

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

Dec 19, 2023 – 09:48 pm GMT

PDB ID	:	8CN9
Title	:	Factor VII binding Fab of the bispecific antibody HMB-001 in complex with
		Factor VII
Authors	:	Schluckebier, G.; Johansson, E.
Deposited on	:	2023-02-22
Resolution	:	3.40 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
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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.



Motria	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
R <sub>free</sub>	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	Δ	914	5%		
1	A	214	6%	15%	•
1	F	214	78%	20%	·
1	K	214	2% <b>88</b> %	11%	-
1	Р	214	80%	18%	·
2	В	220	2% <b>8</b> 3%	15%	••



Mol	Chain	Length	Quality of chain	
2	G	220	80%	17% ··
2	L	220	<u>2%</u> 80%	18% •
2	Q	220	82%	16% ·
3	С	254	2% <b>7</b> 9%	20%
3	Н	254	2% 83%	16% ·
3	М	254	78%	19% ••
3	R	254	.% <b>7</b> 4%	23% ••
4	D	107	2% 66% 20%	• 12%
4	Ι	107	2% 81%	7% 11%
4	Ν	107	4% 68% 20%	• 11%
4	S	107	% 66% 18%	• 14%
5	Е	219	7% 75% 1	6% 9%
5	J	219	6% 65% 22%	12%
5	О	219	9% 58% 20%	22%
5	Т	219	9% 59% 15% •	26%

Continued from previous page...



# 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 29516 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1 1	010	Total	С	Ν	0	$\mathbf{S}$	0	0	0	
	A	212	1630	1025	274	327	4	0	0	0
1	F	F 209	Total	С	Ν	0	S	0	0	0
	Г		1607	1013	267	323	4			
1	K	019	Total	С	Ν	0	S	0	0	0
	213	1639	1030	275	330	4	0	0	0	
1 P	210	Total	С	Ν	0	$\mathbf{S}$	0	0	0	
		1617	1016	271	326	4	0		U	

• Molecule 1 is a protein called Fab light chain.

• Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
0	D	217	Total	С	Ν	0	$\mathbf{S}$	0	0	0	
	D	217	1627	1027	272	323	5	0	0	0	
0	C	216	Total C	С	Ν	0	S	0	0	0	0
	Z G	210	1621	1024	271	321	5		0	0	
0	т	916	Total	С	Ν	0	S	0	0	0	
	210	1616	1020	268	323	5	0	0	U		
2 Q	0	916	Total	С	Ν	0	S	0	0	0	
	210	1621	1024	271	321	5	0	0	0		

• Molecule 3 is a protein called Coagulation factor VII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2 (	С	254	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
J	U	204	1974	1253	351	357	13		0	0
2	Ц	254	Total	С	Ν	0	S	0	0	0
з п	204	1974	1253	351	357	13	0	0	0	
2	М	940	Total	С	Ν	0	S	0	0	0
5 M	249	1938	1232	343	350	13	0	0	0	
3 R	240	Total	С	Ν	0	S	0	0	0	
	n	249	1938	1232	343	350	13	0	0	



- Residues ZeroOcc AltConf Mol Chain Trace Atoms Total С Ν Ο S 4 D 940 0 0 70642512314513С Ν S Total Ο 4 Ι 950 0 0 42912471414813S Total С Ν 0 4 Ν 950 0 0 71442912414813Total С Ν 0 S  $\mathbf{S}$ 0 4 920 0 689 41412014213
- Molecule 4 is a protein called Coagulation factor VII.

• Molecule 5 is a protein called Tissue factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
F D	F	200	Total	С	Ν	0	$\mathbf{S}$	0	0	0
5		200	1603	1014	259	325	5	0	0	0
5	т	102	Total	С	Ν	0	S	0	0	0
D J	195	1552	987	250	310	5	0	0	0	
E.	0	171	Total	С	Ν	0	S	0	0	0
D D	1/1	1376	874	223	274	5	0	0		
5	E T	162	Total	С	Ν	0	S	0	0	0
	105	1316	840	212	259	5	0	0	U	

• Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total Ca 1 1	0	0
6	С	1	Total Ca 1 1	0	0
6	F	1	Total Ca 1 1	0	0
6	Н	2	Total Ca 2 2	0	0
6	K	1	Total Ca 1 1	0	0
6	М	2	Total Ca 2 2	0	0
6	R	2	Total Ca 2 2	0	0

• Molecule 7 is beta-D-glucopyranose (three-letter code: BGC) (formula:  $C_6H_{12}O_6$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total         C         O           11         6         5	0	0
7	Ι	1	Total         C         O           11         6         5	0	0
7	S	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 11  6  5 \end{array}$	0	0

 $\bullet\,$  Molecule 8 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	Р	1	Total Cs 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: Fab light chain





• Molecule 3: Coagulation factor VII



• Molecule 3: Coagulation factor VII Chain M: 78% 19% LEU ASP ARG GLY ALA • Molecule 3: Coagulation factor VII Chain R: 74% 23% • • LEU ASP ARG GLY ALA • Molecule 4: Coagulation factor VII Chain D: 66% 20% 12% • ASP GLY ASP ASN ALA SER SER SER PRO GLY GLY • Molecule 4: Coagulation factor VII Chain I: 81% 7% 11%









# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	144.78Å 100.79Å 181.74Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $101.22^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	48.50 - 3.40	Depositor
Resolution (A)	46.66 - 3.40	EDS
% Data completeness	93.0 (48.50-3.40)	Depositor
(in resolution range)	92.3(46.66-3.40)	EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.15 (at 3.40 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
B B.	0.303 , $0.356$	Depositor
$n, n_{free}$	0.304 , $0.354$	DCC
$R_{free}$ test set	1878 reflections $(2.86\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	65.9	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.23, 19.1	EDS
L-test for $twinning^2$	$ < L >=0.37, < L^2>=0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	29516	wwPDB-VP
Average B, all atoms $(Å^2)$	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 46.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1541e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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: BGC, CA, CS

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

Mal	Chain	Bond lengths		Bond	angles
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.25	0/1668	0.48	0/2267
1	F	0.26	0/1645	0.48	0/2237
1	Κ	0.25	0/1677	0.48	0/2279
1	Р	0.25	0/1654	0.46	0/2246
2	В	0.25	0/1667	0.49	0/2277
2	G	0.26	0/1661	0.50	0/2269
2	L	0.25	0/1656	0.48	0/2263
2	Q	0.25	0/1661	0.49	0/2269
3	С	0.24	0/2024	0.49	0/2755
3	Н	0.23	0/2024	0.49	0/2755
3	М	0.24	0/1987	0.49	0/2704
3	R	0.24	0/1987	0.50	0/2704
4	D	0.24	0/719	0.48	0/971
4	Ι	0.24	0/727	0.48	0/982
4	Ν	0.25	0/727	0.50	0/982
4	S	0.26	0/701	0.50	0/945
5	Ε	0.24	0/1637	0.48	0/2229
5	J	0.24	0/1583	0.48	0/2152
5	0	0.24	0/1402	0.48	0/1905
5	Т	0.24	0/1347	0.49	0/1831
All	All	0.25	0/30154	0.49	0/41022

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1630	0	1587	19	0
1	F	1607	0	1565	23	0
1	K	1639	0	1593	15	0
1	Р	1617	0	1567	27	0
2	В	1627	0	1599	20	0
2	G	1621	0	1594	23	0
2	L	1616	0	1584	26	0
2	Q	1621	0	1594	23	0
3	С	1974	0	1950	33	0
3	Н	1974	0	1951	24	0
3	М	1938	0	1912	34	0
3	R	1938	0	1913	39	0
4	D	706	0	639	12	0
4	Ι	714	0	644	4	0
4	Ν	714	0	644	14	0
4	S	689	0	620	14	0
5	Е	1603	0	1543	20	0
5	J	1552	0	1511	32	0
5	0	1376	0	1337	25	0
5	Т	1316	0	1270	21	0
6	А	1	0	0	0	0
6	С	1	0	0	0	0
6	F	1	0	0	0	0
6	Н	2	0	0	0	0
6	Κ	1	0	0	0	0
6	М	2	0	0	0	0
6	R	2	0	0	0	0
7	D	11	0	8	0	0
7	Ι	11	0	9	0	0
7	S	11	0	8	0	0
8	Р	1	0	0	0	0
All	All	29516	0	28642	415	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 7.

