	0.43	
1:B:204:LYS:NZ	1:B:205:HIS:HE1	2.16	0.43	
1:B:226:ARG:HD3	1:B:300:TRP:CE3	2.53	0.43	
1:C:163:HIS:O	1:C:165:TYR:N	2.52	0.43	



	i a s pagem	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:131:ASN:CG	2:F:502:THR:HG23	2.39	0.43	
1:C:37:LEU:HD23	1:C:37:LEU:HA	1.82	0.43	
1:B:182:GLN:O	1:B:184:ASN:N	2.52	0.43	
1:B:226:ARG:HD3	1:B:300:TRP:CZ3	2.53	0.43	
1:B:239:GLU:O	1:B:240:LEU:C	2.57	0.43	
1:C:26:SER:OG	1:C:29:GLU:HG3	2.17	0.43	
1:C:195:ARG:HG3	1:C:195:ARG:HH11	1.83	0.43	
1:D:76:GLN:N	1:D:76:GLN:CD	2.70	0.43	
1:B:182:GLN:C	1:B:184:ASN:H	2.21	0.43	
1:C:30:LEU:HB2	1:C:53:ALA:HB2	2.01	0.43	
1:C:174:ARG:O	1:C:178:LEU:HD13	2.19	0.43	
1:C:215:LEU:CD2	1:D:219:VAL:HG21	2.48	0.43	
2:H:507:GLU:O	2:H:507:GLU:HG3	2.19	0.43	
1:A:111:TYR:HB3	1:A:147:ARG:HG3	2.00	0.43	
1:B:77:PRO:HB2	1:B:78:GLU:H	1.63	0.43	
1:B:182:GLN:HG3	1:B:198:GLN:CD	2.38	0.43	
1:B:243:GLU:HB3	1:B:255:ARG:HB2	1.99	0.43	
1:D:254:ASP:C	1:D:256:LYS:H	2.22	0.43	
2:F:507:GLU:O	2:F:507:GLU:HG3	2.19	0.43	
1:B:30:LEU:HB2	1:B:53:ALA:HB2	2.01	0.43	
1:C:284:ASN:ND2	1:D:284:ASN:ND2	2.62	0.43	
1:D:77:PRO:HB2	1:D:78:GLU:H	1.63	0.43	
1:A:81:LEU:HD22	1:A:101:LEU:HD12	2.00	0.43	
1:B:134:ASP:O	1:B:138:SER:HB2	2.19	0.43	
1:B:182:GLN:OE1	1:B:183:ARG:HB2	2.19	0.43	
1:B:247:THR:HB	1:B:248:PRO:CD	2.49	0.43	
1:C:235:LYS:HD3	1:C:235:LYS:HA	1.85	0.43	
1:A:235:LYS:HA	1:A:235:LYS:HD3	1.82	0.43	
1:C:81:LEU:HD22	1:C:101:LEU:HD12	2.01	0.43	
1:C:96:LYS:HA	2:G:505:MET:HE1	2.01	0.43	
1:D:182:GLN:HG3	1:D:198:GLN:CD	2.38	0.43	
1:B:228:ILE:HD12	1:B:294:PHE:HE2	1.84	0.43	
1:C:258:ILE:HD13	1:C:281:LEU:CD1	2.49	0.43	
1:C:287:MET:O	1:C:288:LYS:C	2.57	0.43	
1:D:170:ILE:HG22	1:D:171:ALA:N	2.33	0.43	
1:B:61:ALA:O	1:B:62:VAL:C	2.58	0.42	
1:B:254:ASP:C	1:B:256:LYS:H	2.22	0.42	
1:C:43:TYR:N	1:C:44:PRO:HD2	2.34	0.42	
1:D:294:PHE:O	1:D:298:ASN:ND2	2.52	0.42	
1:A:50:TYR:OH	2:E:508:VAL:HG11	2.19	0.42	
1:B:76:GLN:N	1:B:76:GLN:CD	2.70	0.42	



