

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	4YZF
Title	:	Crystal structure of the anion exchanger domain of human erythrocyte Band
		3
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Deposited on	:	2015-03-25
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

:	4.02b-467
:	1.8.5 (274361), CSD as541be (2020)
:	1.13
:	2.37.1
:	1.1.7(2018)
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	5.8.0158
:	7.0.044 (Gargrove)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.37.1
	: : : : : : : : : : : : : : : : : : : :



1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	
_		011	.%			
1	А	911	32%	19% •	• 48%	
	_		3%			
1	В	911	32%	20%	48%	
			.%			
1	С	911	32%	20%	48%	
			3%			
1	D	911	32%	20%	48%	
			9%			
2	E	223		76%		22% ·



Mol	Chain	Length	Quality of chain	
2	G	223	9%	16%
2	Ι	223	71%	27% •
2	K	223	9%	20%
3	F	218	8%	21%
3	Н	218	83%	17%
3	J	218	20%	23%
3	L	218	85%	14% •



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 28724 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	475	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	475	3769	2535	598	619	17	0	0	0
1	D	475	Total	С	Ν	0	S	0	0	0
	D	475	3769	2535	598	619	17	0	0	
1	C	475	Total	С	Ν	0	S	0	0	0
		475	3769	2535	598	619	17	0	0	0
1	П	475	Total	С	Ν	0	S	0	0	0
	D	415	3769	2535	598	619	17	0	0	0

• Molecule 1 is a protein called Band 3 anion transport protein.

• Molecule 2 is a protein called FAB fragment of Immunoglobulin (IgG) molecule.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	F	002	Total	С	Ν	0	S	0	0	0
		220	1690	1077	274	334	5	0	0	0
0	C	002	Total	С	Ν	0	S	0	0	0
	G	220	1690	1077	274	334	5	0	0	0
0	т	202	Total	С	Ν	0	S	0	0	0
	1	220	1690	1077	274	334	5	0	0	0
0	V	002	Total	С	Ν	0	S	0	0	0
	K	К 223	1690	1077	274	334	5	0	0	0

• Molecule 3 is a protein called FAB fragment of Immunoglobulin (IgG) molecule.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
9	Б	010	Total	С	Ν	0	S	0	0	0
3	Г	210	1694	1055	285	346	8	0	0	0
9	п	010	Total	С	Ν	0	S	0	0	0
3	п	210	1694	1055	285	346	8	0	0	0
9	т	919	Total	С	Ν	0	S	0	0	0
3	J	218	1694	1055	285	346	8	0	0	0
9	т	010	Total	С	Ν	0	S	0	0	0
3		210	1694	1055	285	346	8	0	0	0





• Molecule 4 is 2,2'-ethane-1,2-diylbis{5-[(sulfanylmethyl)amino]benzenesulfonic acid} (three-letter code: 4KU) (formula: $C_{16}H_{20}N_2O_6S_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	Δ	1	Total	С	Ν	0	S	0	0
4	A	L	28	16	2	6	4	0	0
4	В	1	Total	С	Ν	0	S	0	0
4	D	I	28	16	2	6	4	0	0
4	С	1	Total	С	Ν	0	S	0	0
4	U	L	28	16	2	6	4	0	0
4	Л	1	Total	С	Ν	0	S	0	0
4	D		28	16	2	6	4	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: Band 3 anion transport protein



PHE ASP GLU GLU GLU GLU TYR ASP GLU VAL MET PRO VAL

• Molecule 1: Band 3 anion transport protein











• Molecule 2: FAB fragment of Immunoglobulin (IgG) molecule









• Molecule 3: FAB fragment of Immunoglobulin (IgG) molecule





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	152.82Å 171.96Å 271.70Å	Deperitor
a, b, c, α , β , γ	90.00° 101.16° 90.00°	Depositor
Bosolution(A)	37.72 - 3.50	Depositor
Resolution (A)	48.84 - 3.50	EDS
% Data completeness	94.6 (37.72-3.50)	Depositor
(in resolution range)	94.7 (48.84 - 3.50)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.59 (at 3.48 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1951)	Depositor
D D.	0.274 , 0.290	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.276 , 0.292	DCC
R_{free} test set	4135 reflections (5.01%)	wwPDB-VP
Wilson B-factor $(Å^2)$	115.1	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.25 , 67.5	EDS
L-test for twinning ²	$< L >=0.42, < L^2>=0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	28724	wwPDB-VP
Average B, all atoms $(Å^2)$	145.0	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 51.75 % 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 5.3662e-05. 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: $4\mathrm{KU}$

