

Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 07:13 pm GMT

PDB ID	:	4BH6
Title	:	Insights into degron recognition by APC coactivators from the structure of an
		Acm1-Cdh1 complex
Authors	:	He, J.; Chao, W.C.H.; Zhang, Z.; Yang, J.; Cronin, N.; Barford, D.
Deposited on	:	2013-03-29
Resolution	:	2.90 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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	308	73%	23%	•••
1	В	308	% • 74%	21%	•••
1	С	308	74%	21%	•••
1	D	308	77%	20%	••
1	Е	308	% 70%	26%	• •



2

2

Ο

Р

70

70

21%

24%

4%

• •

•••

• •

7%

10%

7%

71%

70%

Conti	nued from	n previous	page				
Mol	Chain	Length		Qualit	ty of chain	L	
1	F	308	2%	71%			24%
1	C	208	3%				
	G	308	12%	/3%			22%
1	Н	308		70%			24%
2	Ι	70	.% •	51%		33%	9%
2	J	70	.% •	56%		26%	9%
2	К	70		57%		24%	11%
2	L	70		51%	16%	6% •	26%
2	М	70	20%	6% •	70	0%	
2	Ν	70	21%	6% •	719	%	

7%

• •



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21491 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	204	Total	С	Ν	Ο	S	0	0	0
	A	304	2371	1488	419	452	12	0	0	0
1	В	304	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	D	504	2358	1480	415	452	11	0	0	0
1	С	304	Total	С	Ν	Ο	\mathbf{S}	0	Ο	0
1	U	504	2359	1480	416	451	12	0	0	0
1	Л	305	Total	С	Ν	Ο	S	0	0	0
1	D	505	2364	1483	417	452	12	0		0
1	F	303	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	Ľ	505	2344	1472	410	450	12	0	0	0
1	F	304	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	Ľ	504	2347	1475	411	449	12	0	0	
1	C	303	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	G	303	2350	1474	413	451	12	0	0	0
1	Ц	200	Total	С	Ν	Ο	S	0	0	0
	11	299	2321	1457	406	446	12	0	0	0

• Molecule 1 is a protein called APC/C ACTIVATOR PROTEIN CDH1.

• Molecule 2 is a protein called APC/C-CDH1 MODULATOR 1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	Ι	65	Total C N O P S 528 320 98 107 1 2	0	0	0
2	J	63	Total C N O P S 508 309 93 103 1 2	0	0	0
2	K	65	Total C N O P S 528 320 98 107 1 2	0	0	0
2	L	52	Total C N O P S 430 259 78 90 1 2	0	0	0
2	М	21	Total C N O S 179 110 33 35 1	0	0	0
2	Ν	20	Total C N O S 157 97 29 30 1	0	0	0



Continued	from	nrovioue	naae
Commuta	jiom	pretious	paye

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	Ο	20	Total C N O S 170 105 32 32 1	0	0	0
2	Р	21	Total C N O 149 93 24 32	0	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	7	Total O 7 7	0	0
3	В	8	Total O 8 8	0	0
3	С	5	$\begin{array}{cc} \text{Total} & \text{O} \\ 5 & 5 \end{array}$	0	0
3	D	3	Total O 3 3	0	0
3	Ε	4	Total O 4 4	0	0
3	F	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: APC/C ACTIVATOR PROTEIN CDH1



H520 S524 S524 S532 S532 D536 L539 L539 L539 L539 L539 S548

\bullet Molecule 1: APC/C ACTIVATOR PROTEIN CDH1





CEO2 S361 CIV FEO8 S361 CIV FEO8 D365 CIVS FEO8 D365 CIVS FEO1 R365 CIVS SS2 CIV CIV SS3 CIV CIV SS4 CIV CIV SS4 CIV SS4 CIV

• Molecule 1: APC/C ACTIVATOR PROTEIN CDH1







4 Data and refinement statistics (i)

Property	Value	Source	
Space group	C 1 2 1	Depositor	
Cell constants	198.43Å 188.14Å 93.44Å	Descrite	
a, b, c, α , β , γ	90.00° 92.13° 90.00°	Depositor	
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	69.27 - 2.90	Depositor	
Resolution (A)	$69.27 \ - \ 2.90$	EDS	
% Data completeness	96.1 (69.27-2.90)	Depositor	
(in resolution range)	96.1 (69.27-2.90)	EDS	
R _{merge}	0.10	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$1.94 (at 2.91 \text{\AA})$	Xtriage	
Refinement program	REFMAC 5.7.0029	Depositor	
D D.	0.219 , 0.257	Depositor	
Π, Π_{free}	0.218 , 0.256	DCC	
R_{free} test set	3671 reflections $(5.04%)$	wwPDB-VP	
Wilson B-factor $(Å^2)$	55.7	Xtriage	
Anisotropy	0.182	Xtriage	
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.30 , 62.6	EDS	
L-test for twinning ²	$< L >=0.47, < L^2>=0.30$	Xtriage	
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage	
F_o, F_c correlation	0.92	EDS	
Total number of atoms	21491	wwPDB-VP	
Average B, all atoms $(Å^2)$	65.0	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 38.28 % 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 3.7776e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: SEP

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	Bo	ond lengths	Bond angles		
			# Z > 5	RMSZ	# Z > 5	
1	А	0.63	0/2425	0.79	2/3297~(0.1%)	
1	В	0.71	4/2412~(0.2%)	0.80	6/3283~(0.2%)	
1	С	0.62	0/2413	0.80	2/3284~(0.1%)	
1	D	0.56	0/2418	0.75	1/3291~(0.0%)	
1	Е	0.56	0/2397	0.75	1/3262~(0.0%)	
1	F	0.51	0/2401	0.72	2/3269~(0.1%)	
1	G	0.52	0/2403	0.72	1/3270~(0.0%)	
1	Н	0.46	0/2374	0.67	1/3230~(0.0%)	
2	Ι	0.79	4/524~(0.8%)	0.87	0/703	
2	J	0.58	0/504	0.80	0/677	
2	Κ	0.66	0/524	0.88	1/703~(0.1%)	
2	L	0.61	0/427	0.80	0/576	
2	М	0.46	0/182	0.72	1/244~(0.4%)	
2	Ν	0.53	0/160	0.76	0/216	
2	0	0.44	0/173	0.71	0/232	
2	Р	0.52	0/151	0.64	0/206	
All	All	0.58	8/21888~(0.0%)	0.76	18/29743~(0.1%)	

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	В	0	1
2	Ι	0	1
2	J	0	1
2	Κ	0	1
2	L	0	2
All	All	0	6



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	545	PHE	CG-CD2	-9.56	1.24	1.38
1	В	545	PHE	CG-CD1	-9.13	1.25	1.38
2	Ι	92	ASN	CG-ND2	-6.11	1.17	1.32
2	Ι	100	ASN	CG-ND2	-5.72	1.18	1.32
2	Ι	100	ASN	CG-OD1	-5.69	1.11	1.24
1	В	545	PHE	CE2-CZ	-5.64	1.26	1.37
2	Ι	92	ASN	CG-OD1	-5.52	1.11	1.24
1	В	545	PHE	CE1-CZ	-5.39	1.27	1.37

All (8) bond length outliers are listed below:

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	452	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	А	452	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	Н	497	LEU	CA-CB-CG	7.00	131.40	115.30
1	С	497	LEU	CA-CB-CG	6.60	130.47	115.30
1	F	497	LEU	CA-CB-CG	6.53	130.32	115.30
1	Е	497	LEU	CA-CB-CG	6.50	130.25	115.30
1	D	497	LEU	CA-CB-CG	6.46	130.16	115.30
1	А	497	LEU	CA-CB-CG	6.40	130.02	115.30
1	В	545	PHE	CE1-CZ-CE2	-6.19	108.86	120.00
1	В	452	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	G	497	LEU	CA-CB-CG	5.82	128.69	115.30
1	F	452	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	В	497	LEU	CA-CB-CG	5.42	127.76	115.30
1	В	545	PHE	CB-CG-CD1	5.33	124.53	120.80
1	В	452	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	Κ	111	ARG	NE-CZ-NH2	5.10	122.85	120.30
2	М	63	LEU	CA-CB-CG	5.03	126.88	115.30
1	В	545	PHE	CD1-CG-CD2	-5.02	111.78	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	362	ARG	Peptide
2	Ι	107	CYS	Peptide
2	J	107	CYS	Peptide
2	Κ	107	CYS	Peptide
2	L	107	CYS	Peptide
2	L	110	GLU	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	2371	0	2309	45	0
1	В	2358	0	2280	54	0
1	С	2359	0	2281	42	0
1	D	2364	0	2283	38	0
1	Е	2344	0	2262	59	0
1	F	2347	0	2266	55	0
1	G	2350	0	2269	52	0
1	Н	2321	0	2246	57	0
2	Ι	528	0	498	24	0
2	J	508	0	476	23	0
2	Κ	528	0	495	24	0
2	L	430	0	390	24	0
2	М	179	0	158	7	0
2	Ν	157	0	128	6	0
2	0	170	0	152	2	0
2	Р	149	0	107	4	0
3	А	7	0	0	3	0
3	В	8	0	0	2	0
3	С	5	0	0	1	0
3	D	3	0	0	0	0
3	Е	4	0	0	1	0
3	F	1	0	0	0	0
All	All	21491	0	20600	433	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 10.

All (433) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:264:PHE:H	2:L:92:ASN:HD21	1.08	0.99
1:G:264:PHE:H	2:J:92:ASN:HD21	1.14	0.92
1:B:544:LEU:HB3	1:B:545:PHE:CE1	2.04	0.91
1:E:494:LYS:HE3	3:E:2003:HOH:O	1.75	0.86
1:B:544:LEU:C	1:B:545:PHE:HD1	1.77	0.86



	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:D:264:PHE:H	2:L:100:ASN:HD21	1.23	0.83
1:B:264:PHE:H	2:J:100:ASN:HD21	1.26	0.82
1:E:306:THR:HG22	1:E:347:VAL:O	1.80	0.82
2:J:119:ARG:HA	2:L:111:ARG:HH21	1.48	0.78
1:G:473:GLN:HE21	2:J:91:GLU:HG3	1.47	0.77
1:G:473:GLN:NE2	2:J:91:GLU:HG3	2.00	0.77
1:F:306:THR:HG22	1:F:347:VAL:O	1.84	0.77
1:H:386:GLN:OE1	2:L:88:VAL:HB	1.84	0.76
1:C:264:PHE:H	2:K:100:ASN:HD21	1.30	0.76
1:H:306:THR:HG22	1:H:347:VAL:O	1.88	0.74
1:H:323:ASN:O	2:P:78:HIS:HE1	1.71	0.73
1:A:501:ASP:O	1:A:502:CYS:HB2	1.89	0.72
1:B:544:LEU:C	1:B:545:PHE:CD1	2.63	0.72
1:G:268:LEU:H	1:G:520:HIS:HD2	1.38	0.71
2:L:110:GLU:OE2	2:L:110:GLU:N	2.23	0.71
1:F:268:LEU:H	1:F:520:HIS:HD2	1.39	0.71
1:E:268:LEU:H	1:E:520:HIS:HD2	1.39	0.70
1:H:323:ASN:O	2:P:78:HIS:CE1	2.45	0.70
1:B:501:ASP:O	1:B:502:CYS:HB2	1.91	0.69
1:B:268:LEU:H	1:B:520:HIS:HD2	1.38	0.69
1:E:386:GLN:OE1	2:I:88:VAL:HB	1.92	0.69
1:E:473:GLN:HE21	2:I:91:GLU:HG3	1.58	0.68
1:H:371:VAL:HG13	2:P:63:LEU:HD22	1.75	0.68
1:F:495:TYR:CZ	2:K:105:LYS:HD3	2.28	0.68
1:B:306:THR:HG22	1:B:347:VAL:O	1.94	0.67
2:I:112:ALA:C	2:K:113:PHE:HA	2.14	0.67
1:B:268:LEU:H	1:B:520:HIS:CD2	2.12	0.67
1:C:501:ASP:O	1:C:502:CYS:HB2	1.95	0.67
1:C:268:LEU:H	1:C:520:HIS:HD2	1.41	0.67
1:C:245:ARG:NH1	1:C:485:GLU:OE2	2.29	0.66
1:G:253:ARG:HD3	2:J:124:ASP:OD2	1.94	0.66
1:H:268:LEU:H	1:H:520:HIS:HD2	1.40	0.66
1:H:473:GLN:HE21	2:L:91:GLU:HG3	1.61	0.66
1:B:544:LEU:HB3	1:B:545:PHE:CD1	2.31	0.66
1:E:473:GLN:NE2	2:I:91:GLU:HG3	2.10	0.66
1:F:268:LEU:H	1:F:520:HIS:CD2	2.14	0.66
1:A:306:THR:HG22	1:A:347:VAL:O	1.96	0.65
1:H:473:GLN:NE2	2:L:91:GLU:HG3	2.12	0.65
1:F:473:GLN:HE21	2:K:91:GLU:HG3	1.61	0.65
1:F:501:ASP:O	1:F:502:CYS:HB2	1.96	0.64
1:C:306:THR:HG22	1:C:347:VAL:O	1.98	0.64



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:332:MET:HG3	1:H:333:LYS:N	2.10	0.64
1:E:268:LEU:H	1:E:520:HIS:CD2	2.16	0.64
1:D:501:ASP:O	1:D:502:CYS:HB2	1.98	0.63
1:C:268:LEU:H	1:C:520:HIS:CD2	2.16	0.63
1:E:501:ASP:O	1:E:502:CYS:HB2	1.98	0.63
1:G:268:LEU:H	1:G:520:HIS:CD2	2.17	0.63
1:E:302:GLU:CD	1:E:302:GLU:H	2.01	0.63
1:A:429:ALA:HB3	2:I:99:GLU:HG3	1.79	0.63
1:G:247:ILE:HD13	1:G:499:LEU:HD23	1.79	0.63
1:B:544:LEU:HB3	1:B:545:PHE:HE1	1.58	0.62
1:F:473:GLN:NE2	2:K:91:GLU:HG3	2.13	0.62
1:G:501:ASP:O	1:G:502:CYS:HB2	1.99	0.62
1:F:330:ASP:HB2	1:F:337:ILE:HG12	1.81	0.62
1:B:330:ASP:HB2	1:B:337:ILE:HG12	1.82	0.62
1:E:341:SER:HB2	2:N:78:HIS:HD2	1.64	0.62
1:D:345:ASP:OD2	1:D:362:ARG:HD2	1.98	0.62
1:F:264:PHE:H	2:K:92:ASN:HD21	1.46	0.62
1:H:268:LEU:H	1:H:520:HIS:CD2	2.17	0.62
1:A:316:HIS:HE1	3:A:2003:HOH:O	1.83	0.62
1:E:258:PRO:HB3	2:I:119:ARG:HG2	1.81	0.62
1:G:306:THR:HG22	1:G:347:VAL:O	1.98	0.61
2:I:109:TYR:O	2:I:110:GLU:C	2.39	0.60
1:E:537:GLU:OE1	2:I:119:ARG:NH2	2.35	0.59
1:A:268:LEU:H	1:A:520:HIS:CD2	2.20	0.59
1:A:330:ASP:HB2	1:A:337:ILE:HG12	1.84	0.59
1:A:268:LEU:H	1:A:520:HIS:HD2	1.50	0.59
1:G:330:ASP:HB2	1:G:337:ILE:HG12	1.85	0.59
1:B:371:VAL:HG13	2:J:63:LEU:HD13	1.86	0.58
1:D:514:HIS:HE1	1:D:532:SER:OG	1.86	0.58
1:H:330:ASP:HB2	1:H:337:ILE:HG12	1.85	0.58
1:B:345:ASP:OD2	1:B:362:ARG:HD2	2.03	0.58
1:H:501:ASP:O	1:H:502:CYS:HB2	2.03	0.58
1:A:459:VAL:O	1:A:461:THR:N	2.36	0.58
1:D:268:LEU:H	1:D:520:HIS:CD2	2.22	0.58
1:G:427:LYS:HE3	2:J:82:TYR:CE2	2.39	0.58
1:B:514:HIS:HE1	1:B:532:SER:OG	1.86	0.57
1:C:345:ASP:OD2	1:C:362:ARG:HD2	2.04	0.57
1:H:345:ASP:OD2	1:H:362:ARG:HD2	2.04	0.57
3:B:2008:HOH:O	2:J:102:SEP:HB2	2.03	0.57
1:D:268:LEU:H	1:D:520:HIS:HD2	1.52	0.57
1:H:514:HIS:HE1	1:H:532:SER:OG	1.88	0.57