All (415) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom 2	Interatomic	Clash
	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:G:157:GLU:HG3	2:G:158:PRO:HA	1.57	0.84
1:K:113:PRO:HB3	1:K:139:PHE:HB3	1.67	0.76
2:B:210:LYS:HG3	2:B:211:PRO:HD3	1.66	0.76
5:J:134:VAL:HG23	5:J:141:LEU:HB2	1.72	0.71
1:K:187:GLU:HA	1:K:211:ARG:HH12	1.55	0.71
2:B:128:PRO:HB3	2:B:154:TYR:HB3	1.76	0.68
3:R:223:ARG:NH1	3:R:251:PRO:O	2.28	0.67
5:E:151:LEU:HA	5:E:193:ILE:HG22	1.77	0.66
5:O:20:LYS:HD2	5:O:60:THR:HG21	1.77	0.66
3:C:216:HIS:ND1	3:C:220:GLU:OE1	2.28	0.65
3:H:275:PHE:HB3	5:J:45:TRP:HB2	1.79	0.64
5:O:127:VAL:HG21	5:O:189:VAL:HG11	1.78	0.64
2:L:51:TYR:HE1	2:L:59:ASN:HB3	1.63	0.64
5:T:40:THR:HG23	5:T:43:GLY:HA3	1.79	0.64
2:L:128:PRO:HB3	2:L:154:TYR:HB3	1.79	0.64
5:J:36:VAL:HG22	5:J:75:VAL:HG22	1.78	0.63
3:M:273:LEU:HD11	3:M:357:TYR:HB2	1.81	0.63
1:A:42:GLU:OE1	1:A:45:ARG:NH2	2.31	0.63
2:Q:128:PRO:HB3	2:Q:154:TYR:HB3	1.81	0.63
5:J:6:THR:HG21	5:J:32:GLN:HB3	1.81	0.63
3:R:353:ARG:NH1	4:S:98:CYS:O	2.31	0.63
2:G:98:ARG:HG2	2:G:111:TYR:HB2	1.80	0.63
3:H:182:LEU:HD13	3:H:208:LEU:HD11	1.81	0.63
3:C:178:CYS:SG	3:C:344:SER:OG	2.56	0.62
3:C:184:ASN:HD21	3:C:187:TRP:HD1	1.47	0.62
5:O:113:ILE:HA	5:O:127:VAL:HG22	1.82	0.61
4:D:102:CYS:HA	4:D:112:CYS:HA	1.83	0.61
5:J:16:SER:O	5:J:107:ASN:ND2	2.34	0.61
5:O:113:ILE:HG23	5:O:125:VAL:HG13	1.82	0.61
2:L:53:GLN:NE2	2:L:57:SER:OG	2.34	0.61
5:J:6:THR:HG22	5:J:7:VAL:H	1.66	0.60
1:A:193:ALA:HB2	1:A:208:SER:HB3	1.83	0.60
3:M:182:LEU:HD22	3:M:208:LEU:HD11	1.82	0.60
1:F:15:PRO:HG3	1:F:106:ILE:HD11	1.83	0.60
1:K:90:ASN:ND2	1:K:93:SER:O	2.34	0.60
1:A:61:ARG:NH2	1:A:82:ASP:OD1	2.36	0.59
2:Q:103:TYR:HB3	3:R:184:ASN:HD22	1.67	0.59
3:R:255:THR:HG23	3:R:257:HIS:H	1.68	0.59
3:H:379:ARG:NH2	5:J:91:GLU:OE1	2.36	0.59
1:P:111:ALA:HB3	1:P:140:TYR:H	1.68	0.59
3:C:225:VAL:HG21	3:C:246:LEU:HD23	1.84	0.59
2:G:128:PRO:HB3	2:G:154:TYR:HB3	1.84	0.59



	lo us puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:L:103:TYR:HB3	3:M:184:ASN:HD22	1.68	0.59
5:J:155:LEU:HD11	5:J:187:PHE:HB3	1.85	0.58
5:T:111:PRO:HB3	5:T:205:SER:HA	1.84	0.58
2:G:33:SER:HB3	2:G:98:ARG:HH21	1.69	0.58
3:R:228:VAL:HG22	3:R:246:LEU:HG	1.85	0.58
5:T:37:GLN:OE1	5:T:74:ARG:NH2	2.37	0.58
2:G:1:GLN:HG3	2:G:2:VAL:H	1.69	0.58
5:J:9:ALA:HA	5:J:27:PRO:HG3	1.85	0.57
1:P:21:LEU:HD12	1:P:73:LEU:HD23	1.84	0.57
3:R:229:ILE:HG21	3:R:390:LEU:HD13	1.86	0.57
4:S:102:CYS:SG	4:S:103:SER:N	2.76	0.57
1:A:6:GLN:HE21	1:A:102:THR:HG23	1.68	0.57
2:G:2:VAL:HG22	2:G:27:TYR:HB2	1.85	0.57
5:O:156:TYR:HA	5:O:167:THR:HA	1.86	0.57
1:K:14:SER:HA	1:K:107:LYS:HB2	1.87	0.57
1:F:46:LEU:HD21	1:F:49:LYS:HD3	1.86	0.57
5:J:155:LEU:HB3	5:J:168:ALA:HB3	1.87	0.57
3:R:277:ARG:HH21	5:T:43:GLY:H	1.52	0.56
3:C:223:ARG:HG3	3:C:252:VAL:HG12	1.87	0.56
1:P:79:GLU:HG3	1:P:80:PRO:HD2	1.87	0.56
1:P:108:ARG:HG2	1:P:109:THR:N	2.20	0.56
1:P:113:PRO:HB3	1:P:139:PHE:HB3	1.86	0.56
2:G:72:ARG:HE	2:G:74:THR:HG22	1.69	0.56
4:D:70:CYS:H	5:E:20:LYS:HE3	1.71	0.56
1:F:34:HIS:HD2	1:F:50:TYR:H	1.52	0.56
1:F:106:ILE:O	1:F:166:GLN:NE2	2.35	0.56
3:R:159:CYS:HB2	3:R:299:VAL:HG13	1.87	0.56
2:G:157:GLU:HG3	2:G:158:PRO:CA	2.31	0.56
1:P:106:ILE:O	1:P:166:GLN:NE2	2.38	0.56
3:R:300:LEU:HD21	3:R:337:LYS:HB3	1.88	0.56
4:N:102:CYS:SG	4:N:103:SER:N	2.80	0.55
2:G:164:ASN:ND2	2:G:202:THR:O	2.39	0.55
3:M:265:GLU:OE2	4:N:113:ARG:NH1	2.39	0.55
3:M:372:GLY:O	3:M:373:HIS:ND1	2.39	0.55
2:B:209:HIS:CD2	2:B:211:PRO:HD2	2.42	0.55
3:M:327:MET:O	3:M:379:ARG:NH2	2.39	0.55
3:C:338:ASP:OD1	3:C:339:SER:N	2.37	0.55
3:M:172:VAL:HG12	3:M:177:LEU:HB2	1.87	0.55
2:B:73:ASP:OD1	2:B:73:ASP:N	2.39	0.55
5:E:151:LEU:HD12	5:E:153:TYR:HE1	1.71	0.55
3:C:186:ILE:HD13	3:C:251:PRO:HB3	1.89	0.54