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	B	ond angles
WIOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.42	0/3862	0.62	2/5246~(0.0%)
1	В	0.37	0/3862	0.59	2/5246~(0.0%)
1	С	0.40	0/3862	0.60	1/5246~(0.0%)
1	D	0.37	0/3862	0.57	1/5246~(0.0%)
2	Е	0.48	0/1737	0.90	3/2377~(0.1%)
2	G	0.39	0/1737	0.67	1/2377~(0.0%)
2	Ι	0.43	0/1737	0.81	3/2377~(0.1%)
2	K	0.37	0/1737	0.66	1/2377~(0.0%)
3	F	0.44	0/1736	0.64	0/2360
3	Н	0.37	0/1736	0.57	1/2360~(0.0%)
3	J	0.37	0/1736	0.60	0/2360
3	L	0.34	0/1736	0.55	0/2360
All	All	0.40	0/29340	0.64	15/39932~(0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	Η	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	G	68	ARG	NE-CZ-NH1	-7.19	116.70	120.30
2	Е	158	GLU	C-N-CD	-6.51	106.27	120.60
2	Κ	68	ARG	NE-CZ-NH1	-5.98	117.31	120.30
2	Ι	158	GLU	C-N-CD	-5.73	107.99	120.60



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	737	ALA	C-N-CA	5.63	135.79	121.70
2	Ι	215	LYS	N-CA-C	-5.62	95.81	111.00
1	С	737	ALA	C-N-CA	5.58	135.64	121.70
2	Е	97	CYS	N-CA-C	-5.32	96.64	111.00
2	Ι	97	CYS	N-CA-C	-5.29	96.72	111.00
1	В	737	ALA	C-N-CA	5.26	134.84	121.70
1	D	737	ALA	C-N-CA	5.19	134.67	121.70
3	Н	109	GLU	OE1-CD-OE2	-5.14	117.13	123.30
2	Ε	215	LYS	N-CA-C	-5.14	97.13	111.00
1	B	657	SER	C-N-CA	5.07	134.37	121.70
1	А	657	SER	C-N-CA	5.03	134.28	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	Н	111	LYS	Mainchain

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	3769	0	3990	150	0
1	В	3769	0	3990	141	0
1	С	3769	0	3988	138	0
1	D	3769	0	3989	144	0
2	Е	1690	0	1645	40	0
2	G	1690	0	1645	28	0
2	Ι	1690	0	1645	45	0
2	Κ	1690	0	1645	33	0
3	F	1694	0	1609	33	0
3	Н	1694	0	1609	28	0
3	J	1694	0	1609	40	0
3	L	1694	0	1609	26	0
4	А	28	0	15	1	0
4	В	28	0	14	2	0
4	С	28	0	15	3	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	28	0	15	2	0
All	All	28724	0	29032	798	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 14.

All (798) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:828:VAL:HG23	1:A:829:LYS:HG3	1.48	0.94
1:D:851:LYS:HE3	1:D:859:LEU:HD22	1.51	0.92
1:C:828:VAL:HG23	1:C:829:LYS:HG3	1.49	0.92
1:D:828:VAL:HG23	1:D:829:LYS:HG3	1.54	0.90
1:D:737:ALA:HB3	1:D:738:LEU:HB2	1.55	0.89
1:B:737:ALA:HB3	1:B:738:LEU:HB2	1.55	0.89
2:I:124:ALA:HB2	2:I:183:ASP:HB3	1.53	0.89
1:C:851:LYS:HE3	1:C:859:LEU:HD22	1.52	0.89
1:D:592:LYS:HB2	1:D:606:GLY:HA3	1.56	0.88
1:C:592:LYS:HB2	1:C:606:GLY:HA3	1.55	0.88
1:C:737:ALA:HB3	1:C:738:LEU:HB2	1.55	0.87
2:K:30:THR:HA	2:K:55:TRP:HD1	1.38	0.87
1:A:851:LYS:HE3	1:A:859:LEU:HD22	1.57	0.86
1:A:737:ALA:HB3	1:A:738:LEU:HB2	1.54	0.86
1:B:592:LYS:HB2	1:B:606:GLY:HA3	1.58	0.85
3:F:112:ARG:NH1	3:F:174:ASP:O	2.09	0.85
1:B:828:VAL:HG23	1:B:829:LYS:HG3	1.57	0.85
1:A:592:LYS:HB2	1:A:606:GLY:HA3	1.58	0.83
2:E:30:THR:HA	2:E:55:TRP:CD1	2.16	0.81
2:I:30:THR:HA	2:I:55:TRP:CD1	2.16	0.80
2:E:30:THR:HA	2:E:55:TRP:HD1	1.47	0.80
1:B:501:VAL:HG21	1:B:710:VAL:HB	1.64	0.79
2:G:30:THR:HA	2:G:55:TRP:HD1	1.47	0.79
1:D:501:VAL:HG21	1:D:710:VAL:HB	1.64	0.79
1:A:549:LEU:HD22	1:B:569:ASN:HD21	1.47	0.79
1:B:851:LYS:HE3	1:B:859:LEU:HD22	1.63	0.78
1:C:518:ARG:NH1	1:C:804:GLN:OE1	2.17	0.78
1:A:610:VAL:HG13	1:A:791:ILE:HD12	1.65	0.77
3:H:29:VAL:HG23	3:H:96:TRP:HB2	1.66	0.77
1:A:518:ARG:NH1	1:A:804:GLN:OE1	2.18	0.77
1:D:519:TYR:HD2	1:D:867:VAL:HG13	1.49	0.77
1:C:501:VAL:HG21	1:C:710:VAL:HB	1.66	0.76