	A la C	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:E:288:THR:OG1	2:I:122:LEU:HD13	2.05	0.56	
1:F:256:ASP:HB2	2:K:125:LEU:HD21	1.86	0.56	
1:B:247:ILE:HD13	1:B:499:LEU:CD2	2.36	0.56	
1:D:432:ALA:HB1	1:D:477:MET:HB2	1.86	0.56	
1:E:341:SER:HB2	2:N:78:HIS:CD2	2.39	0.56	
2:I:123:LYS:HD3	2:K:111:ARG:CD	2.35	0.56	
1:E:330:ASP:HB2	1:E:337:ILE:HG12	1.86	0.56	
1:G:386:GLN:OE1	2:J:88:VAL:HB	2.06	0.56	
1:C:330:ASP:HB2	1:C:337:ILE:HG12	1.87	0.56	
2:J:119:ARG:HA	2:L:111:ARG:NH2	2.19	0.56	
2:I:69:GLU:O	2:I:73:ILE:HD12	2.07	0.55	
1:B:480:SER:HB2	1:B:545:PHE:CE2	2.40	0.55	
1:G:514:HIS:HE1	1:G:532:SER:OG	1.89	0.55	
1:D:330:ASP:HB2	1:D:337:ILE:HG12	1.88	0.55	
1:G:480:SER:HB3	1:G:483:THR:O	2.06	0.55	
1:A:514:HIS:HE1	1:A:532:SER:OG	1.90	0.55	
2:L:110:GLU:N	2:L:110:GLU:CD	2.60	0.55	
1:B:544:LEU:O	1:B:545:PHE:HD1	1.88	0.55	
1:E:514:HIS:HE1	1:E:532:SER:OG	1.90	0.54	
2:I:123:LYS:HD3	2:K:111:ARG:HD2	1.89	0.54	
1:E:495:TYR:CZ	2:I:105:LYS:HD3	2.42	0.54	
1:B:545:PHE:CD1	1:B:545:PHE:N	2.69	0.54	
1:G:245:ARG:O	1:G:245:ARG:HG2	2.05	0.54	
1:C:517:ARG:HH22	2:K:100:ASN:ND2	2.05	0.54	
1:H:432:ALA:HB1	1:H:477:MET:HB2	1.90	0.54	
1:A:362:ARG:C	1:A:363:ASP:O	2.42	0.54	
1:G:345:ASP:OD2	1:G:362:ARG:HD2	2.08	0.54	
1:C:480:SER:OG	1:C:483:THR:HG23	2.07	0.53	
1:D:480:SER:OG	1:D:483:THR:HG23	2.07	0.53	
1:G:517:ARG:HH22	2:J:92:ASN:ND2	2.07	0.53	
1:A:429:ALA:CB	2:I:99:GLU:HG3	2.38	0.53	
1:F:362:ARG:C	1:F:363:ASP:O	2.43	0.53	
1:H:264:PHE:H	2:L:92:ASN:ND2	1.91	0.53	
1:H:427:LYS:HE3	2:L:82:TYR:CE2	2.44	0.53	
2:M:69:GLU:O	2:M:73:ILE:HG13	2.08	0.53	
1:F:272:SER:HB3	1:F:310:TRP:CE2	2.43	0.53	
1:A:292:THR:HB	1:A:294:ASP:HB2	1.90	0.53	
1:G:268:LEU:HB3	1:G:280:ALA:HB3	1.90	0.53	
1:F:449:THR:N	2:K:91:GLU:OE2	2.39	0.53	
1:F:323:ASN:O	2:M:78:HIS:HE1	1.91	0.52	
1:F:330:ASP:OD1	1:F:332:MET:HG2	2.09	0.52	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:495:TYR:CZ	2:L:105:LYS:HD3	2.45	0.52
1:D:362:ARG:C	1:D:363:ASP:O	2.46	0.52
1:D:272:SER:HB3	1:D:310:TRP:CE2	2.45	0.52
1:H:264:PHE:N	2:L:92:ASN:HD21	1.91	0.52
1:B:253:ARG:HD2	1:B:255:LEU:HD21	1.91	0.52
1:E:256:ASP:OD1	2:I:119:ARG:NH1	2.43	0.52
1:F:269:ILE:O	1:F:269:ILE:HG23	2.10	0.52
1:B:432:ALA:HB1	1:B:477:MET:HB2	1.91	0.52
1:D:459:VAL:O	1:D:461:THR:N	2.43	0.52
1:G:253:ARG:HD2	1:G:255:LEU:HD21	1.92	0.51
1:A:315:SER:OG	1:A:316:HIS:HD2	1.93	0.51
1:C:432:ALA:HB1	1:C:477:MET:HB2	1.91	0.51
1:H:292:THR:HB	1:H:294:ASP:HB2	1.90	0.51
1:E:479:TRP:CZ3	1:E:484:ASN:OD1	2.64	0.51
1:E:480:SER:OG	1:E:483:THR:HG23	2.10	0.51
1:F:292:THR:HB	1:F:294:ASP:HB2	1.93	0.51
1:F:345:ASP:OD2	1:F:362:ARG:HD2	2.11	0.51
1:A:345:ASP:OD2	1:A:362:ARG:HD2	2.10	0.51
1:D:517:ARG:HH22	2:L:100:ASN:ND2	2.09	0.51
1:F:371:VAL:CG1	2:M:63:LEU:HD22	2.41	0.51
1:G:310:TRP:CZ3	1:G:331:VAL:HG21	2.46	0.51
1:B:447:GLY:HA3	1:B:451:ASP:OD2	2.10	0.51
1:F:479:TRP:CZ3	1:F:484:ASN:OD1	2.64	0.51
1:E:292:THR:HB	1:E:294:ASP:HB2	1.92	0.51
2:K:113:PHE:O	2:K:114:LEU:O	2.29	0.51
2:L:69:GLU:O	2:L:73:ILE:HD12	2.10	0.51
1:H:386:GLN:OE1	2:L:88:VAL:CB	2.57	0.50
1:D:269:ILE:HG23	1:D:269:ILE:O	2.10	0.50
1:D:292:THR:HB	1:D:294:ASP:HB2	1.93	0.50
1:C:514:HIS:HE1	1:C:532:SER:OG	1.95	0.50
1:H:311:ILE:HD11	2:P:61:PHE:HE2	1.77	0.50
1:D:306:THR:HG22	1:D:347:VAL:O	2.12	0.50
1:E:345:ASP:OD2	1:E:362:ARG:HD2	2.12	0.50
1:B:261:ALA:O	1:B:520:HIS:HE1	1.94	0.50
1:E:268:LEU:HB3	1:E:280:ALA:HB3	1.92	0.50
1:C:292:THR:HB	1:C:294:ASP:HB2	1.94	0.50
1:H:370:ASP:HB3	1:H:373:MET:HB2	1.94	0.50
1:B:484:ASN:O	1:B:502:CYS:HB2	2.12	0.49
1:F:253:ARG:HD2	1:F:255:LEU:HD21	1.94	0.49
1:F:371:VAL:HG13	2:M:63:LEU:HD22	1.93	0.49
1:G:292:THR:HB	1:G:294:ASP:HB2	1.94	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:432:ALA:HB1	1:A:477:MET:HB2	1.94	0.49
1:F:514:HIS:HE1	1:F:532:SER:OG	1.95	0.49
1:B:271:TRP:CD2	1:B:524:SER:HA	2.48	0.49
2:I:109:TYR:O	2:I:110:GLU:O	2.29	0.49
1:D:459:VAL:CG1	1:D:460:ASN:N	2.76	0.49
2:K:69:GLU:O	2:K:73:ILE:HD12	2.13	0.49
1:G:247:ILE:HD12	1:G:508:ILE:HG22	1.94	0.49
1:A:261:ALA:O	1:A:520:HIS:HE1	1.96	0.49
1:B:543:LYS:NZ	1:B:545:PHE:O	2.40	0.49
1:F:254:VAL:HG12	2:K:125:LEU:HD12	1.95	0.49
1:F:258:PRO:HG3	2:K:119:ARG:HB3	1.93	0.49
1:C:452:ARG:HG2	1:C:472:SER:C	2.33	0.48
1:G:269:ILE:CG2	1:G:520:HIS:HB3	2.42	0.48
1:G:272:SER:HB3	1:G:310:TRP:CE2	2.47	0.48
1:H:517:ARG:HH22	2:L:92:ASN:HD22	1.61	0.48
1:A:272:SER:HB3	1:A:310:TRP:CE2	2.48	0.48
1:E:247:ILE:HD13	1:E:509:ALA:HB2	1.95	0.48
1:H:272:SER:HB3	1:H:310:TRP:CE2	2.48	0.48
1:H:362:ARG:C	1:H:363:ASP:O	2.47	0.48
1:B:362:ARG:C	1:B:363:ASP:O	2.51	0.48
1:E:269:ILE:CG2	1:E:520:HIS:HB3	2.44	0.48
1:A:480:SER:OG	1:A:483:THR:HG23	2.13	0.48
1:E:254:VAL:HG12	2:I:125:LEU:HD12	1.96	0.48
1:G:489:SER:HB2	1:G:518:VAL:HB	1.96	0.48
1:B:292:THR:HB	1:B:294:ASP:HB2	1.95	0.48
1:C:362:ARG:C	1:C:363:ASP:O	2.48	0.48
1:B:480:SER:CB	1:B:545:PHE:CE2	2.97	0.48
1:G:271:TRP:CD2	1:G:524:SER:HA	2.49	0.48
1:G:365:ARG:HG2	1:G:382:GLU:CG	2.44	0.48
1:D:479:TRP:CZ3	1:D:484:ASN:OD1	2.67	0.47
1:F:432:ALA:HB1	1:F:477:MET:HB2	1.95	0.47
1:E:451:ASP:O	1:E:453:ARG:HG2	2.14	0.47
1:B:479:TRP:CZ3	1:B:484:ASN:OD1	2.67	0.47
1:F:268:LEU:HB3	1:F:280:ALA:HB3	1.96	0.47
1:C:269:ILE:CG2	1:C:520:HIS:HB3	2.44	0.47
1:E:310:TRP:CZ3	1:E:331:VAL:HG21	2.49	0.47
1:F:323:ASN:O	2:M:78:HIS:CE1	2.68	0.47
1:H:269:ILE:CG2	1:H:520:HIS:HB3	2.44	0.47
1:A:339:THR:N	2:I:66:GLU:OE2	2.46	0.47
1:A:365:ARG:HG2	1:A:382:GLU:CG	2.45	0.47
1:D:370:ASP:HB3	1:D:373:MET:HB2	1.97	0.47