	lo us puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:H:202:ARG:O	3:H:224:ARG:NH1	2.39	0.54
3:M:277:ARG:HG2	3:M:303:PRO:HA	1.89	0.54
5:0:156:TYR:OH	5:0:204:ASP:OD2	2.25	0.54
4:D:61:CYS:SG	4:D:62:LYS:N	2.80	0.54
2:Q:32:ASP:HB2	3:R:251:PRO:HD3	1.88	0.54
4:S:73:LEU:HD12	4:S:75:ALA:H	1.73	0.54
2:B:154:TYR:HE2	2:B:157:GLU:HG2	1.72	0.54
1:K:47:LEU:HD23	1:K:48:ILE:HG12	1.89	0.54
2:L:209:HIS:CD2	2:L:211:PRO:HD2	2.42	0.54
2:Q:29:ILE:HD11	2:Q:74:THR:HA	1.88	0.54
4:D:73:LEU:HD23	4:D:73:LEU:H	1.73	0.53
5:J:11:ASN:ND2	5:J:26:GLU:OE1	2.39	0.53
5:J:16:SER:HB2	5:J:21:THR:HG23	1.90	0.53
5:E:26:GLU:HB2	5:E:27:PRO:HA	1.91	0.53
3:H:159:CYS:O	3:H:211:HIS:NE2	2.40	0.53
5:E:36:VAL:HG22	5:E:75:VAL:HG22	1.91	0.53
5:O:25:TRP:O	5:O:55:THR:OG1	2.27	0.53
1:P:47:LEU:HD23	1:P:58:ILE:HD12	1.91	0.53
2:Q:36:SER:HA	2:Q:51:TYR:HA	1.90	0.53
2:Q:105:ASN:HD22	4:S:117:GLY:HA3	1.74	0.53
2:L:18:LEU:HD12	2:L:118:VAL:HG11	1.90	0.53
3:H:172:VAL:HG22	3:H:177:LEU:HB2	1.91	0.53
3:H:229:ILE:HG21	3:H:390:LEU:HD13	1.91	0.53
2:Q:161:VAL:HG22	2:Q:207:VAL:HG22	1.91	0.53
3:R:172:VAL:HG21	3:R:198:ILE:HD11	1.90	0.53
3:C:300:LEU:HD21	3:C:337:LYS:HB3	1.91	0.53
5:J:193:ILE:HB	5:J:196:ARG:HD2	1.90	0.53
3:C:235:VAL:O	3:C:238:THR:OG1	2.27	0.52
4:S:68:TYR:OH	4:S:79:ARG:NH1	2.42	0.52
5:T:21:THR:N	5:T:60:THR:OG1	2.42	0.52
5:T:48:LYS:HD2	5:T:62:GLU:HG3	1.91	0.52
1:P:98:PHE:CG	2:Q:46:LEU:HD22	2.45	0.52
4:S:51:ALA:N	4:S:61:CYS:SG	2.72	0.52
3:M:245:LEU:HD13	3:M:387:LEU:HD22	1.91	0.52
1:K:33:LEU:HD21	1:K:88:CYS:HB2	1.91	0.52
5:T:35:THR:HG22	5:T:76:PHE:HB2	1.92	0.52
5:J:114:GLN:HG3	5:J:128:GLU:HB3	1.90	0.52
3:R:182:LEU:HD13	3:R:208:LEU:HD21	1.92	0.52
3:R:245:LEU:HD13	3:R:387:LEU:HD22	1.91	0.52
1:K:29:ILE:HD11	1:K:33:LEU:HD12	1.90	0.52
1:P:133:VAL:HG21	2:Q:133:LEU:HD13	1.91	0.52



	lo uo pugo	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:E:152:ILE:HG12	5:E:194:PRO:HD3	1.92	0.51
1:F:80:PRO:HA	1:F:106:ILE:HD13	1.92	0.51
2:G:67:ARG:NH1	2:G:85:SER:O	2.43	0.51
2:L:92:ALA:HB3	2:L:94:TYR:HE1	1.74	0.51
3:C:208:LEU:HD22	3:C:258:VAL:HG13	1.93	0.51
5:J:113:ILE:HA	5:J:127:VAL:HG22	1.93	0.51
3:M:195:PHE:HB3	3:M:201:TRP:HH2	1.75	0.51
1:F:21:LEU:HD13	1:F:73:LEU:HD23	1.91	0.51
2:L:72:ARG:HA	2:L:79:PHE:HA	1.93	0.51
2:Q:204:THR:HG22	2:Q:219:ARG:HB3	1.91	0.51
4:I:72:CYS:O	5:J:135:ARG:NH2	2.43	0.51
1:K:48:ILE:HD13	1:K:54:PRO:HA	1.93	0.51
5:O:12:LEU:HD22	5:O:97:SER:HB2	1.92	0.51
3:R:353:ARG:HD2	4:S:99:GLU:HA	1.92	0.51
5:T:108:LEU:HD11	5:T:193:ILE:HG13	1.91	0.51
1:A:125:LEU:HB3	1:A:183:LYS:HE3	1.93	0.51
5:T:38:ILE:HD12	5:T:59:LEU:HD13	1.93	0.51
3:C:166:TRP:CD2	3:C:261:LEU:HD13	2.46	0.50
1:P:21:LEU:HD22	1:P:102:THR:HG21	1.92	0.50
3:C:279:SER:HB2	3:C:348:HIS:NE2	2.26	0.50
2:G:130:VAL:HG21	2:G:207:VAL:HG21	1.92	0.50
2:G:164:ASN:HB3	2:G:167:ALA:HB3	1.93	0.50
3:M:217:ASP:OD1	3:M:217:ASP:N	2.43	0.50
4:S:120:LEU:HD21	4:S:124:GLY:HA2	1.92	0.50
1:K:107:LYS:HA	1:K:140:TYR:OH	2.11	0.50
5:O:68:LYS:HG2	5:O:103:TYR:HE2	1.77	0.50
3:R:232:SER:HA	3:R:402:ARG:HG2	1.93	0.49
5:T:145:ASP:O	5:T:147:PHE:N	2.42	0.49
1:P:88:CYS:O	1:P:99:GLY:N	2.45	0.49
3:R:242:ASP:OD2	3:R:363:SER:OG	2.24	0.49
3:C:208:LEU:HD12	3:C:252:VAL:HG11	1.94	0.49
5:J:127:VAL:HG21	5:J:189:VAL:HG21	1.93	0.49
3:C:160:PRO:HB2	3:C:163:GLU:HG3	1.94	0.49
3:C:167:GLN:OE1	3:C:282:SER:OG	2.27	0.49
1:F:13:LEU:HD12	1:F:17:GLU:HB3	1.95	0.49
2:G:2:VAL:HG11	2:G:98:ARG:HD2	1.95	0.49
5:O:100:PHE:CZ	5:O:102:PRO:HA	2.48	0.49
1:P:108:ARG:HD3	1:P:140:TYR:HB2	1.93	0.49
3:H:255:THR:HG23	3:H:257:HIS:H	1.78	0.48
3:M:173:ASN:OD1	3:M:203:ASN:ND2	2.42	0.48
4:S:85:LYS:O	4:S:85:LYS:HD3	2.13	0.48