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:809:ILE:HG12	1:C:841:ILE:HD11	1.66	0.76
1:C:829:LYS:HB3	1:C:833:MET:N	2.00	0.76
1:C:610:VAL:HG13	1:C:791:ILE:HD12	1.68	0.76
2:G:11:LYS:HE3	2:G:126:THR:HG23	1.67	0.76
3:H:41:GLN:HB2	3:H:51:LEU:HD11	1.66	0.75
1:A:389:ARG:NH1	1:A:699:GLY:O	2.19	0.75
3:L:41:GLN:HB2	3:L:51:LEU:HD11	1.68	0.75
1:C:389:ARG:NH1	1:C:699:GLY:O	2.21	0.74
2:E:124:ALA:HB2	2:E:183:ASP:HB3	1.68	0.74
1:B:389:ARG:NH1	1:B:699:GLY:O	2.20	0.74
1:A:501:VAL:HG21	1:A:710:VAL:HB	1.69	0.74
1:B:829:LYS:HB3	1:B:833:MET:N	2.03	0.74
2:K:30:THR:HA	2:K:55:TRP:CD1	2.22	0.73
1:D:829:LYS:HB3	1:D:833:MET:N	2.04	0.73
1:D:518:ARG:NH1	1:D:804:GLN:OE1	2.22	0.73
1:B:519:TYR:HD2	1:B:867:VAL:HG13	1.54	0.72
3:J:112:ARG:NH1	3:J:174:ASP:O	2.20	0.72
2:I:30:THR:HA	2:I:55:TRP:HD1	1.54	0.72
1:D:520:THR:OG1	1:D:521:GLN:N	2.23	0.71
1:A:680:LEU:HD21	1:A:863:LEU:HD23	1.72	0.71
1:B:829:LYS:HB3	1:B:833:MET:H	1.56	0.71
1:D:389:ARG:NH2	1:D:396:ASP:OD2	2.18	0.71
1:C:680:LEU:HD21	1:C:863:LEU:HD23	1.72	0.70
1:D:610:VAL:HG13	1:D:791:ILE:HD12	1.72	0.70
3:J:109:GLU:OE2	3:J:177:TYR:OH	2.06	0.70
3:L:29:VAL:HG23	3:L:96:TRP:HB2	1.72	0.70
1:C:829:LYS:HB3	1:C:833:MET:H	1.56	0.70
1:A:829:LYS:HB3	1:A:833:MET:N	2.05	0.70
1:D:389:ARG:NH1	1:D:699:GLY:O	2.25	0.70
2:G:30:THR:HA	2:G:55:TRP:CD1	2.26	0.70
2:G:165:ASN:O	2:G:168:SER:OG	2.09	0.70
1:C:488:VAL:HG21	1:C:654:GLY:HA2	1.74	0.69
1:A:851:LYS:HB2	1:A:859:LEU:HD13	1.74	0.69
1:C:522:GLU:OE1	1:C:805:LEU:N	2.22	0.69
3:J:112:ARG:HH12	3:J:174:ASP:HB2	1.58	0.69
1:C:812:LEU:HA	1:C:834:HIS:CE1	2.28	0.68
3:F:29:VAL:HG23	3:F:96:TRP:HB2	1.76	0.68
1:A:812:LEU:HA	1:A:834:HIS:CE1	2.28	0.68
1:A:522:GLU:OE1	1:A:805:LEU:N	2.23	0.68
2:E:13:GLN:HB2	2:E:16:GLN:CD	2.14	0.68
1:C:447:GLN:HG2	1:C:712:MET:HB3	1.74	0.68