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Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:421:LEU:HD21	1:A:462:SER:OG	2.15	0.47	
1:B:492:TYR:HA	1:B:493:SER:HA	1.75	0.47	
1:F:269:ILE:CG2	1:F:520:HIS:HB3	2.45	0.47	
1:F:370:ASP:HB3	1:F:373:MET:HB2	1.97	0.47	
1:G:258:PRO:O	1:G:259:SER:HB2	2.15	0.47	
1:H:365:ARG:HG2	1:H:382:GLU:CG	2.45	0.47	
1:D:371:VAL:HG13	2:L:63:LEU:HD13	1.97	0.46	
1:E:432:ALA:HB1	1:E:477:MET:HB2	1.96	0.46	
1:E:272:SER:HB3	1:E:310:TRP:CE2	2.50	0.46	
1:F:452:ARG:HG2	1:F:472:SER:C	2.36	0.46	
1:A:271:TRP:CD2	1:A:524:SER:HA	2.50	0.46	
1:A:316:HIS:CE1	3:A:2003:HOH:O	2.65	0.46	
1:F:271:TRP:CD2	1:F:524:SER:HA	2.50	0.46	
1:G:247:ILE:HD13	1:G:499:LEU:CD2	2.44	0.46	
1:H:261:ALA:O	1:H:520:HIS:HE1	1.98	0.46	
1:H:361:SER:OG	1:H:362:ARG:N	2.48	0.46	
1:C:517:ARG:HH22	2:K:100:ASN:HD22	1.62	0.46	
1:G:362:ARG:C	1:G:363:ASP:O	2.50	0.46	
1:G:370:ASP:HB3	1:G:373:MET:HB2	1.97	0.46	
1:B:310:TRP:CZ3	1:B:331:VAL:HG21	2.50	0.46	
1:B:338:ARG:HA	2:J:66:GLU:OE1	2.16	0.46	
1:D:361:SER:O	1:D:363:ASP:O	2.33	0.46	
1:E:362:ARG:C	1:E:363:ASP:O	2.49	0.46	
1:A:492:TYR:CE1	2:I:102:SEP:HB2	2.51	0.46	
1:E:339:THR:HG21	2:N:75:VAL:HG23	1.98	0.46	
1:H:492:TYR:HA	1:H:493:SER:HA	1.73	0.46	
1:H:271:TRP:CD2	1:H:524:SER:HA	2.51	0.46	
2:I:120:ILE:H	2:K:111:ARG:NH2	2.13	0.46	
1:D:421:LEU:HD13	1:D:423:PHE:CZ	2.51	0.46	
1:B:269:ILE:HG23	1:B:269:ILE:O	2.16	0.46	
1:D:514:HIS:HD2	1:D:536:ASP:OD2	1.99	0.46	
1:E:372:ARG:O	2:N:64:TYR:HB2	2.15	0.46	
1:B:338:ARG:HA	2:J:66:GLU:CD	2.36	0.46	
1:B:545:PHE:HD2	3:B:2007:HOH:O	1.99	0.46	
1:D:452:ARG:HG2	1:D:472:SER:C	2.36	0.46	
1:E:271:TRP:CD2	1:E:524:SER:HA	2.50	0.46	
2:M:77:ARG:O	2:M:77:ARG:NE	2.45	0.46	
1:A:268:LEU:HB3	1:A:280:ALA:HB3	1.97	0.45	
1:C:370:ASP:HB3	1:C:373:MET:HB2	1.98	0.45	
1:C:492:TYR:HA	1:C:493:SER:HA	1.73	0.45	
1:G:288:THR:OG1	2:J:122:LEU:HD13	2.16	0.45	