	t i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:S:103:SER:HB2	4:S:113:ARG:HE	1.78	0.48
3:C:161:LYS:NZ	3:C:217:ASP:OD2	2.37	0.48
2:G:219:ARG:H	2:G:219:ARG:HD3	1.78	0.48
3:H:239:THR:HB	3:H:364:TRP:CD1	2.48	0.48
3:M:190:SER:OG	3:M:191:ALA:N	2.46	0.48
2:Q:98:ARG:HB3	2:Q:111:TYR:HB2	1.96	0.48
3:R:336:SER:OG	3:R:337:LYS:NZ	2.43	0.48
3:C:195:PHE:HE2	3:C:204:LEU:HD21	1.78	0.48
2:G:93:VAL:HG22	2:G:117:LEU:HD12	1.95	0.48
5:E:39:SER:HB3	5:E:45:TRP:HA	1.94	0.48
3:H:279:SER:HB3	3:H:348:HIS:NE2	2.29	0.48
5:O:117:GLU:HB2	5:O:124:ASN:HB3	1.96	0.48
3:C:344:SER:HA	3:C:362:VAL:HG13	1.96	0.48
4:N:118:TYR:OH	4:N:135:CYS:O	2.30	0.48
1:F:37:GLN:HB2	1:F:47:LEU:HD11	1.96	0.48
5:T:143:LEU:HD23	5:T:143:LEU:H	1.78	0.48
2:G:154:TYR:OH	2:G:187:LEU:HD23	2.14	0.48
3:R:187:TRP:CZ3	3:R:247:ARG:HB2	2.49	0.48
4:S:102:CYS:HA	4:S:112:CYS:HA	1.95	0.48
2:G:36:SER:HA	2:G:51:TYR:HA	1.96	0.47
5:J:35:THR:HG23	5:J:50:PHE:HA	1.96	0.47
3:M:262:CYS:N	4:N:135:CYS:SG	2.87	0.47
3:R:153:ILE:N	3:R:343:ASP:OD2	2.47	0.47
3:M:338:ASP:OD1	3:M:339:SER:N	2.48	0.47
5:T:106:THR:O	5:T:196:ARG:NH1	2.48	0.47
5:J:136:ARG:HD3	5:J:141:LEU:HD21	1.96	0.47
5:J:143:LEU:O	5:J:146:VAL:N	2.47	0.47
2:L:37:TRP:HB3	2:L:49:ILE:HD11	1.96	0.47
4:N:69:ILE:HD12	5:O:20:LYS:HB3	1.95	0.47
5:O:6:THR:OG1	5:O:32:GLN:NE2	2.45	0.47
4:D:92:VAL:HG11	5:E:51:TYR:HE2	1.79	0.47
5:O:156:TYR:HB3	5:O:167:THR:HG22	1.97	0.47
3:R:338:ASP:OD1	3:R:339:SER:N	2.48	0.47
1:A:113:PRO:HB3	1:A:139:PHE:CB	2.45	0.47
1:K:94:PHE:HB2	4:N:130:THR:OG1	2.14	0.47
3:R:343:ASP:OD1	3:R:343:ASP:N	2.33	0.47
3:M:287:LEU:HD11	3:M:294:ALA:HB2	1.97	0.47
3:R:165:PRO:HB2	3:R:259:VAL:HG12	1.97	0.47
2:B:18:LEU:HB2	2:B:86:VAL:HG11	1.96	0.46
2:B:18:LEU:HD11	2:B:118:VAL:HG11	1.97	0.46
4:D:103:SER:N	4:D:111:SER:O	2.43	0.46



	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:E:28:LYS:HD3	5:E:55:THR:HG21	1.97	0.46
2:L:4:LEU:HD21	2:L:35:TRP:HZ3	1.79	0.46
1:F:134:CYS:HB2	1:F:148:TRP:CZ2	2.51	0.46
5:O:195:SER:HB3	5:O:196:ARG:HH21	1.80	0.46
5:O:110:GLN:HB3	5:O:203:THR:HG23	1.97	0.46
2:Q:51:TYR:CE1	2:Q:59:ASN:HB3	2.51	0.46
2:L:36:SER:HA	2:L:51:TYR:HA	1.97	0.46
1:F:161:GLU:HB3	1:F:175:LEU:HD21	1.98	0.46
2:L:103:TYR:HB3	3:M:184:ASN:ND2	2.30	0.46
4:N:69:ILE:HG23	5:O:20:LYS:HB2	1.97	0.46
1:P:118:PHE:HB2	1:P:133:VAL:HG23	1.98	0.46
5:T:32:GLN:NE2	5:T:34:TYR:OH	2.45	0.46
5:O:196:ARG:HB3	5:O:199:ASN:OD1	2.16	0.46
1:A:15:PRO:HG3	1:A:106:ILE:HD11	1.98	0.45
1:K:183:LYS:HZ2	1:K:186:TYR:HD2	1.63	0.45
4:D:77:GLU:HB3	4:D:85:LYS:HD2	1.98	0.45
5:J:132:THR:OG1	5:J:141:LEU:O	2.33	0.45
2:B:6:GLU:OE2	2:B:115:GLY:N	2.49	0.45
3:C:234:TYR:HD2	3:C:402:ARG:HH12	1.64	0.45
1:F:61:ARG:HH21	1:F:82:ASP:CG	2.19	0.45
1:P:70:ASP:OD1	1:P:70:ASP:N	2.49	0.45
3:C:166:TRP:CD1	3:C:261:LEU:HD22	2.52	0.45
4:I:64:GLN:OE1	4:I:67:SER:OG	2.33	0.45
1:P:138:ASN:HA	1:P:172:THR:HB	1.98	0.45
2:Q:53:GLN:HE21	2:Q:57:SER:HB2	1.82	0.45
3:R:190:SER:OG	3:R:191:ALA:N	2.50	0.45
3:C:172:VAL:HG12	3:C:177:LEU:HB2	1.99	0.45
5:E:86:THR:HA	5:E:89:ALA:HB2	1.99	0.45
1:F:142:ARG:HD3	1:F:163:VAL:HG11	1.99	0.45
2:G:37:TRP:CD2	2:G:81:LEU:HD23	2.52	0.45
1:K:170:ASP:OD1	1:K:170:ASP:N	2.43	0.45
1:K:187:GLU:N	1:K:211:ARG:HH22	2.15	0.45
3:M:229:ILE:HB	3:M:245:LEU:HB3	1.98	0.45
2:Q:16:GLN:HG3	2:Q:17:THR:H	1.82	0.45
2:B:161:VAL:HG22	2:B:207:VAL:HG22	1.98	0.45
3:C:229:ILE:HD13	3:C:390:LEU:HD13	1.98	0.45
5:O:38:ILE:HD11	5:O:59:LEU:HD13	1.98	0.45
2:Q:209:HIS:ND1	2:Q:211:PRO:HD2	2.32	0.45
3:R:273:LEU:HD11	3:R:357:TYR:HB2	1.98	0.45
1:A:32:TYR:HB2	1:A:92:HIS:HB2	1.98	0.45
1:A:36:TYR:N	1:A:87:TYR:O	2.46	0.45