	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:239:GLU:O	1:D:240:LEU:C	2.57	0.42	
1:A:195:ARG:HG3	1:A:195:ARG:HH11	1.84	0.42	
1:B:215:LEU:O	1:B:218:GLN:HB2	2.20	0.42	
1:C:178:LEU:HD12	1:C:178:LEU:N	2.35	0.42	
1:A:230:ASP:C	1:A:232:LEU:N	2.73	0.42	
1:B:203:ALA:HA	1:B:206:ASP:OD2	2.19	0.42	
1:B:241:MET:CE	1:B:254:ASP:N	2.82	0.42	
1:B:145:LYS:NZ	1:B:304:TYR:HB3	2.35	0.42	
1:C:57:ASN:C	1:C:57:ASN:HD22	2.21	0.42	
1:C:176:ARG:HA	1:C:180:GLU:HB2	2.01	0.42	
1:C:284:ASN:OD1	1:C:287:MET:HB2	2.18	0.42	
1:A:178:LEU:N	1:A:178:LEU:HD12	2.35	0.42	
1:B:145:LYS:CD	1:B:304:TYR:HB3	2.50	0.42	
1:D:247:THR:HB	1:D:248:PRO:HD2	2.00	0.42	
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.82	0.42	
1:A:154:ARG:O	1:A:154:ARG:HG3	2.19	0.42	
1:B:69:LEU:HD23	2:F:508:VAL:HG23	2.01	0.42	
1:B:170:ILE:HG22	1:B:171:ALA:N	2.33	0.42	
1:D:113:GLU:O	1:D:116:ALA:HB3	2.19	0.42	
1:D:182:GLN:NE2	1:D:198:GLN:NE2	2.67	0.42	
1:A:176:ARG:HA	1:A:180:GLU:HB2	2.01	0.42	
1:C:154:ARG:HG3	1:C:154:ARG:O	2.20	0.42	
1:D:228:ILE:HD12	1:D:294:PHE:HE2	1.85	0.42	
1:D:243:GLU:HB3	1:D:255:ARG:HB2	2.00	0.42	
1:C:163:HIS:O	1:C:164:SER:C	2.57	0.42	
1:D:85:ARG:HH11	1:D:85:ARG:CG	2.32	0.42	
1:A:31:LYS:HB3	1:A:31:LYS:HE2	1.86	0.42	
1:A:237:SER:O	1:A:238:PHE:HB2	2.20	0.42	
1:C:113:GLU:O	1:C:116:ALA:HB3	2.19	0.41	
1:C:169:LEU:HD22	1:D:173:GLU:CD	2.41	0.41	
1:D:38:PHE:O	1:D:40:GLY:N	2.53	0.41	
1:D:107:GLU:OE1	1:D:107:GLU:HA	2.20	0.41	
1:D:178:LEU:C	1:D:180:GLU:H	2.23	0.41	
1:A:31:LYS:HD3	1:A:63:TYR:HE1	1.85	0.41	
1:A:105:GLN:OE1	1:A:113:GLU:HB3	2.19	0.41	
1:B:85:ARG:HH11	1:B:85:ARG:CG	2.32	0.41	
1:B:254:ASP:O	1:B:258:ILE:HD11	2.20	0.41	
1:C:38:PHE:CE1	2:G:508:VAL:HG23	2.54	0.41	
1:D:148:TRP:O	1:D:150:SER:N	2.53	0.41	
1:A:95:VAL:HG11	1:A:125:ALA:HB2	2.02	0.41	
1:A:113:GLU:O	1:A:116:ALA:HB3	2.20	0.41	