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:308:LEU:HB2	1:B:317:LEU:HD11	1.98	0.45
1:E:479:TRP:HZ3	1:E:484:ASN:OD1	1.99	0.45
1:B:258:PRO:O	1:B:259:SER:HB2	2.17	0.45
1:H:497:LEU:HD22	1:H:518:VAL:HG11	1.99	0.45
1:G:459:VAL:O	1:G:461:THR:N	2.50	0.45
1:H:269:ILE:HG23	1:H:269:ILE:O	2.17	0.45
1:C:371:VAL:HG13	2:K:63:LEU:HD13	1.99	0.44
1:G:479:TRP:CZ3	1:G:484:ASN:OD1	2.70	0.44
1:A:299:CYS:HB3	1:A:329:TYR:CE2	2.53	0.44
1:C:451:ASP:O	1:C:453:ARG:HG2	2.16	0.44
1:F:479:TRP:HZ3	1:F:484:ASN:OD1	2.00	0.44
1:H:427:LYS:HE3	2:L:82:TYR:CZ	2.52	0.44
1:G:247:ILE:CD1	1:G:508:ILE:HG22	2.48	0.44
1:G:269:ILE:HG23	1:G:269:ILE:O	2.17	0.44
1:H:479:TRP:CZ3	1:H:484:ASN:OD1	2.71	0.44
1:B:337:ILE:HD13	1:B:337:ILE:HA	1.74	0.44
1:E:459:VAL:CG1	1:E:460:ASN:N	2.79	0.44
1:F:264:PHE:HA	1:F:519:LEU:HD22	2.00	0.44
1:E:268:LEU:N	1:E:520:HIS:HD2	2.11	0.44
1:G:361:SER:OG	1:G:362:ARG:N	2.50	0.44
1:A:269:ILE:HG21	1:A:520:HIS:HB3	2.00	0.44
1:A:315:SER:OG	1:A:316:HIS:CD2	2.70	0.44
1:A:516:PHE:HB3	3:A:2001:HOH:O	2.18	0.44
1:E:394:ASN:CG	1:E:397:ASP:HB2	2.37	0.44
1:G:337:ILE:HD13	1:G:337:ILE:HA	1.78	0.44
1:H:254:VAL:HG22	1:H:540:ARG:HG2	1.99	0.44
1:C:479:TRP:CZ3	1:C:484:ASN:OD1	2.71	0.44
1:E:370:ASP:HB3	1:E:373:MET:HB2	2.00	0.44
1:A:484:ASN:O	1:A:502:CYS:HB2	2.18	0.44
1:E:459:VAL:HG12	1:E:460:ASN:N	2.33	0.44
1:G:517:ARG:HH22	2:J:92:ASN:HD22	1.64	0.44
1:H:451:ASP:O	1:H:453:ARG:HG2	2.17	0.44
1:A:459:VAL:CG1	1:A:460:ASN:N	2.81	0.43
1:C:268:LEU:HB3	1:C:280:ALA:HB3	2.00	0.43
1:C:269:ILE:HG21	1:C:520:HIS:HB3	2.00	0.43
1:B:368:HIS:HB2	1:B:379:GLU:HB3	1.99	0.43
1:E:253:ARG:HD2	1:E:255:LEU:HD21	1.99	0.43
1:E:365:ARG:HG2	1:E:382:GLU:CG	2.48	0.43
1:F:490:HIS:CD2	1:F:498:THR:HG23	2.52	0.43
1:G:368:HIS:HB2	1:G:379:GLU:HB3	2.00	0.43
1:H:264:PHE:HA	1:H:519:LEU:HD22	2.00	0.43