	to do pagon	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:192:TYR:HB2	1:F:209:PHE:HE1	1.81	0.45
3:M:256:ASP:OD1	4:N:133:TYR:OH	2.28	0.45
1:P:33:LEU:HD22	1:P:71:PHE:CG	2.52	0.45
5:E:193:ILE:HG13	5:E:193:ILE:O	2.15	0.45
3:M:242:ASP:HB3	3:M:378:THR:HG21	1.99	0.45
3:M:208:LEU:HD22	3:M:258:VAL:HG22	1.98	0.45
3:M:227:GLN:HB2	3:M:247:ARG:HB3	1.98	0.45
3:R:232:SER:HB3	3:R:404:PRO:HA	1.97	0.45
1:A:28:GLY:HA3	4:D:113:ARG:HG2	1.98	0.45
1:F:110:VAL:HG23	1:F:140:TYR:O	2.16	0.45
3:H:161:LYS:HD3	3:H:211:HIS:CG	2.52	0.45
2:L:126:LYS:HA	2:L:126:LYS:HD3	1.71	0.45
2:Q:18:LEU:HD11	2:Q:118:VAL:HG11	1.98	0.45
2:G:126:LYS:HD2	2:G:184:LEU:HD21	1.99	0.44
3:H:169:LEU:HD11	3:H:176:GLN:HG2	1.98	0.44
3:M:161:LYS:NZ	3:M:217:ASP:OD2	2.50	0.44
1:A:133:VAL:HG22	1:A:178:THR:HB	2.00	0.44
3:C:300:LEU:HD11	3:C:337:LYS:HD3	1.99	0.44
2:Q:35:TRP:HB3	2:Q:79:PHE:CZ	2.53	0.44
5:T:17:THR:HG21	5:T:110:GLN:OE1	2.16	0.44
1:F:149:LYS:HE3	1:F:149:LYS:HB2	1.72	0.44
2:G:154:TYR:OH	2:G:177:ALA:HB2	2.17	0.44
1:P:187:GLU:HA	1:P:211:ARG:HH12	1.82	0.44
3:R:221:GLN:HE21	3:R:258:VAL:HG21	1.83	0.44
3:H:208:LEU:HD22	3:H:258:VAL:HG13	1.98	0.44
5:J:111:PRO:HG2	5:J:205:SER:OG	2.16	0.44
1:K:135:LEU:HD22	2:L:190:VAL:HG21	1.99	0.44
2:L:39:ARG:HH22	2:L:64:LEU:HD11	1.81	0.44
3:R:274:ALA:HB1	3:R:304:ARG:NH2	2.32	0.44
3:M:184:ASN:HD21	3:M:187:TRP:HD1	1.64	0.44
2:B:204:THR:HA	2:B:219:ARG:HA	1.99	0.44
5:J:45:TRP:CH2	5:J:74:ARG:HD3	2.52	0.44
4:N:106:THR:OG1	4:N:107:GLY:N	2.50	0.44
3:M:225:VAL:HG11	3:M:246:LEU:HD23	1.99	0.44
3:R:227:GLN:HB3	3:R:247:ARG:HB3	2.00	0.44
1:A:51:THR:HG21	1:A:71:PHE:HD2	1.83	0.44
3:C:232:SER:HA	3:C:402:ARG:HD2	2.00	0.44
5:E:172:THR:OG1	5:E:173:ASN:N	2.51	0.44
5:O:153:TYR:HE1	5:O:173:ASN:HA	1.82	0.44
3:C:168:VAL:HG21	3:C:188:VAL:HG21	2.00	0.43
2:L:54:TYR:HA	2:L:72:ARG:HH12	1.83	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:M:187:TRP:CD1	3:M:391:MET:HG3	2.53	0.43
3:M:208:LEU:HD23	3:M:209:GLY:N	2.33	0.43
2:B:6:GLU:HA	2:B:22:CYS:HA	2.01	0.43
1:F:94:PHE:O	1:F:96:LEU:N	2.51	0.43
2:L:49:ILE:HG22	2:L:64:LEU:HD12	2.00	0.43
3:M:187:TRP:CZ3	3:M:247:ARG:HB2	2.52	0.43
1:A:77:SER:O	1:A:77:SER:OG	2.30	0.43
3:H:159:CYS:HB2	3:H:299:VAL:HB	2.00	0.43
3:R:277:ARG:O	3:R:303:PRO:HA	2.18	0.43
2:B:164:ASN:HB3	2:B:167:ALA:HB3	1.99	0.43
3:C:225:VAL:HA	3:C:248:LEU:HA	2.01	0.43
5:J:32:GLN:HE22	5:J:77:SER:HB3	1.83	0.43
2:L:102:TYR:HD1	2:L:107:PHE:HB3	1.84	0.43
5:O:194:PRO:HA	5:O:200:ARG:CZ	2.48	0.43
1:P:89:GLN:HG3	1:P:98:PHE:CZ	2.54	0.43
3:R:214:SER:HB3	3:R:295:LEU:HD21	2.01	0.43
1:A:6:GLN:NE2	1:A:102:THR:HG23	2.33	0.43
1:A:6:GLN:OE1	1:A:99:GLY:HA3	2.19	0.43
1:F:120:PRO:HD3	1:F:132:VAL:HG22	2.01	0.43
5:J:157:TYR:HD2	5:J:165:LYS:HB3	1.83	0.43
1:F:105:GLU:OE1	1:F:173:TYR:OH	2.29	0.43
5:J:188:SER:HB2	5:J:207:VAL:HG22	2.00	0.43
5:T:39:SER:HB3	5:T:45:TRP:HD1	1.83	0.43
5:J:154:THR:HG23	5:J:190:GLN:HB3	2.01	0.43
3:C:217:ASP:OD1	3:C:217:ASP:N	2.43	0.43
3:R:272:THR:HG21	4:S:95:ASN:HB2	2.01	0.43
5:T:19:PHE:H	5:T:106:THR:HG23	1.83	0.43
2:B:51:TYR:CE1	2:B:59:ASN:HB3	2.54	0.43
2:L:93:VAL:HG22	2:L:117:LEU:HD13	2.00	0.43
2:B:34:ALA:HB1	2:B:51:TYR:CD2	2.54	0.42
5:E:144:ARG:HH11	5:E:151:LEU:HG	1.83	0.42
2:L:11:LEU:HD12	2:L:156:PRO:HG3	1.99	0.42
2:L:53:GLN:HG2	2:L:54:TYR:N	2.34	0.42
3:R:316:LYS:HE3	3:R:316:LYS:HB3	1.83	0.42
2:B:98:ARG:HD2	2:B:111:TYR:HD2	1.84	0.42
2:L:32:ASP:HB2	3:M:251:PRO:HD3	2.01	0.42
3:M:386:TRP:CD1	3:M:405:PHE:HA	2.55	0.42
4:D:70:CYS:N	5:E:20:LYS:HE3	2.34	0.42
3:H:263:LEU:HD12	3:H:264:PRO:HD2	2.01	0.42
3:H:338:ASP:OD1	3:H:339:SER:N	2.53	0.42
4:N:48:ASP:HB3	4:N:63:ASP:OD2	2.19	0.42