	is as page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:J:29:VAL:HG23	3:J:96:TRP:HB2	1.74	0.68
1:B:520:THR:OG1	1:B:521:GLN:N	2.24	0.68
1:B:480:GLU:O	2:G:108:TYR:OH	2.09	0.68
1:A:829:LYS:HB3	1:A:833:MET:H	1.60	0.67
1:B:526:PHE:CD2	1:B:844:LEU:HD21	2.29	0.67
1:B:610:VAL:HG13	1:B:791:ILE:HD12	1.74	0.67
2:G:60:TYR:CD1	3:H:98:ILE:HG21	2.29	0.67
1:A:520:THR:HG22	1:A:867:VAL:HG11	1.75	0.67
1:D:708:LEU:O	1:D:712:MET:HG2	1.95	0.67
2:E:13:GLN:HB2	2:E:16:GLN:NE2	2.10	0.67
1:A:526:PHE:CD2	1:A:844:LEU:HD21	2.30	0.67
1:B:809:ILE:HG12	1:B:841:ILE:HD11	1.76	0.67
1:D:809:ILE:HG12	1:D:841:ILE:HD11	1.77	0.66
1:D:829:LYS:HB3	1:D:833:MET:H	1.59	0.66
3:H:197:THR:OG1	3:H:212:SER:OG	2.14	0.66
1:C:803:ILE:HG22	1:C:806:PHE:H	1.59	0.66
2:E:54:TRP:CH2	2:E:60:TYR:HD2	2.14	0.66
3:H:84:GLU:HA	3:H:110:ILE:HD11	1.75	0.66
3:J:189:GLU:HA	3:J:192:ARG:HG3	1.77	0.66
1:D:480:GLU:O	2:K:108:TYR:OH	2.10	0.66
1:C:526:PHE:CD2	1:C:844:LEU:HD21	2.31	0.66
3:J:197:THR:HG1	3:J:212:SER:HG	1.39	0.65
1:B:588:LEU:HD12	1:B:609:GLY:HA2	1.78	0.65
1:A:519:TYR:HD2	1:A:867:VAL:HG13	1.62	0.65
1:B:689:VAL:HG12	1:B:696:MET:HE1	1.79	0.65
3:L:197:THR:HG1	3:L:212:SER:HG	1.44	0.65
1:D:522:GLU:OE1	1:D:805:LEU:N	2.24	0.65
1:A:447:GLN:HG2	1:A:712:MET:HB3	1.78	0.65
1:C:520:THR:OG1	1:C:521:GLN:N	2.28	0.65
3:H:51:LEU:HA	3:H:62:VAL:HG21	1.79	0.64
2:I:129:PRO:HB3	2:I:155:TYR:HB3	1.79	0.64
1:A:488:VAL:HG21	1:A:654:GLY:HA2	1.79	0.64
1:A:413:TYR:CD1	1:A:769:LEU:HB3	2.32	0.64
1:C:708:LEU:O	1:C:712:MET:HG2	1.97	0.64
2:K:60:TYR:CD1	3:L:98:ILE:HG21	2.32	0.64
1:B:820:PRO:HD3	1:B:826:LYS:HD2	1.78	0.64
2:E:6:GLU:O	2:E:117:THR:HB	1.98	0.64
1:C:482:ASN:HB3	2:I:56:SER:OG	1.97	0.64
1:D:680:LEU:HD21	1:D:863:LEU:HD23	1.80	0.64
1:A:803:ILE:HG22	1:A:806:PHE:H	1.62	0.63
1:A:809:ILE:HG12	1:A:841:ILE:HD11	1.81	0.63