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:M:72:ASN:HD22	2:M:72:ASN:HA	1.67	0.43	
1:E:484:ASN:O	1:E:502:CYS:HB2	2.19	0.43	
1:F:514:HIS:CE1	1:F:540:ARG:HD2	2.54	0.43	
1:D:271:TRP:CD2	1:D:524:SER:HA	2.53	0.43	
1:G:264:PHE:HA	1:G:519:LEU:HD22	2.00	0.43	
2:J:114:LEU:HD13	2:J:118:GLY:HA3	1.99	0.43	
1:A:310:TRP:CZ3	1:A:331:VAL:HG21	2.53	0.43	
1:C:394:ASN:CG	1:C:397:ASP:HB2	2.39	0.43	
1:F:253:ARG:HD3	2:K:124:ASP:OD2	2.18	0.43	
1:F:412:TYR:CD1	1:F:412:TYR:N	2.86	0.43	
1:F:514:HIS:HD2	1:F:536:ASP:OD2	2.01	0.43	
1:G:432:ALA:HB1	1:G:477:MET:HB2	2.00	0.43	
1:H:368:HIS:HB2	1:H:379:GLU:HB3	2.01	0.43	
2:I:79:ASN:O	2:I:83:ASN:ND2	2.47	0.43	
2:K:120:ILE:O	2:K:121:ALA:C	2.56	0.43	
1:C:468:ILE:HD13	1:C:505:MET:HE2	1.99	0.43	
1:F:492:TYR:HA	1:F:493:SER:HA	1.67	0.43	
2:O:69:GLU:O	2:O:73:ILE:CD1	2.66	0.43	
1:C:271:TRP:CD2	1:C:524:SER:HA	2.53	0.43	
1:E:372:ARG:HG2	2:N:62:MET:O	2.18	0.43	
1:F:261:ALA:O	1:F:520:HIS:HE1	2.02	0.43	
1:F:337:ILE:HD13	1:F:337:ILE:HA	1.74	0.43	
1:F:480:SER:OG	1:F:483:THR:HG23	2.19	0.43	
2:I:106:ILE:HG22	2:I:108:PRO:HB3	2.01	0.43	
1:C:459:VAL:CG1	1:C:460:ASN:N	2.82	0.43	
1:D:490:HIS:CD2	1:D:498:THR:HG23	2.54	0.43	
2:J:79:ASN:O	2:J:83:ASN:ND2	2.50	0.43	
1:C:253:ARG:HD2	1:C:255:LEU:HD21	2.01	0.43	
1:C:514:HIS:HD2	1:C:536:ASP:OD2	2.02	0.43	
1:E:412:TYR:N	1:E:412:TYR:CD1	2.86	0.43	
1:F:268:LEU:N	1:F:520:HIS:HD2	2.11	0.43	
1:F:459:VAL:CG1	1:F:460:ASN:N	2.81	0.43	
1:A:479:TRP:CZ3	1:A:484:ASN:OD1	2.71	0.43	
1:B:452:ARG:HG2	1:B:472:SER:C	2.39	0.43	
1:C:310:TRP:CZ3	1:C:331:VAL:HG21	2.53	0.43	
1:F:459:VAL:HG12	1:F:460:ASN:N	2.34	0.43	
1:A:269:ILE:CG2	1:A:520:HIS:HB3	2.48	0.42	
1:A:338:ARG:HA	2:I:66:GLU:CD	2.39	0.42	
1:F:459:VAL:O	1:F:461:THR:N	2.50	0.42	
1:F:275:ASP:OD1	1:F:525:ASN:HB3	2.19	0.42	
1:H:268:LEU:N	1:H:520:HIS:HD2	2.14	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:H:394:ASN:CG	1:H:397:ASP:HB2	2.40	0.42	
1:H:517:ARG:HH22	2:L:92:ASN:ND2	2.17	0.42	
1:A:394:ASN:O	1:A:395:VAL:HB	2.19	0.42	
1:A:501:ASP:O	1:A:502:CYS:CB	2.61	0.42	
1:B:247:ILE:CD1	1:B:499:LEU:CD2	2.96	0.42	
1:C:358:THR:HA	1:C:367:LEU:O	2.19	0.42	
1:C:361:SER:HA	3:C:2003:HOH:O	2.19	0.42	
1:G:497:LEU:CD2	1:G:518:VAL:HG11	2.49	0.42	
1:A:269:ILE:O	1:A:269:ILE:HG23	2.18	0.42	
1:C:269:ILE:HG23	1:C:269:ILE:O	2.19	0.42	
1:D:261:ALA:O	1:D:520:HIS:HE1	2.03	0.42	
1:F:394:ASN:CG	1:F:397:ASP:HB2	2.39	0.42	
1:G:459:VAL:CG1	1:G:460:ASN:N	2.83	0.42	
2:L:106:ILE:HG22	2:L:108:PRO:HB3	2.00	0.42	
1:B:459:VAL:CG1	1:B:460:ASN:N	2.81	0.42	
1:G:275:ASP:OD1	1:G:525:ASN:HB3	2.20	0.42	
1:A:489:SER:HB2	1:A:518:VAL:HB	2.01	0.42	
1:C:490:HIS:CD2	1:C:498:THR:HG23	2.55	0.42	
1:B:514:HIS:HD2	1:B:536:ASP:OD2	2.03	0.42	
1:C:264:PHE:HA	1:C:519:LEU:HD22	2.01	0.42	
1:E:433:MET:HE3	1:E:433:MET:HB3	1.85	0.42	
1:H:449:THR:N	2:L:91:GLU:OE2	2.42	0.42	
1:C:505:MET:HE3	1:C:505:MET:HB3	1.91	0.42	
1:E:247:ILE:O	1:E:249:LYS:HE3	2.20	0.42	
1:B:269:ILE:CG2	1:B:520:HIS:HB3	2.48	0.42	
1:B:480:SER:OG	1:B:483:THR:HG23	2.19	0.42	
1:C:484:ASN:O	1:C:502:CYS:HB2	2.19	0.42	
1:E:269:ILE:HG23	1:E:269:ILE:O	2.19	0.42	
1:E:459:VAL:O	1:E:461:THR:N	2.52	0.42	
1:E:546:ASP:HB3	1:E:547:LYS:H	1.48	0.42	
2:K:102:SEP:O2P	2:K:105:LYS:HG3	2.20	0.42	
1:A:490:HIS:CD2	1:A:498:THR:HG23	2.55	0.42	
1:B:501:ASP:O	1:B:502:CYS:CB	2.64	0.42	
1:E:247:ILE:HD12	1:E:247:ILE:H	1.84	0.42	
1:H:386:GLN:OE1	2:L:88:VAL:CG2	2.68	0.42	
1:H:452:ARG:HG2	1:H:472:SER:C	2.40	0.42	
1:A:468:ILE:HD13	1:A:505:MET:HE2	2.02	0.41	
1:C:433:MET:HE2	1:C:445:THR:HG22	2.02	0.41	
1:D:479:TRP:HZ3	1:D:484:ASN:OD1	2.02	0.41	
1:F:310:TRP:CZ3	1:F:331:VAL:HG21	2.55	0.41	
1:H:459:VAL:O	1:H:461:THR:N	2.49	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:O:69:GLU:O	2:O:73:ILE:HD12	2.20	0.41	
1:B:517:ARG:HH22	2:J:100:ASN:ND2	2.17	0.41	
1:D:353:ASN:HB2	1:D:393:TRP:CD2	2.55	0.41	
1:C:459:VAL:HG12	1:C:460:ASN:N	2.34	0.41	
2:J:85:ASN:N	2:J:85:ASN:HD22	2.18	0.41	
1:B:479:TRP:HZ3	1:B:484:ASN:OD1	2.03	0.41	
1:B:489:SER:HB2	1:B:518:VAL:HB	2.02	0.41	
1:C:315:SER:OG	1:C:316:HIS:HD2	2.04	0.41	
1:D:253:ARG:HD2	1:D:255:LEU:HD21	2.02	0.41	
1:D:451:ASP:O	1:D:453:ARG:HG2	2.20	0.41	
1:F:365:ARG:HG2	1:F:382:GLU:CG	2.51	0.41	
1:H:459:VAL:CG1	1:H:460:ASN:N	2.83	0.41	
2:K:79:ASN:O	2:K:83:ASN:ND2	2.52	0.41	
1:E:322:ALA:HA	1:E:346:ARG:HB3	2.02	0.41	
1:F:451:ASP:O	1:F:453:ARG:HG2	2.20	0.41	
1:H:268:LEU:HB3	1:H:280:ALA:HB3	2.03	0.41	
1:H:310:TRP:CZ3	1:H:331:VAL:HG21	2.55	0.41	
1:D:459:VAL:HG12	1:D:460:ASN:N	2.35	0.41	
1:E:341:SER:CB	2:N:78:HIS:HD2	2.31	0.41	
1:F:495:TYR:CE2	2:K:105:LYS:HD3	2.55	0.41	
1:H:489:SER:HB2	1:H:518:VAL:HB	2.02	0.41	
1:E:264:PHE:HA	1:E:519:LEU:HD22	2.01	0.41	
1:F:547:LYS:HA	1:F:548:PRO:HD2	1.79	0.41	
1:H:480:SER:HB3	1:H:483:THR:O	2.21	0.41	
1:A:459:VAL:HG12	1:A:460:ASN:N	2.36	0.41	
1:B:459:VAL:HG12	1:B:460:ASN:N	2.35	0.41	
1:D:324:GLY:HA2	1:D:347:VAL:HG23	2.03	0.41	
1:D:489:SER:HB2	1:D:518:VAL:HB	2.03	0.41	
2:J:69:GLU:O	2:J:73:ILE:HD12	2.20	0.41	
1:A:433:MET:HA	1:A:444:ALA:O	2.20	0.41	
1:D:517:ARG:HH22	2:L:100:ASN:HD22	1.69	0.41	
1:E:368:HIS:HB2	1:E:379:GLU:HB3	2.03	0.41	
1:G:484:ASN:O	1:G:502:CYS:HB2	2.21	0.41	
1:A:254:VAL:HG22	1:A:540:ARG:HG2	2.02	0.41	
1:C:272:SER:HB3	1:C:310:TRP:CE2	2.56	0.41	
1:D:497:LEU:HD22	1:D:518:VAL:HG11	2.02	0.41	
1:E:261:ALA:O	1:E:520:HIS:HE1	2.04	0.41	
1:E:492:TYR:HA	1:E:493:SER:HA	1.75	0.41	
1:G:394:ASN:CG	1:G:397:ASP:HB2	2.41	0.41	
1:H:492:TYR:CE1	1:H:517:ARG:HD3	2.56	0.41	
2:K:106:ILE:HG22	2:K:108:PRO:HB3	2.03	0.41	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
1:G:269:ILE:HG21	1:G:520:HIS:HB3	2.03	0.40
1:G:495:TYR:CZ	2:J:105:LYS:HD3	2.56	0.40
1:H:258:PRO:O	1:H:259:SER:HB2	2.21	0.40
1:D:310:TRP:CZ3	1:D:331:VAL:HG21	2.56	0.40
1:B:365:ARG:HG2	1:B:382:GLU:CG	2.51	0.40
1:E:492:TYR:CZ	2:I:94:PRO:HB3	2.57	0.40
1:F:497:LEU:CD2	1:F:518:VAL:HG11	2.51	0.40
1:G:258:PRO:HG3	2:J:119:ARG:HB2	2.02	0.40
1:G:480:SER:OG	1:G:483:THR:HG23	2.22	0.40
1:H:269:ILE:HG21	1:H:520:HIS:HB3	2.03	0.40
1:A:324:GLY:HA2	1:A:347:VAL:HG23	2.03	0.40
1:B:278:ALA:HB2	1:B:310:TRP:CZ2	2.56	0.40
1:B:358:THR:HA	1:B:367:LEU:O	2.21	0.40
1:D:501:ASP:HB2	1:D:508:ILE:HD11	2.03	0.40
1:E:489:SER:HB2	1:E:518:VAL:HB	2.04	0.40
1:H:275:ASP:OD1	1:H:525:ASN:HB3	2.22	0.40
1:B:370:ASP:HB3	1:B:373:MET:HB2	2.04	0.40
1:G:492:TYR:HA	1:G:493:SER:HA	1.71	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	302/308~(98%)	282 (93%)	16 (5%)	4 (1%)	12	37
1	В	302/308~(98%)	278 (92%)	20 (7%)	4 (1%)	12	37
1	С	302/308~(98%)	279~(92%)	20 (7%)	3(1%)	15	45
1	D	303/308~(98%)	278 (92%)	22 (7%)	3(1%)	15	45
1	Ε	301/308~(98%)	274 (91%)	24 (8%)	3(1%)	15	45
1	F	302/308~(98%)	277 (92%)	21 (7%)	4 (1%)	12	37