	i i i i i i i i i i i i i i i i i i i	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:P:158:ASN:OD1	1:P:158:ASN:N	2.52	0.42
5:T:15:LYS:HE3	5:T:15:LYS:HB2	1.91	0.42
3:H:245:LEU:HD13	3:H:387:LEU:HD22	2.01	0.42
1:P:187:GLU:HA	1:P:211:ARG:NH1	2.35	0.42
3:C:187:TRP:CZ3	3:C:247:ARG:HB2	2.54	0.42
4:D:118:TYR:HD1	4:D:129:PRO:HA	1.84	0.42
3:H:306:MET:SD	5:J:74:ARG:NH2	2.92	0.42
2:L:52:ILE:HA	2:L:58:THR:HG22	2.01	0.42
3:M:193:HIS:ND1	3:M:242:ASP:OD2	2.52	0.42
1:F:192:TYR:HB2	1:F:209:PHE:CE1	2.55	0.42
2:G:125:THR:HG23	2:G:156:PRO:HD2	2.01	0.42
5:E:67:VAL:O	5:E:102:PRO:HG2	2.19	0.42
2:Q:35:TRP:HB2	2:Q:52:ILE:HG23	2.02	0.42
2:B:154:TYR:HB2	2:B:209:HIS:CE1	2.55	0.41
4:N:62:LYS:HD3	4:N:62:LYS:HA	1.87	0.41
4:N:138:ILE:HG22	4:N:140:ILE:HG12	2.02	0.41
5:E:111:PRO:HG2	5:E:205:SER:HB3	2.01	0.41
5:O:40:THR:HG22	5:O:71:TYR:HE1	1.85	0.41
1:P:95:PRO:HG3	2:Q:62:PRO:HD2	2.02	0.41
1:P:108:ARG:HG2	1:P:109:THR:H	1.84	0.41
2:Q:51:TYR:HE1	2:Q:59:ASN:HB3	1.85	0.41
5:T:101:THR:HG21	5:T:104:LEU:HB2	2.02	0.41
3:H:265:GLU:OE2	4:I:113:ARG:NH2	2.52	0.41
5:J:136:ARG:HH11	5:J:141:LEU:HD21	1.85	0.41
4:N:120:LEU:HA	4:N:127:CYS:HA	2.03	0.41
1:P:115:VAL:HA	1:P:135:LEU:O	2.21	0.41
3:R:201:TRP:HE1	3:R:228:VAL:HG21	1.85	0.41
4:D:96:GLY:O	4:D:110:ARG:NE	2.52	0.41
5:E:16:SER:HA	5:E:20:LYS:O	2.20	0.41
3:M:329:CYS:HA	3:M:376:VAL:HA	2.02	0.41
5:O:136:ARG:HB2	5:O:141:LEU:HD21	2.01	0.41
3:C:182:LEU:HD13	3:C:208:LEU:HD11	2.03	0.41
1:F:188:LYS:HE3	1:F:189:HIS:CE1	2.55	0.41
1:K:120:PRO:HD3	1:K:132:VAL:HG22	2.03	0.41
5:T:111:PRO:HD3	5:T:203:THR:CG2	2.50	0.41
2:B:150:LEU:HD21	2:B:152:LYS:HD3	2.01	0.41
3:C:348:HIS:O	3:C:359:THR:HG22	2.20	0.41
4:D:69:ILE:HG22	5:E:20:LYS:HD2	2.03	0.41
1:F:207:LYS:HB3	1:F:207:LYS:HE2	1.87	0.41
1:P:39:LYS:HG2	1:P:84:ALA:HB2	2.01	0.41
1:P:50:TYR:CE2	3:R:392:ARG:HG3	2.56	0.41



	in a second s	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:Q:24:VAL:HG11	2:Q:35:TRP:CH2	2.56	0.41	
3:R:185:THR:HG22	3:R:254:LEU:HD21	2.02	0.41	
1:A:4:LEU:HD21	1:A:88:CYS:SG	2.60	0.41	
1:A:34:HIS:HD2	1:A:50:TYR:H	1.67	0.41	
1:F:78:LEU:HD21	1:F:104:LEU:HD21	2.02	0.41	
3:M:173:ASN:HA	3:M:203:ASN:ND2	2.36	0.41	
4:S:73:LEU:HB2	4:S:74:PRO:HD2	2.02	0.41	
3:H:254:LEU:HD22	3:H:260:PRO:HD3	2.02	0.41	
3:H:277:ARG:HE	3:H:303:PRO:HB3	1.86	0.41	
3:M:354:GLY:O	4:N:137:LYS:NZ	2.53	0.41	
3:R:357:TYR:OH	4:S:100:GLN:HG3	2.21	0.41	
1:A:11:LEU:HD21	1:A:13:LEU:HD12	2.03	0.41	
2:B:195:SER:HA	2:B:198:LEU:HD13	2.02	0.41	
3:C:338:ASP:HB3	3:C:369:ALA:H	1.85	0.41	
2:G:11:LEU:HD12	2:G:156:PRO:HG3	2.02	0.41	
3:H:217:ASP:OD1	3:H:217:ASP:N	2.43	0.41	
2:L:41:PRO:HD2	2:L:45:GLY:O	2.21	0.41	
2:Q:72:ARG:HA	2:Q:79:PHE:HA	2.02	0.41	
3:R:389:LYS:HG2	3:R:390:LEU:HG	2.02	0.41	
5:E:33:VAL:HG23	5:E:78:TYR:HB2	2.03	0.41	
2:G:41:PRO:HA	2:G:92:ALA:HA	2.03	0.41	
5:J:157:TYR:CE2	5:J:166:LYS:HG3	2.56	0.41	
2:Q:156:PRO:C	2:Q:158:PRO:HD3	2.41	0.41	
1:F:39:LYS:HG3	1:F:40:PRO:HD2	2.03	0.40	
5:J:37:GLN:OE1	5:J:47:SER:OG	2.33	0.40	
2:L:52:ILE:HD11	2:L:72:ARG:HD3	2.03	0.40	
2:L:53:GLN:HG2	2:L:54:TYR:H	1.86	0.40	
2:B:91:THR:HG23	2:B:119:THR:HA	2.03	0.40	
3:C:261:LEU:HD12	3:C:261:LEU:HA	1.91	0.40	
3:C:332:TYR:CE1	3:C:337:LYS:HD2	2.57	0.40	
3:H:230:ILE:HD12	3:H:400:LEU:HD11	2.04	0.40	
1:P:77:SER:O	1:P:77:SER:OG	2.37	0.40	
1:P:139:PHE:HZ	1:P:175:LEU:HB2	1.86	0.40	
3:H:229:ILE:HB	3:H:245:LEU:HB3	2.02	0.40	
4:I:62:LYS:HD3	4:I:69:ILE:HD11	2.03	0.40	
5:O:150:ASP:O	5:O:193:ILE:HG22	2.21	0.40	
5:T:111:PRO:HG3	5:T:204:ASP:O	2.21	0.40	
1:A:12:SER:HA	1:A:105:GLU:O	2.21	0.40	
2:B:53:GLN:HG2	2:B:54:TYR:O	2.22	0.40	
5:E:155:LEU:O	5:E:168:ALA:N	2.46	0.40	
5:J:178:ASP:OD1	5:J:178:ASP:N	2.50	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
5:T:111:PRO:HD3	5:T:203:THR:HG23	2.04	0.40	
5:O:153:TYR:H	5:0:153:TYR:HD1	1.70	0.40	
3:R:366:GLN:HG2	3:R:373:HIS:CD2	2.57	0.40	
3:R:383:TYR:O	3:R:387:LEU:N	2.43	0.40	