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:413:TYR:CD1	1:B:769:LEU:HB3	2.33	0.63
1:D:867:VAL:HB	1:D:868:PRO:HD3	1.80	0.63
1:D:832:ARG:HD3	1:D:835:LEU:HD12	1.80	0.63
3:J:40:TYR:HE2	3:J:93:GLN:HG2	1.64	0.63
1:B:806:PHE:HA	1:B:809:ILE:HD12	1.81	0.62
1:C:689:VAL:HG12	1:C:696:MET:HE1	1.80	0.62
1:B:488:VAL:HG21	1:B:654:GLY:HA2	1.80	0.62
1:C:658:GLU:HG2	2:I:59:LYS:CG	2.30	0.62
1:D:526:PHE:CD2	1:D:844:LEU:HD21	2.34	0.62
1:A:492:TRP:CD2	1:A:664:MET:HB2	2.35	0.62
1:A:520:THR:OG1	1:A:521:GLN:N	2.31	0.62
2:I:34:ILE:HG23	2:I:99:ARG:HD2	1.81	0.62
1:A:824:TYR:O	1:A:828:VAL:HG22	2.00	0.62
1:D:432:ARG:HG2	3:L:96:TRP:CZ3	2.35	0.62
1:B:867:VAL:HB	1:B:868:PRO:HD3	1.81	0.62
1:C:588:LEU:HD12	1:C:609:GLY:HA2	1.82	0.61
1:C:824:TYR:O	1:C:828:VAL:HG22	2.00	0.61
3:F:112:ARG:HH12	3:F:174:ASP:HB2	1.64	0.61
3:F:197:THR:OG1	3:F:212:SER:OG	2.17	0.61
1:D:811:LEU:HD22	1:D:826:LYS:HZ1	1.64	0.61
1:B:518:ARG:NH1	1:B:804:GLN:OE1	2.34	0.61
1:D:851:LYS:HA	1:D:856:SER:HB2	1.83	0.61
1:C:413:TYR:CD1	1:C:769:LEU:HB3	2.36	0.61
1:C:519:TYR:HD2	1:C:867:VAL:HG13	1.66	0.61
1:C:867:VAL:HB	1:C:868:PRO:HD3	1.82	0.61
1:A:820:PRO:HD3	1:A:826:LYS:HD2	1.83	0.61
1:B:447:GLN:HG2	1:B:712:MET:HB3	1.83	0.61
1:D:808:ARG:NH2	1:D:840:GLN:HG3	2.14	0.61
1:A:651:HIS:CD2	1:A:653:LEU:HB2	2.34	0.61
1:D:757:LYS:HB3	1:D:759:GLN:HE22	1.66	0.61
1:C:658:GLU:HG2	2:I:59:LYS:HG2	1.82	0.61
1:C:820:PRO:HD3	1:C:826:LYS:HD2	1.83	0.61
1:C:484:LEU:HD13	1:C:663:MET:HG2	1.83	0.60
1:C:691:LYS:HE2	1:C:694:ARG:HE	1.64	0.60
1:D:820:PRO:HD3	1:D:826:LYS:HD2	1.82	0.60
1:B:832:ARG:HD3	1:B:835:LEU:HD12	1.82	0.60
1:B:824:TYR:O	1:B:828:VAL:HG22	2.02	0.60
1:D:689:VAL:HG12	1:D:696:MET:HE1	1.82	0.60
1:C:780:LEU:HA	1:C:783:ILE:HD12	1.83	0.60
4:C:1000:4KU:H18	4:C:1000:4KU:SAH	2.41	0.60
1:D:824:TYR:O	1:D:828:VAL:HG22	2.02	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:716:ALA:HB1	1:A:721:MET:HB2	1.84	0.60
1:B:836:PHE:CD2	1:B:886:LEU:HD13	2.37	0.60
1:C:851:LYS:HB2	1:C:859:LEU:HD13	1.84	0.60
1:C:520:THR:HG22	1:C:867:VAL:HG11	1.84	0.60
1:C:492:TRP:CE2	1:C:664:MET:HB2	2.37	0.60
1:C:716:ALA:HB1	1:C:721:MET:HB2	1.82	0.60
3:H:189:GLU:HA	3:H:192:ARG:HG3	1.85	0.59
2:I:198:TRP:CH2	2:I:222:PRO:HG3	2.38	0.59
1:A:584:PHE:HE2	1:A:616:ILE:HG21	1.67	0.59
1:B:389:ARG:NH2	1:B:396:ASP:OD2	2.24	0.59
1:B:466:GLY:O	1:B:470:VAL:HG23	2.02	0.59
1:A:867:VAL:HB	1:A:868:PRO:HD3	1.84	0.59
1:C:492:TRP:CD2	1:C:664:MET:HB2	2.37	0.59
4:A:1000:4KU:H18	4:A:1000:4KU:SAH	2.42	0.59
1:D:447:GLN:HG2	1:D:712:MET:HB3	1.84	0.59
1:B:426:LEU:O	1:B:430:LYS:HG2	2.03	0.59
1:B:661:ILE:O	1:B:664:MET:HG2	2.03	0.59
1:C:389:ARG:NH2	1:C:396:ASP:OD2	2.21	0.59
1:C:866:THR:O	1:C:870:ARG:HB2	2.02	0.58
3:F:12:ALA:HA	3:F:109:GLU:O	2.03	0.58
2:K:165:ASN:O	2:K:168:SER:OG	2.21	0.58
1:C:851:LYS:HA	1:C:856:SER:HB2	1.84	0.58
1:D:696:MET:HB2	1:D:756:VAL:HG22	1.86	0.58
1:B:686:THR:O	1:B:690:SER:OG	2.22	0.58
1:A:484:LEU:HD23	2:E:58:SER:HB2	1.84	0.58
1:D:864:ILE:O	1:D:868:PRO:HD2	2.03	0.58
1:A:708:LEU:O	1:A:712:MET:HG2	2.03	0.58
2:I:60:TYR:CD1	3:J:98:ILE:HG21	2.38	0.58
3:L:40:TYR:HE2	3:L:93:GLN:HG2	1.69	0.58
2:E:60:TYR:CD1	3:F:98:ILE:HG21	2.38	0.57
1:D:413:TYR:CD1	1:D:769:LEU:HB3	2.39	0.57
1:C:411:PHE:CD1	1:C:610:VAL:HG11	2.39	0.57
3:L:189:GLU:HA	3:L:192:ARG:HG3	1.87	0.57
3:J:41:GLN:HB2	3:J:51:LEU:HD11	1.86	0.57
1:B:696:MET:HB2	1:B:756:VAL:HG22	1.85	0.57
1:D:588:LEU:HD12	1:D:609:GLY:HA2	1.87	0.57
1:A:472:GLU:OE1	1:A:490:ARG:NH1	2.38	0.57
1:B:808:ARG:NH2	1:B:840:GLN:HG3	2.19	0.57
1:B:551:LYS:O	1:B:552:THR:OG1	2.22	0.57
2:G:177:PRO:O	3:H:166:SER:OG	2.19	0.56
1:A:866:THR:O	1:A:870:ARG:HB2	2.05	0.56