	to as pagem	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:258:ILE:HD13	1:A:281:LEU:CD1	2.50	0.41	
1:D:61:ALA:O	1:D:62:VAL:C	2.59	0.41	
1:D:148:TRP:CZ2	1:D:300:TRP:HB3	2.55	0.41	
1:A:163:HIS:O	1:A:164:SER:C	2.58	0.41	
1:A:163:HIS:O	1:A:165:TYR:N	2.54	0.41	
1:B:178:LEU:C	1:B:180:GLU:H	2.24	0.41	
1:C:268:PHE:HA	1:C:274:SER:O	2.21	0.41	
1:D:26:SER:HB3	1:D:29:GLU:CG	2.51	0.41	
1:B:166:LEU:O	1:B:169:LEU:N	2.53	0.41	
1:C:235:LYS:HB2	1:C:253:TYR:CE2	2.56	0.41	
1:A:248:PRO:HA	1:B:282:ILE:CD1	2.46	0.41	
1:A:268:PHE:HA	1:A:274:SER:O	2.21	0.41	
1:B:107:GLU:OE1	1:B:107:GLU:HA	2.21	0.41	
1:C:248:PRO:HD2	1:C:276:LEU:HD13	2.03	0.41	
1:D:134:ASP:O	1:D:138:SER:HB2	2.21	0.41	
1:D:145:LYS:CD	1:D:304:TYR:HB3	2.50	0.41	
1:D:254:ASP:O	1:D:258:ILE:HD11	2.21	0.41	
1:D:288:LYS:HE3	1:D:288:LYS:HB2	1.87	0.41	
1:A:37:LEU:HD13	1:A:45:GLU:HB3	2.03	0.41	
1:A:96:LYS:HA	2:E:505:MET:HE1 2.02		0.41	
1:A:134:ASP:O	1:A:135:ASP:C	2.57	0.41	
1:A:248:PRO:HD2	1:A:276:LEU:HD13	2.03	0.41	
1:B:140:LEU:O	1:B:141:ARG:C	2.58	0.41	
1:B:247:THR:HB	1:B:248:PRO:HD2	2.02	0.41	
1:C:230:ASP:C	1:C:232:LEU:N	2.75	0.41	
1:D:215:LEU:O	1:D:218:GLN:HB2	2.21	0.41	
1:D:255:ARG:O	1:D:255:ARG:HG3	2.21	0.41	
2:E:507:GLU:O	2:E:507:GLU:HG3	2.21	0.41	
1:A:156:ILE:C	1:A:158:GLN:H	2.25	0.41	
1:C:251:ILE:N	1:C:251:ILE:CD1	2.78	0.41	
1:D:131:ASN:ND2	1:D:131:ASN:O	2.54	0.41	
1:B:38:PHE:O	1:B:40:GLY:N	2.54	0.40	
1:D:241:MET:CE	1:D:254:ASP:N	2.84	0.40	
1:B:37:LEU:HD12	1:B:46:ALA:HA	2.03	0.40	
1:C:156:ILE:C	1:C:158:GLN:H	2.25	0.40	
1:D:203:ALA:HA	203:ALA:HA 1:D:206:ASP:OD2		0.40	
1:A:136:ILE:N	1:A:137:PRO:HD2	2.36	0.40	
1:C:71:TYR:CG	1:C:79:GLN:HB2	2.57	0.40	
1:D:85:ARG:HG3	1:D:85:ARG:NH1	2.35	0.40	
1:A:141:ARG:HG3	1:A:141:ARG:HH11	1.86	0.40	
1:A:194:ILE:O	1:A:198:GLN:HB2	2.22	0.40	



Atom-1 Atom-2		Interatomic distance (Å)	Clash overlap (Å)	
1:C:302:GLU:HA	1:C:302:GLU:OE2	2.22	0.40	
1:B:241:MET:SD	1:B:252:THR:HG22	2.61	0.40	

There are no symmetry-related clashes.

#### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	279/281~(99%)	223 (80%)	45 (16%)	11 (4%)	3	18
1	В	279/281~(99%)	214 (77%)	51 (18%)	14 (5%)	2	14
1	С	279/281~(99%)	223 (80%)	46 (16%)	10 (4%)	3	20
1	D	279/281~(99%)	216 (77%)	48 (17%)	15 (5%)	2	12
2	Е	7/9~(78%)	3(43%)	2(29%)	2 (29%)	0	0
2	F	7/9~(78%)	3 (43%)	2(29%)	2 (29%)	0	0
2	G	7/9~(78%)	3(43%)	2(29%)	2 (29%)	0	0
2	Н	7/9~(78%)	3 (43%)	2 (29%)	2 (29%)	0	0
All	All	1144/1160~(99%)	888 (78%)	198 (17%)	58 (5%)	2	13

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	159	GLU
1	А	181	CYS
1	А	300	TRP
1	А	301	VAL
1	В	38	PHE
1	В	77	PRO
1	В	134	ASP
1	В	182	GLN



Mol	Chain	Res	Type
1	В	264	ARG
1	С	159	GLU
1	C	181	CYS
1	C	300	TRP
1	C	301	VAL
1	D	38	PHE
1	D	77	PRO
1	D	134	ASP
1	D	182	GLN
1	D	264	ARG
2	Е	502	THR
2	F	502	THR
2	G	502	THR
2	H	502	THR
1	В	74	MET
1	В	75	GLN
1	В	180	GLU
1	D	74	MET
1	D	75	GLN
1	D	180	GLU
2	Е	503	SER
2	F	503	SER
2	G	503	SER
2	Н	503	SER
1	А	133	GLY
1	А	158	GLN
1	А	160	SER
1	В	30	LEU
1	В	227	ASP
1	В	255	ARG
1	С	158	GLN
1	С	160	SER
1	D	30	LEU
1	D	183	ARG
1	D	227	ASP
1	D	255	ARG
1	В	183	ARG
1	С	133	GLY
1	А	190	ASP
1	В	178	LEU
1	С	164	SER
1	С	190	ASP