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	210/214~(98%)	203~(97%)	7 (3%)	0	100	100
1	F	207/214~(97%)	192 (93%)	15 (7%)	0	100	100
1	K	211/214~(99%)	202 (96%)	9 (4%)	0	100	100
1	Р	206/214~(96%)	197 (96%)	9 (4%)	0	100	100
2	В	213/220~(97%)	204 (96%)	9 (4%)	0	100	100
2	G	212/220~(96%)	201 (95%)	11 (5%)	0	100	100
2	L	212/220~(96%)	205 (97%)	7 (3%)	0	100	100
2	Q	212/220~(96%)	199 (94%)	13 (6%)	0	100	100
3	С	252/254~(99%)	245 (97%)	7 (3%)	0	100	100
3	Н	252/254~(99%)	246 (98%)	6 (2%)	0	100	100
3	М	245/254~(96%)	242 (99%)	3 (1%)	0	100	100
3	R	245/254~(96%)	237 (97%)	8 (3%)	0	100	100
4	D	92/107~(86%)	85 (92%)	7 (8%)	0	100	100
4	Ι	93/107~(87%)	84 (90%)	9 (10%)	0	100	100
4	Ν	93/107~(87%)	88 (95%)	5 (5%)	0	100	100
4	S	88/107 (82%)	77 (88%)	11 (12%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
5	Ε	194/219~(89%)	187~(96%)	7 (4%)	0	100	100
5	J	185/219~(84%)	178~(96%)	7 (4%)	0	100	100
5	Ο	159/219~(73%)	149 (94%)	10 (6%)	0	100	100
5	Т	155/219~(71%)	146 (94%)	9~(6%)	0	100	100
All	All	3736/4056~(92%)	3567~(96%)	169 (4%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	184/186~(99%)	183 (100%)	1 (0%)	88	94	
1	F	182/186~(98%)	180~(99%)	2(1%)	73	86	
1	Κ	185/186~(100%)	181 (98%)	4 (2%)	52	75	
1	Р	183/186~(98%)	181 (99%)	2(1%)	73	86	
2	В	188/191~(98%)	183~(97%)	5(3%)	44	70	
2	G	187/191~(98%)	181 (97%)	6 (3%)	39	67	
2	L	187/191~(98%)	184 (98%)	3~(2%)	62	81	
2	Q	187/191~(98%)	184 (98%)	3 (2%)	62	81	
3	С	216/216~(100%)	210~(97%)	6 (3%)	43	70	
3	Н	216/216~(100%)	209~(97%)	7 (3%)	39	67	
3	М	213/216~(99%)	208 (98%)	5 (2%)	50	74	
3	R	213/216~(99%)	205~(96%)	8 (4%)	33	61	
4	D	82/92~(89%)	74 (90%)	8 (10%)	8	28	
4	Ι	83/92~(90%)	81 (98%)	2(2%)	49	74	
4	Ν	83/92~(90%)	78~(94%)	5~(6%)	19	49	
4	S	80/92~(87%)	76~(95%)	4 (5%)	24	54	
5	Е	185/200~(92%)	177~(96%)	8 (4%)	29	59	



Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
5	J	179/200~(90%)	175~(98%)	4 (2%)	52	75	
5	Ο	160/200~(80%)	155~(97%)	5(3%)	40	68	
5	Т	151/200~(76%)	148 (98%)	3~(2%)	55	77	
All	All	3344/3540~(94%)	3253~(97%)	91 (3%)	44	70	

Continued from previous page...

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

Mol	Mol Chain		Type
1	А	77	SER
2	В	6	GLU
2	В	39	ARG
2	В	72	ARG
2	В	90	ASP
2	В	98	ARG
3	С	157	LYS
3	С	159	CYS
3	С	166	TRP
3	С	193	HIS
3	С	329	CYS
3	С	340	CYS
4	D	50	CYS
4	D	52	SER
4	D	61	CYS
4	D	72	CYS
4	D	73	LEU
4	D	81	CYS
4	D	98	CYS
4	D	135	CYS
5	Е	44	ASP
5	Е	48	LYS
5	Ε	61	ASP
5	Е	74	ARG
5	Е	129	ASP
5	Е	151	LEU
5	Е	186	CYS
5	Е	209	CYS
1	F	63	SER
1	F	186	TYR
2	G	22	CYS
2	G	40	GLN
2	G	51	TYR



Mol	Chain	Res	Type
2	G	121	SER
2	G	149	CYS
2	G	219	ARG
3	H	202	ARG
3	Н	256	ASP
3	Н	277	ARG
3	Н	310	CYS
3	Н	340	CYS
3	Н	368	CYS
3	Н	392	ARG
4	Ι	110	ARG
4	Ι	127	CYS
5	J	32	GLN
5	J	185	TYR
5	J	186	CYS
5	J	210	MET
1	K	6	GLN
1	K	61	ARG
1	K	122	ASP
1	K	211	ARG
2	L	22	CYS
2	L	96	CYS
2	L	217	ASP
3	М	161	LYS
3	М	166	TRP
3	М	199	LYS
3	М	277	ARG
3	М	329	CYS
4	Ν	50	CYS
4	Ν	61	CYS
4	N	102	CYS
4	Ν	110	ARG
4	N	114	CYS
5	Ο	28	LYS
5	Ο	72	LEU
5	0	116	PHE
5	0	144	ARG
5	0	155	LEU
1	Р	11	LEU
1	Р	142	ARG
2	Q	65	LYS
2	Q	98	ARG



00.000	e ontentaca from procee ac page										
Mol	Chain	Res	Type								
2	Q	180	GLN								
3	R	159	CYS								
3	R	201	TRP								
3	R	217	ASP								
3	R	278	PHE								
3	R	284	TRP								
3	R	340	CYS								
3	R	343	ASP								
3	R	381	SER								
4	S	61	CYS								
4	S	70	CYS								
4	S	102	CYS								
4	S	110	ARG								
5	Т	19	PHE								
5	Т	61	ASP								
5	Т	74	ARG								

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	3 H 184		ASN
5	J	18	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 11 are monoatomic - leaving 3 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	Type	Chain	Dec	Tinle	Bo	ond leng	$_{\rm sths}$	B	ond ang	les
	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BGC	D	201	-	11,11,12	1.36	1 (9%)	15,16,17	1.10	2 (13%)
7	BGC	Ι	201	-	11,11,12	1.31	1 (9%)	15,16,17	1.48	4 (26%)
7	BGC	S	201	-	11,11,12	1.18	1 (9%)	15,16,17	0.96	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BGC	D	201	-	-	-	0/1/1/1
7	BGC	Ι	201	-	-	-	0/1/1/1
7	BGC	S	201	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
7	D	201	BGC	O5-C1	3.37	1.51	1.42
7	Ι	201	BGC	O5-C1	3.30	1.51	1.42
7	S	201	BGC	O5-C1	2.94	1.50	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
7	Ι	201	BGC	O5-C5-C4	2.65	114.28	109.52
7	Ι	201	BGC	C6-C5-C4	-2.62	108.24	113.07
7	Ι	201	BGC	C1-C2-C3	2.46	115.42	110.31
7	D	201	BGC	O5-C5-C4	2.24	113.54	109.52
7	D	201	BGC	C6-C5-C4	-2.08	109.22	113.07
7	Ι	201	BGC	O5-C1-C2	2.07	113.97	110.28

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

No monomer is involved in short contacts.

# 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$<$ RSRZ $>$	# <b>RSRZ</b>	>2	$OWAB(Å^2)$	Q<0.9
1	А	212/214~(99%)	0.34	11 (5%) 27	27	34, 68, 108, 118	0
1	F	209/214~(97%)	0.27	12 (5%) 23	24	28, 58, 93, 106	0
1	K	213/214~(99%)	0.22	4 (1%) 66	65	32, 63, 96, 109	0
1	Р	210/214~(98%)	0.21	3 (1%) 75	74	31, 60, 90, 119	0
2	В	217/220~(98%)	0.08	4 (1%) 68	67	29, 64, 94, 110	0
2	G	216/220~(98%)	0.11	7 (3%) 47	46	33, 62, 88, 115	0
2	L	216/220~(98%)	0.01	4 (1%) 66	65	36, 64, 88, 111	0
2	Q	216/220~(98%)	-0.05	1 (0%) 91	90	32, 64, 86, 98	0
3	С	254/254~(100%)	0.20	6 (2%) 59	57	24, 52, 85, 132	0
3	Н	254/254~(100%)	0.20	5 (1%) 65	64	25, 53, 87, 105	0
3	М	249/254~(98%)	0.16	9 (3%) 42	42	28, 55, 89, 135	0
3	R	249/254~(98%)	0.19	3 (1%) 79	77	30, 55, 88, 142	0
4	D	94/107~(87%)	0.00	2 (2%) 63	62	32, 64, 88, 101	0
4	Ι	95/107~(88%)	0.07	2 (2%) 63	62	38, 65, 91, 102	0
4	Ν	95/107~(88%)	-0.02	4 (4%) 36	35	42, 68, 94, 108	0
4	S	92/107~(85%)	0.10	1 (1%) 80	79	43, 72, 101, 109	0
5	Е	200/219~(91%)	0.27	15 (7%) 14	16	30, 64, 99, 113	0
5	J	193/219~(88%)	0.29	13 (6%) 17	19	29, 67, 115, 132	0
5	Ο	171/219~(78%)	0.51	19 (11%) 5	6	35, 82, 124, 138	0
5	Т	163/219~(74%)	0.55	20 (12%) 4	5	35, 73, 114, 127	0
All	All	3818/4056 (94%)	0.19	145 (3%) 40	) 39	24, 61, 101, 142	0