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	G	301/308~(98%)	278~(92%)	19 (6%)	4 (1%)	12	37
1	Н	297/308~(96%)	274 (92%)	20 (7%)	3(1%)	15	45
2	Ι	60/70~(86%)	51 (85%)	6 (10%)	3~(5%)	2	7
2	J	58/70~(83%)	50 (86%)	6 (10%)	2(3%)	3	15
2	Κ	60/70~(86%)	51 (85%)	6 (10%)	3~(5%)	2	7
2	L	49/70~(70%)	41 (84%)	6 (12%)	2(4%)	3	11
2	М	19/70~(27%)	18 (95%)	1 (5%)	0	100	100
2	Ν	18/70~(26%)	18 (100%)	0	0	100	100
2	Ο	18/70~(26%)	18 (100%)	0	0	100	100
2	Р	19/70~(27%)	18 (95%)	0	1 (5%)	2	6
All	All	2711/3024 (90%)	2485 (92%)	187 (7%)	39 (1%)	11	36

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All (39) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	299	CYS
1	А	460	ASN
1	В	299	CYS
1	С	299	CYS
1	D	299	CYS
1	Е	299	CYS
1	Е	460	ASN
1	F	246	GLN
1	F	299	CYS
1	G	299	CYS
1	Н	299	CYS
2	Ι	86	ASN
2	J	86	ASN
2	Κ	86	ASN
2	Κ	108	PRO
2	Κ	114	LEU
2	L	86	ASN
1	В	460	ASN
1	С	460	ASN
1	D	460	ASN
1	F	460	ASN
1	G	460	ASN
1	Н	460	ASN



Mol	Chain	Res	Type
2	Ι	108	PRO
2	Ι	110	GLU
2	J	108	PRO
2	L	108	PRO
1	А	502	CYS
1	Е	303	ASN
1	В	502	CYS
1	F	303	ASN
1	G	303	ASN
1	Н	303	ASN
1	А	303	ASN
1	В	303	ASN
1	С	303	ASN
1	D	303	ASN
2	Р	79	ASN
1	G	269	ILE

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	262/266~(98%)	240 (92%)	22 (8%)	11	31
1	В	259/266~(97%)	239~(92%)	20 (8%)	13	35
1	С	259/266~(97%)	238~(92%)	21 (8%)	11	33
1	D	259/266~(97%)	240~(93%)	19 (7%)	14	38
1	Е	257/266~(97%)	238~(93%)	19 (7%)	13	38
1	F	257/266~(97%)	236~(92%)	21 (8%)	11	32
1	G	258/266~(97%)	238~(92%)	20 (8%)	12	34
1	Н	256/266~(96%)	237~(93%)	19 (7%)	13	38
2	Ι	56/61~(92%)	49 (88%)	7(12%)	4	14
2	J	54/61~(88%)	47 (87%)	7 (13%)	4	12
2	K	56/61~(92%)	49 (88%)	7 (12%)	4	14



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	47/61~(77%)	42 (89%)	5 (11%)	6 20
2	М	18/61~(30%)	15 (83%)	3~(17%)	2 6
2	Ν	14/61~(23%)	12 (86%)	2(14%)	3 10
2	Ο	17/61~(28%)	14 (82%)	3 (18%)	2 5
2	Р	11/61~(18%)	9~(82%)	2(18%)	1 5
All	All	2340/2616 (89%)	2143 (92%)	197 (8%)	11 31

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All (197) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type	
1	А	245	ARG	
1	А	246	GLN	
1	А	269	ILE	
1	А	279	VAL	
1	А	297	HIS	
1	А	302	GLU	
1	А	337	ILE	
1	А	340	LEU	
1	А	371	VAL	
1	А	373	MET	
1	А	380	THR	
1	А	386	GLN	
1	А	415	THR	
1	А	466	SER	
1	А	478	VAL	
1	А	483	THR	
1	А	486	LEU	
1	А	497	LEU	
1	А	498	THR	
1	А	539	LEU	
1	А	543	LYS	
1	А	544	LEU	
1	В	246	GLN	
1	В	269	ILE	
1	В	279	VAL	
1	В	297	HIS	
1	В	337	ILE	
1	В	340	LEU	
1	В	371	VAL	
1	В	373	MET	



Mol	Chain	Res	Type
1	В	380	THR
1	В	386	GLN
1	В	415	THR
1	В	466	SER
1	В	483	THR
1	В	486	LEU
1	В	497	LEU
1	В	498	THR
1	В	539	LEU
1	В	544	LEU
1	В	545	PHE
1	В	547	LYS
1	С	245	ARG
1	С	269	ILE
1	С	279	VAL
1	С	297	HIS
1	С	327	GLU
1	С	337	ILE
1	С	340	LEU
1	С	371	VAL
1	С	373	MET
1	С	380	THR
1	С	386	GLN
1	С	397	ASP
1	С	415	THR
1	С	466	SER
1	С	478	VAL
1	С	483	THR
1	С	486	LEU
1	С	497	LEU
1	С	498	THR
1	С	539	LEU
1	С	544	LEU
1	D	269	ILE
1	D	279	VAL
1	D	297	HIS
1	D	337	ILE
1	D	340	LEU
1	D	371	VAL
1	D	373	MET
1	D	380	THR
1	D	386	GLN



Mol	Chain Res Typ		Type
1	D	397	ASP
1	D	415	THR
1	D	466	SER
1	D	483	THR
1	D	486	LEU
1	D	497	LEU
1	D	498	THR
1	D	539	LEU
1	D	543	LYS
1	D	544	LEU
1	Е	247	ILE
1	Е	269	ILE
1	Е	279	VAL
1	Е	297	HIS
1	Ε	337	ILE
1	Е	340	LEU
1	Е	371	VAL
1	Е	373	MET
1	Е	380	THR
1	Е	386	GLN
1	Ε	415	THR
1	Е	466	SER
1	Ε	478	VAL
1	Ε	483	THR
1	Ε	486	LEU
1	Ε	497	LEU
1	Ε	498	THR
1	Ε	539	LEU
1	Е	544	LEU
1	F	247	ILE
1	F	269	ILE
1	F	279	VAL
1	F	297	HIS
1	F	327	GLU
1	F	332	MET
1	F	337	ILE
1	F	340	LEU
1	F	371	VAL
1	F	373	MET
1	F	380	THR
1	F	386	GLN
1	F	415	THR



Mol	Chain	Res	Type	
1	F	466	SER	
1	F	478	VAL	
1	F	483	THR	
1	F	486	LEU	
1	F	497	LEU	
1	F	498	THR	
1	F	539	LEU	
1	F	544	LEU	
1	G	245	ARG	
1	G	253	ARG	
1	G	269	ILE	
1	G	279	VAL	
1	G	297	HIS	
1	G	337	ILE	
1	G	340	LEU	
1	G	371	VAL	
1	G	373	MET	
1	G	380	THR	
1	G	386	GLN	
1	G	415	THR	
1	G	466	SER	
1	G	478	VAL	
1	G	483	THR	
1	G	486	LEU	
1	G	497	LEU	
1	G	498	THR	
1	G	539	LEU	
1	G	544	LEU	
1	Н	269	ILE	
1	Н	279	VAL	
1	Н	297	HIS	
1	Н	302	GLU	
1	Н	332	MET	
1	Н	337	ILE	
1	Н	340	LEU	
1	Н	371	VAL	
1	Н	373	MET	
1	Н	380	THR	
1	Н	386	GLN	
1	Н	415	THR	
1	Н	478	VAL	
1	Н	483	THR	