	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:807:ASP:O	1:B:811:LEU:HG	2.06	0.56
2:K:34:ILE:HG23	2:K:99:ARG:HD2	1.87	0.56
2:E:6:GLU:OE2	2:E:114:GLY:HA3	2.06	0.56
2:E:6:GLU:HG3	2:E:97:CYS:HB2	1.87	0.56
1:A:822:VAL:O	1:A:825:VAL:HG22	2.05	0.56
1:B:708:LEU:O	1:B:712:MET:HG2	2.05	0.56
2:K:11:LYS:HG3	2:K:12:LEU:N	2.20	0.56
3:L:197:THR:OG1	3:L:212:SER:OG	2.17	0.56
1:A:492:TRP:CE2	1:A:664:MET:HB2	2.40	0.56
1:B:658:GLU:HG2	2:G:59:LYS:HG2	1.88	0.56
3:H:84:GLU:HA	3:H:110:ILE:CD1	2.35	0.56
1:A:811:LEU:HD22	1:A:826:LYS:HZ1	1.71	0.56
1:B:864:ILE:O	1:B:868:PRO:HD2	2.06	0.56
1:B:680:LEU:HD21	1:B:863:LEU:HD23	1.88	0.56
1:D:488:VAL:HG21	1:D:654:GLY:HA2	1.87	0.56
1:D:492:TRP:CE2	1:D:664:MET:HB2	2.41	0.56
1:A:411:PHE:CD1	1:A:610:VAL:HG11	2.40	0.55
1:B:811:LEU:HD22	1:B:826:LYS:HZ1	1.71	0.55
1:D:661:ILE:O	1:D:664:MET:HG2	2.06	0.55
1:B:472:GLU:OE1	1:B:490:ARG:NH1	2.40	0.55
1:C:865:LEU:O	1:C:869:LEU:HB3	2.06	0.55
1:D:412:ILE:HG13	1:D:734:HIS:HD2	1.70	0.55
1:B:845:ALA:O	1:B:849:VAL:HG23	2.06	0.55
1:C:820:PRO:HG2	1:C:822:VAL:O	2.05	0.55
1:B:853:THR:O	1:B:856:SER:HB3	2.07	0.55
1:C:496:TRP:CE2	1:C:668:ALA:HB2	2.41	0.55
1:D:757:LYS:HB3	1:D:759:GLN:NE2	2.21	0.55
1:B:402:SER:HB2	1:B:405:VAL:HG23	1.89	0.55
3:F:112:ARG:HG2	3:F:113:ALA:N	2.22	0.55
1:A:818:TYR:O	1:A:826:LYS:NZ	2.28	0.55
1:A:819:HIS:HA	1:A:826:LYS:HD2	1.89	0.55
1:B:733:THR:HG21	1:B:795:MET:HG2	1.87	0.55
1:D:734:HIS:CE1	1:D:762:SER:HG	2.25	0.55
1:A:544:PHE:HZ	1:A:572:LEU:HD23	1.71	0.55
1:C:490:ARG:NH2	1:C:722:PRO:HA	2.21	0.55
2:E:27:PHE:CZ	2:E:99:ARG:HD3	2.42	0.55
1:B:522:GLU:OE1	1:B:805:LEU:N	2.31	0.55
1:C:862:VAL:HA	1:C:865:LEU:HB3	1.87	0.55
2:I:18:LEU:HD23	2:I:84:ILE:HD12	1.89	0.55
1:C:733:THR:HG21	1:C:795:MET:HG2	1.88	0.55
1:C:853:THR:O	1:C:856:SER:HB3	2.07	0.55