All (145) RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
5	0	112	THR	6.2
1	F	148	TRP	6.0
5	Т	132	THR	5.0
1	F	132	VAL	4.9
3	С	397	PRO	4.5
2	G	220	VAL	4.5
5	Е	183	GLU	4.2
5	Т	90	GLY	4.2
5	Т	134	VAL	4.2
2	L	9	PRO	4.1
5	Т	182	GLY	4.0
2	G	135	PRO	3.9
3	С	291	GLY	3.9
5	J	123	VAL	3.9
5	J	180	ASP	3.9
1	F	134	CYS	3.9
3	М	243	ILE	3.8
1	А	147	GLN	3.7
5	Т	108	LEU	3.6
3	Н	290	ARG	3.6
5	0	103	TYR	3.5
5	0	156	TYR	3.5
5	0	111	PRO	3.5
5	Е	88	SER	3.5
5	Е	175	PHE	3.5
5	Т	183	GLU	3.4
5	Т	133	LEU	3.4
1	А	156	SER	3.4
5	Т	161	SER	3.4
5	Е	182	GLY	3.4
5	Е	145	ASP	3.3
5	J	131	ARG	3.3
4	D	108	THR	3.3
2	В	136	CYS	3.3
5	J	117	GLU	3.3
3	С	288	LEU	3.2
5	0	123	VAL	3.2
5	Т	109	GLY	3.2
5	J	133	LEU	3.2
2	L	11	LEU	3.1
3	М	179	GLY	3.1
5	Ο	137	ASN	3.1
5	Е	176	LEU	3.1



8CN9
------

Mol	Chain	Res	Type	RSRZ
3	М	200	ASN	3.0
5	0	118	GLN	3.0
1	F	63	SER	3.0
3	R	201	TRP	3.0
2	G	129	SER	2.9
5	J	140	PHE	2.9
1	F	185	ASP	2.9
5	Т	153	TYR	2.9
5	J	156	TYR	2.8
5	Е	123	VAL	2.8
3	М	319	ASP	2.8
4	N	58	GLY	2.8
1	А	202	SER	2.8
5	Ο	147	PHE	2.8
5	Т	189	VAL	2.8
1	F	131	SER	2.8
5	J	181	LYS	2.8
1	F	4	LEU	2.8
5	Т	110	GLN	2.8
4	D	117	GLY	2.8
3	Н	287	LEU	2.7
1	Κ	206	THR	2.7
1	А	143	GLU	2.7
1	А	201	LEU	2.7
5	Т	111	PRO	2.7
1	А	121	SER	2.7
5	Т	185	TYR	2.7
5	Е	139	THR	2.7
2	L	95	TYR	2.6
1	Р	191	VAL	2.6
1	F	119	PRO	2.6
1	А	122	ASP	2.6
3	М	178	CYS	2.6
3	R	278	PHE	2.6
2	G	1	GLN	2.6
1	Р	124	GLN	2.6
5	Т	26	GLU	2.6
5	J	82	ASN	2.6
5	0	188	SER	2.5
5	J	175	PHE	2.5
2	В	1	GLN	2.5
5	Е	146	VAL	2.5



Mol	Chain	Res	Type	RSRZ
5	0	174	GLU	2.5
5	0	90	GLY	2.5
1	F	120	PRO	2.5
2	В	12	VAL	2.5
2	Q	147	LEU	2.4
1	А	149	LYS	2.4
1	Κ	63	SER	2.4
3	Н	282	SER	2.4
5	0	113	ILE	2.4
3	М	176	GLN	2.4
5	Е	108	LEU	2.4
5	J	124	ASN	2.4
3	С	203	ASN	2.4
3	М	287	LEU	2.4
5	Т	188	SER	2.4
3	R	347	PRO	2.4
1	А	123	GLU	2.3
5	0	207	VAL	2.3
5	Ε	140	PHE	2.3
5	0	169	LYS	2.3
3	С	319	ASP	2.3
1	F	147	GLN	2.3
2	G	190	VAL	2.3
4	Ν	64	GLN	2.3
5	Т	158	TRP	2.2
1	А	18	ARG	2.2
5	Т	10	TYR	2.2
5	0	134	VAL	2.2
1	K	1	GLU	2.2
1	K	39	LYS	2.2
5	Е	114	GLN	2.2
5	Е	133	LEU	2.2
1	A	103	LYS	2.2
5	Ō	4	THR	2.2
5	0	191	ALA	2.2
5	0	128	GLU	2.2
5	J	188	SER	2.2
1	F	124	GLN	2.2
1	Р	123	GLU	2.2
4	Ι	97	GLY	2.2
3	М	282	SER	2.2
2	G	147	LEU	2.1



Mol	Chain	Res	Type	RSRZ
2	G	200	THR	2.1
3	Н	364	TRP	2.1
4	Ι	106	THR	2.1
2	L	147	LEU	2.1
4	N	71	PHE	2.1
4	N	84	HIS	2.1
5	0	143	LEU	2.1
1	F	135	LEU	2.1
5	J	118	GLN	2.1
3	С	163	GLU	2.1
5	Т	157	TYR	2.0
5	Е	206	PRO	2.0
3	Н	203	ASN	2.0
5	Т	81	GLY	2.0
3	М	280	LEU	2.0
2	В	147	LEU	2.0
4	S	80	ASN	2.0
5	Е	192	VAL	2.0

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
6	CA	М	502	1/1	0.73	0.12	$57,\!57,\!57,\!57$	0
6	CA	R	502	1/1	0.74	0.10	$65,\!65,\!65,\!65$	0
7	BGC	S	201	11/12	0.78	0.15	72,91,108,114	0
7	BGC	Ι	201	11/12	0.79	0.22	70,80,93,96	0
7	BGC	D	201	11/12	0.84	0.17	75,89,107,112	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
6	CA	С	501	1/1	0.84	0.13	66, 66, 66, 66	0
6	CA	Н	502	1/1	0.84	0.10	49,49,49,49	0
6	CA	Κ	301	1/1	0.88	0.23	80,80,80,80	0
6	CA	R	501	1/1	0.88	0.13	52,52,52,52	0
6	CA	М	501	1/1	0.89	0.12	52,52,52,52	0
6	CA	А	301	1/1	0.90	0.17	36,36,36,36	0
6	CA	Н	501	1/1	0.94	0.19	71,71,71,71	0
8	CS	Р	301	1/1	0.95	0.05	115,115,115,115	0
6	CA	F	301	1/1	0.97	0.11	54,54,54,54	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