Mol	Chain	Res	Type	
1	Н	486	LEU	
1	Н	497	LEU	
1	Н	498	THR	
1	Н	539	LEU	
1	Н	544	LEU	
2	Ι	63	LEU	
2	Ι	88	VAL	
2	Ι	89	SER	
2	Ι	107	CYS	
2	Ι	114	LEU	
2	Ι	115	ARG	
2	Ι	119	ARG	
2	J	63	LEU	
2	J	88	VAL	
2	J	89	SER	
2	J	97	VAL	
2	J	107	CYS	
2	J	114	LEU	
2	J	119	ARG	
2	К	63	LEU	
2	К	88	VAL	
2	Κ	89	SER	
2	К	107	CYS	
2	Κ	110	GLU	
2	Κ	124	ASP	
2	К	125	LEU	
2	L	88	VAL	
2	L	89	SER	
2	L	107	CYS	
2	L	110	GLU	
2	L	111	ARG	
2	М	71	ARG	
2	М	77	ARG	
2	М	78	HIS	
2	Ν	77	ARG	
2	N	78	HIS	
2	Ο	72	ASN	
2	0	77	ARG	
2	Ο	78	HIS	
2	Р	61	PHE	
2	Р	78	HIS	

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49)



such sidechains are listed below:

Mol	Chain	Res	Type
1	А	316	HIS
1	А	496	ASN
1	А	514	HIS
1	А	520	HIS
1	В	316	HIS
1	В	496	ASN
1	В	514	HIS
1	В	520	HIS
1	С	316	HIS
1	С	514	HIS
1	С	520	HIS
1	D	316	HIS
1	D	496	ASN
1	D	514	HIS
1	D	520	HIS
1	Е	316	HIS
1	Е	496	ASN
1	Е	514	HIS
1	Е	520	HIS
1	F	316	HIS
1	F	514	HIS
1	F	520	HIS
1	G	316	HIS
1	G	514	HIS
1	G	520	HIS
1	Н	316	HIS
1	Н	496	ASN
1	Н	514	HIS
1	Н	520	HIS
2	Ι	78	HIS
2	Ι	85	ASN
2	J	85	ASN
2	J	86	ASN
2	J	92	ASN
2	J	96	GLN
2	J	100	ASN
2	K	85	ASN
2	Κ	92	ASN
2	K	100	ASN
2	L	85	ASN
2	L	86	ASN
2	L	92	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)

4 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	Bond I Bond		ond leng	gths	Bond angles		
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	SEP	J	102	2	8,9,10	0.76	0	8,12,14	1.47	2 (25%)
2	SEP	Ι	102	2	8,9,10	0.95	0	8,12,14	1.73	1 (12%)
2	SEP	K	102	2	8,9,10	0.60	0	8,12,14	1.49	1 (12%)
2	SEP	L	102	2	8,9,10	0.78	0	8,12,14	0.97	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	J	102	2	-	0/5/8/10	-
2	SEP	Ι	102	2	-	0/5/8/10	-
2	SEP	K	102	2	-	0/5/8/10	-
2	SEP	L	102	2	-	0/5/8/10	-



Chain Mol Res Type 2L 100ASN 2М 72ASN 2Μ 78HIS 2 ASN Μ 79 $\overline{2}$ Ν HIS 782Р 78HIS $\mathbf{2}$ Р ASN 79

Continued from previous page...

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Ι	102	SEP	O3P-P-OG	-3.34	97.84	106.73
2	J	102	SEP	O3P-P-OG	-2.96	98.86	106.73
2	Κ	102	SEP	O3P-P-OG	-2.56	99.93	106.73
2	J	102	SEP	O3P-P-O2P	2.10	115.66	107.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	102	SEP	1	0
2	Ι	102	SEP	1	0
2	Κ	102	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	304/308~(98%)	-0.21	1 (0%) 94 94	23, 45, 70, 87	0
1	В	304/308~(98%)	0.00	2 (0%) 87 87	38, 59, 80, 95	0
1	С	304/308~(98%)	-0.29	0 100 100	26, 46, 72, 89	0
1	D	305/308~(99%)	-0.19	0 100 100	31, 55, 87, 101	0
1	E	303/308~(98%)	-0.01	2 (0%) 87 87	27, 59, 99, 121	0
1	F	304/308~(98%)	0.06	6 (1%) 65 63	33, 62, 96, 115	0
1	G	303/308~(98%)	0.02	8 (2%) 56 52	40, 62, 87, 104	0
1	Н	299/308~(97%)	0.66	38 (12%) 3 2	36, 98, 183, 227	0
2	Ι	64/70~(91%)	-0.10	1 (1%) 72 71	29, 62, 95, 102	0
2	J	62/70~(88%)	0.08	1 (1%) 72 71	41, 77, 111, 115	0
2	K	64/70~(91%)	-0.15	0 100 100	29, 62, 96, 109	0
2	L	51/70~(72%)	-0.18	0 100 100	41, 71, 103, 106	0
2	М	21/70~(30%)	0.99	5(23%) 0 0	127, 146, 159, 166	0
2	Ν	20/70~(28%)	0.31	0 100 100	98, 113, 129, 145	0
2	Ο	20/70~(28%)	0.45	0 100 100	100, 112, 142, 166	0
2	Р	$2\overline{1/70}~(30\%)$	1.00	3(14%) 2 2	98, 130, 155, 179	0
All	All	2749/3024 (90%)	0.02	67 (2%) 59 56	23, 59, 121, 227	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Н	329	TYR	4.8
1	Н	357	LEU	4.4
1	Н	318	ALA	4.4
1	Е	548	PRO	4.3
1	Н	546	ASP	4.1



Mol	Chain	Res	Type	RSRZ
1	Н	337	ILE	4.1
1	Н	316	HIS	4.1
1	Н	313	ALA	3.8
1	Н	508	ILE	3.7
1	Н	248	ALA	3.6
1	Н	539	LEU	3.5
1	Н	310 TRP		3.1
2	Р	68 ALA		3.1
1	Н	302	GLU	3.1
2	М	64	TYR	3.0
1	G	331	VAL	2.9
1	Н	545	PHE	2.9
1	Η	533	GLY	2.8
1	H	317	LEU	2.8
1	Н	331	VAL	2.8
1	G	288	THR	2.7
1	В	542	TRP	2.7
1	Н	276	VAL	2.7
1	G	544	LEU	2.7
2	М	67	THR	2.5
1	F	337	ILE	2.5
1	G	337	ILE	2.4
1	G	326	VAL	2.4
1	H	325	LEU	2.4
2	М	63	LEU	2.4
1	G	340	LEU	2.4
1	F	332	MET	2.4
1	Н	280	ALA	2.4
1	Н	350	LEU	2.4
1	H	369	ARG	2.3
1	H	530	VAL	2.3
1	G	277		2.3
1	E	325	LEU	2.3
1	F	367	LEU	2.3
1	F	331	VAL	2.3
2	P	70	GLU	2.3
1	H	341	SER	2.3
1	H	330	ASP	2.3
1	H	352	TRP	2.3
1	H	278	ALA	2.3
1	Н	340	LEU	2.2
1	H	367	LEU	2.2



Mol	Chain	Res Type		RSRZ	
2	М	74	ALA	2.2	
1	Н	358	THR	2.2	
1	Н	376	PRO	2.2	
1	Н	326	VAL	2.2	
1	Н	291	ASN	2.1	
1	F	319	VAL	2.1	
1	Н	336	CYS	2.1	
1	Н	324	GLY	2.1	
1	А	256	ASP	2.1	
1	Н	356	VAL	2.1	
1	Н	390	GLY	2.1	
2	Р	63	LEU	2.1	
1	F	358	THR	2.1	
2	М	77	ARG	2.1	
1	G	332	MET	2.1	
2	Ι	110	GLU	2.1	
1	Н	328	ILE	2.0	
1	Н	543	LYS	2.0	
1	В	290	ASN	2.0	
2	J	62	MET	2.0	

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	$B-factors(A^2)$	Q<0.9
2	SEP	L	102	10/11	0.93	0.17	52,54,59,60	0
2	SEP	K	102	10/11	0.96	0.15	39,42,44,45	0
2	SEP	J	102	10/11	0.96	0.14	47,48,49,51	0
2	SEP	Ι	102	10/11	0.98	0.15	29,31,32,32	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.



6.5 Other polymers (i)

There are no such residues in this entry.