	to do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:807:ASP:O	1:D:811:LEU:HG	2.07	0.55
3:F:2:ILE:HB	3:F:94:HIS:NE2	2.22	0.55
1:A:496:TRP:CE2	1:A:668:ALA:HB2	2.41	0.54
1:D:737:ALA:CB	1:D:738:LEU:HB2	2.33	0.54
3:J:197:THR:OG1	3:J:212:SER:OG	2.15	0.54
2:K:13:GLN:HB2	2:K:16:GLN:NE2	2.22	0.54
1:A:806:PHE:HA	1:A:809:ILE:HD12	1.88	0.54
1:C:549:LEU:HD22	1:D:569:ASN:HD21	1.72	0.54
1:D:695:LYS:HG2	1:D:755:GLU:HA	1.88	0.54
1:A:658:GLU:HG2	2:E:59:LYS:HD2	1.90	0.54
1:B:490:ARG:NH2	1:B:722:PRO:HA	2.22	0.54
1:C:432:ARG:HG2	3:J:96:TRP:CZ3	2.42	0.54
1:D:658:GLU:HG2	2:K:59:LYS:HG2	1.89	0.54
1:D:806:PHE:HA	1:D:809:ILE:HD12	1.88	0.54
2:E:34:ILE:HG23	2:E:99:ARG:HD2	1.88	0.54
1:D:432:ARG:HG2	3:L:96:TRP:CH2	2.42	0.54
2:G:54:TRP:CH2	2:G:60:TYR:HD2	2.26	0.54
1:B:651:HIS:CD2	1:B:653:LEU:HB2	2.43	0.54
1:D:829:LYS:HE2	1:D:878:PHE:CD2	2.42	0.54
1:C:829:LYS:HE2	1:C:878:PHE:CD2	2.42	0.54
2:I:29:LEU:O	2:I:55:TRP:HB2	2.06	0.54
1:A:527:LEU:HD11	1:A:848:TRP:HD1	1.73	0.54
1:A:829:LYS:HE2	1:A:878:PHE:CD2	2.43	0.54
3:F:41:GLN:HB2	3:F:51:LEU:HD11	1.90	0.54
1:A:482:ASN:HB3	2:E:56:SER:OG	2.07	0.54
3:L:84:GLU:HA	3:L:110:ILE:HD13	1.90	0.54
1:A:851:LYS:CE	1:A:859:LEU:HD22	2.34	0.54
1:B:829:LYS:HE2	1:B:878:PHE:CD2	2.42	0.54
1:C:472:GLU:OE1	1:C:490:ARG:NH1	2.40	0.54
3:F:2:ILE:HD12	3:F:94:HIS:CE1	2.42	0.54
2:I:87:VAL:HG12	2:I:121:VAL:HG11	1.89	0.54
1:B:820:PRO:HG2	1:B:822:VAL:O	2.09	0.53
1:D:845:ALA:O	1:D:849:VAL:HG23	2.09	0.53
2:I:126:THR:HG23	2:I:157:PRO:HD3	1.90	0.53
1:B:716:ALA:HB1	1:B:721:MET:HB2	1.90	0.53
1:B:737:ALA:CB	1:B:738:LEU:HB2	2.34	0.53
1:D:657:SER:HB2	1:D:658:GLU:O	2.09	0.53
1:B:851:LYS:HA	1:B:856:SER:HB2	1.91	0.53
1:C:768:VAL:O	1:C:772:LEU:HG	2.08	0.53
1:D:466:GLY:O	1:D:470:VAL:HG23	2.08	0.53
1:D:866:THR:O	1:D:870:ARG:HB2	2.08	0.53



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:J:12:ALA:HA	3:J:109:GLU:O	2.08	0.53
1:C:397:ILE:HG23	1:C:761:ILE:HD11	1.89	0.53
1:A:661:ILE:O	1:A:664:MET:HG2	2.09	0.53
1:D:426:LEU:O	1:D:430:LYS:HG2	2.08	0.53
1:A:651:HIS:CD2	1:A:653:LEU:H	2.27	0.53
1:C:657:SER:HB2	1:C:658:GLU:O	2.08	0.53
3:J:40:TYR:HE2	3:J:93:GLN:CG	2.21	0.53
2:G:18:LEU:HD23	2:G:84:ILE:HD12	1.90	0.53
1:B:773:SER:HA	1:B:776:MET:HG3	1.91	0.53
1:C:773:SER:HA	1:C:776:MET:HG3	1.90	0.53
1:D:490:ARG:NH2	1:D:722:PRO:HA	2.23	0.53
1:D:851:LYS:HB2	1:D:859:LEU:HD13	1.91	0.53
1:B:519:TYR:CD2	1:B:867:VAL:HG13	2.39	0.52
1:C:808:ARG:NH2	1:C:840:GLN:HG3	2.25	0.52
3:H:112:ARG:HG3	3:H:113:ALA:N	2.24	0.52
1:B:440:LEU:HD11	1:B:464:PHE:HB2	1.91	0.52
2:K:18:LEU:HD23	2:K:84:ILE:HD12	1.91	0.52
1:D:412:ILE:HG13	1:D:734:HIS:CD2	2.44	0.52
1:D:716:ALA:HB1	1:D:721:MET:HB2	1.90	0.52
1:A:440:LEU:HD11	1:A:464:PHE:HB2	1.90	0.52
1:B:520:THR:HG22	1:B:867:VAL:HG11	1.90	0.52
3:H:39:TRP:HB2	3:H:52:ILE:HB	1.92	0.52
1:A:526:PHE:HD2	1:A:844:LEU:HD21	1.74	0.52
1:B:419:PRO:O	1:B:423:PHE:HB2	2.09	0.52
1:C:811:LEU:HD23	1:C:814:LYS:HD2	1.91	0.52
1:D:773:SER:HA	1:D:776:MET:HG3	1.92	0.52
1:D:853:THR:O	1:D:856:SER:HB3	2.10	0.52
3:H:110:ILE:N	3:H:170:GLN:OE1	2.38	0.52
2:I:4:LEU:HD13	2:I:24:PHE:HB3	1.92	0.52
1:A:757:LYS:HB3	1:A:759:GLN:NE2	2.25	0.52
1:C:832:ARG:HD3	1:C:835:LEU:HD12	1.92	0.52
1:D:432:ARG:HH22	1:D:480:GLU:CD	2.14	0.52
1:A:597:PHE:HB3	1:A:602:ARG:HB2	1.91	0.51
1:B:878:PHE:HD2	1:B:882:GLU:HB3	1.74	0.51
1:C:552:THR:HB	1:C:553:TYR:HB3	1.93	0.51
1:D:836:PHE:CD2	1:D:886:LEU:HD13	2.45	0.51
2:K:54:TRP:CH2	2:K:60:TYR:HD2	2.28	0.51
1:A:426:LEU:O	1:A:430:LYS:HG2	2.10	0.51
3:J:3:VAL:HB	3:J:26:SER:HB3	1.92	0.51
1:B:811:LEU:HD23	1:B:814:LYS:HD2	1.91	0.51
1:C:551:LYS:O	1:C:552:THR:OG1	2.25	0.51