Continued from prettous page								
Mol	Chain	Res	Type					
1	А	111	TYR					
1	А	164	SER					
1	D	178	LEU					
1	А	270	PRO					
1	С	270	PRO					
1	В	76	GLN					
1	D	76	GLN					
1	D	39	VAL					

#### 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	entiles
1	А	244/244~(100%)	224 (92%)	20 (8%)	11	36
1	В	244/244~(100%)	220~(90%)	24 (10%)	8	29
1	С	244/244~(100%)	223~(91%)	21 (9%)	10	35
1	D	244/244~(100%)	220 (90%)	24 (10%)	8	29
2	Ε	9/9~(100%)	8 (89%)	1 (11%)	6	23
2	F	9/9~(100%)	9 (100%)	0	100	100
2	G	9/9~(100%)	9~(100%)	0	100	100
2	Н	9/9~(100%)	8 (89%)	1 (11%)	6	23
All	All	1012/1012~(100%)	921 (91%)	91 (9%)	9	32

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	49	CYS
1	А	55	THR
1	А	57	ASN
1	А	103	GLN
1	А	135	ASP
1	А	141	ARG
1	А	149	ASN



Mol	Chain	Res	Type
1	А	151	ILE
1	А	195	ARG
1	A	198	GLN
1	А	204	LYS
1	А	208	TYR
1	А	227	ASP
1	А	240	LEU
1	А	242	ARG
1	А	257	ASP
1	А	273	ARG
1	А	280	GLN
1	А	288	LYS
1	А	289	GLU
1	В	24	SER
1	В	32	GLU
1	В	41	ARG
1	В	55	THR
1	В	57	ASN
1	В	75	GLN
1	В	76	GLN
1	В	104	CYS
1	В	106	LEU
1	В	131	ASN
1	В	135	ASP
1	В	146	LYS
1	В	154	ARG
1	В	161	GLU
1	В	166	LEU
1	В	175	GLU
1	В	195	ARG
1	В	198	GLN
1	В	213	ASP
1	В	223	ARG
1	В	258	ILE
1	В	273	ARG
1	В	278	GLN
1	В	292	ASP
1	С	49	CYS
1	С	55	THR
1	С	57	ASN
1	C	83	ASP
1	С	103	GLN

Continued from previous page...



Mol	Chain	Res	Type
1	С	135	ASP
1	C	141	ARG
1	C	149	ASN
1	C	151	ILE
1	C	195	ARG
1	C	198	GLN
1	C	204	LYS
1	C	208	TYR
1	C	227	ASP
1	C	240	LEU
1	С	242	ARG
1	C	257	ASP
1	С	273	ARG
1	C	280	GLN
1	C	288	LYS
1	С	289	GLU
1	D	24	SER
1	D	32	GLU
1	D	41	ARG
1	D	55	THR
1	D	57	ASN
1	D	75	GLN
1	D	76	GLN
1	D	104	CYS
1	D	106	LEU
1	D	131	ASN
1	D	135	ASP
1	D	146	LYS
1	D	154	ARG
1	D	161	GLU
1	D	166	LEU
1	D	175	GLU
1	D	195	ARG
1	D	198	GLN
1	D	213	ASP
1	D	223	ARG
1	D	258	ILE
1	D	273	ARG
1	D	278	GLN
1	D	292	ASP
2	Е	509	ASP
2	Н	509	ASP



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Chain Res	
1	А	57	ASN
1	А	66	ASN
1	А	79	GLN
1	А	117	ASN
1	А	131	ASN
1	А	182	GLN
1	А	198	GLN
1	А	205	HIS
1	А	218	GLN
1	А	280	GLN
1	А	284	ASN
1	A	298	ASN
1	В	28	GLN
1	В	57	ASN
1	В	93	GLN
1	В	131	ASN
1	В	184	ASN
1	В	198	GLN
1	В	205	HIS
1	В	267	HIS
1	В	278	GLN
1	В	280	GLN
1	С	66	ASN
1	С	79	GLN
1	С	93	GLN
1	С	117	ASN
1	С	131	ASN
1	С	182	GLN
1	С	198	GLN
1	С	205	HIS
1	С	218	GLN
1	C	280	GLN
1	С	284	ASN
1	С	298	ASN
1	D	57	ASN
1	D	131	ASN
1	D	184	ASN
1	D	198	GLN
1	D	205	HIS
1	D	267	HIS
1	D	278	GLN



Continued from previous page...

Mol	Chain	$\operatorname{Res}$	Type
1	D	280	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)

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	ol Typo Chain Bos Li		Tinle	Bond lengths			Bond angles			
Moi Type C	Chain	nes	nes Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2	
3	SO4	A	1305	-	4,4,4	0.23	0	$6,\!6,\!6$	0.07	0
3	SO4	А	1307	-	4,4,4	0.52	0	$6,\!6,\!6$	0.15	0
3	SO4	С	1305	-	4,4,4	0.27	0	$6,\!6,\!6$	0.10	0
3	SO4	В	1305	-	4,4,4	0.29	0	$6,\!6,\!6$	0.15	0
3	SO4	D	1305	-	4,4,4	0.33	0	$6,\!6,\!6$	0.14	0
3	SO4	В	1306	-	4,4,4	0.28	0	$6,\!6,\!6$	0.13	0
3	SO4	А	1306	-	4,4,4	0.30	0	$6,\!6,\!6$	0.07	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	1307	SO4	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<sup>th</sup> 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	281/281~(100%)	0.41	10 (3%) 42 40	36, 74, 120, 136	0
1	В	281/281~(100%)	0.34	5 (1%) 68 67	36, 78, 117, 136	0
1	С	281/281~(100%)	0.37	9 (3%) 47 46	36, 74, 120, 135	0
1	D	281/281~(100%)	0.40	6 (2%) 63 62	36, 78, 117, 136	0
2	Ε	9/9~(100%)	0.56	1 (11%) 5 5	95, 103, 114, 120	0
2	F	9/9~(100%)	1.11	2(22%) 0 1	95, 103, 115, 120	0
2	G	9/9~(100%)	0.50	0 100 100	96, 102, 115, 120	0
2	Н	9/9~(100%)	1.10	3 (33%) 0 0	95, 103, 116, 121	0
All	All	1160/1160 (100%)	0.39	36 (3%) 49 48	36, 78, 120, 136	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res Type		RSRZ	
1	А	182	GLN	5.2	
1	С	182	GLN	4.7	
1	D	188	HIS	4.2	
1	D	189	GLU	3.7	
1	А	189	GLU	3.7	
2	F	501	ASP	3.4	
1	В	189	GLU	3.3	
1	А	188	HIS	3.2	
1	С	180	GLU	3.1	
1	D	187	GLY	3.1	
1	D	186	GLU	3.1	
1	А	172	ALA	2.7	
1	А	185	HIS	2.7	
2	Н	501	ASP	2.6	
1	А	178	LEU	2.6	
1	С	216	PHE	2.5	



Mol	Chain	Res	Type	RSRZ	
1	С	151	ILE	2.5	
1	А	220	ASP	2.5	
1	С	68	ALA	2.4	
1	В	43	TYR	2.4	
1	В	185	HIS	2.4	
1	D	44	PRO	2.3	
1	В	186	GLU	2.3	
1	А	166	LEU	2.3	
1	А	216	PHE	2.2	
2	Ε	508	VAL	2.2	
2	Н	506	GLU	2.2	
1	С	178	LEU	2.2	
2	F	506	GLU	2.2	
1	А	111	TYR	2.2	
1	D	121	ALA	2.2	
1	С	253	TYR	2.1	
2	Н	509	ASP	2.1	
1	С	189	GLU	2.0	
1	В	240	LEU	2.0	
1	С	258	ILE	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
4	NI	В	1310	1/1	-0.41	0.30	200,200,200,200	0
4	NI	В	1308	1/1	<mark>-0.38</mark>	0.57	200,200,200,200	0
4	NI	В	1309	1/1	0.08	0.47	200,200,200,200	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
4	NI	В	1307	1/1	0.37	0.57	200,200,200,200	0
3	SO4	D	1305	5/5	0.90	0.21	105,106,107,107	0
3	SO4	А	1307	5/5	0.92	0.60	108,109,111,112	0
3	SO4	В	1305	5/5	0.93	0.28	82,83,85,86	0
3	SO4	С	1305	5/5	0.94	0.20	88,89,90,91	0
3	SO4	А	1306	5/5	0.94	0.21	78,79,80,80	0
3	SO4	А	1305	5/5	0.95	0.27	89,90,90,91	0
3	SO4	В	1306	5/5	0.96	0.24	89,89,91,91	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