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Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:162:LEU:HD12	2:E:207:VAL:HG22	1.92	0.51
3:F:40:TYR:HE2	3:F:93:GLN:HG2	1.75	0.51
2:I:6:GLU:HG3	2:I:97:CYS:HB2	1.92	0.51
3:J:52:ILE:CD1	3:J:58:LEU:HG	2.40	0.51
1:A:590:LYS:O	1:A:594:SER:N	2.42	0.51
1:C:443:SER:OG	1:C:447:GLN:NE2	2.43	0.51
1:D:438:SER:OG	1:D:639:LYS:O	2.27	0.51
1:D:696:MET:HB2	1:D:756:VAL:CG2	2.41	0.51
3:H:110:ILE:O	3:H:170:GLN:NE2	2.32	0.51
1:A:520:THR:HG22	1:A:867:VAL:CG1	2.40	0.51
1:B:526:PHE:HD2	1:B:844:LEU:HD21	1.75	0.51
1:B:803:ILE:HG22	1:B:806:PHE:H	1.74	0.51
1:D:803:ILE:HG22	1:D:806:PHE:H	1.74	0.51
1:A:657:SER:HB2	1:A:658:GLU:O	2.10	0.51
1:C:581:THR:HG21	1:C:787:VAL:HG13	1.92	0.51
1:D:811:LEU:HD22	1:D:826:LYS:NZ	2.24	0.51
1:B:739:THR:HG23	1:B:756:VAL:HG12	1.92	0.51
2:E:158:GLU:HG3	2:E:159:PRO:HA	1.92	0.51
1:C:739:THR:HG23	1:C:756:VAL:HG12	1.92	0.51
1:C:822:VAL:O	1:C:825:VAL:HG22	2.11	0.51
1:A:524:PHE:CZ	1:A:528:ILE:HD11	2.46	0.51
1:A:691:LYS:HD2	1:A:693:GLU:OE1	2.11	0.51
1:A:739:THR:HG23	1:A:756:VAL:HG12	1.92	0.51
2:E:2:VAL:HG11	2:E:112:TYR:CD1	2.46	0.51
3:L:40:TYR:HE2	3:L:93:GLN:CG	2.24	0.51
1:A:540:LEU:HD22	1:A:578:MET:SD	2.51	0.51
1:C:818:TYR:O	1:C:826:LYS:NZ	2.39	0.51
1:D:411:PHE:CD1	1:D:610:VAL:HG11	2.46	0.51
2:E:87:VAL:HG12	2:E:121:VAL:HG11	1.93	0.51
1:B:658:GLU:HG2	2:G:59:LYS:CG	2.41	0.50
1:C:487:ILE:HG13	1:C:650:ILE:HD13	1.93	0.50
1:C:864:ILE:O	1:C:868:PRO:HD2	2.10	0.50
1:D:482:ASN:HB3	2:K:56:SER:OG	2.11	0.50
1:D:520:THR:HG22	1:D:867:VAL:HG11	1.92	0.50
1:C:455:GLY:O	1:C:760:ARG:NH1	2.45	0.50
1:A:811:LEU:HD23	1:A:814:LYS:HD2	1.93	0.50
1:D:552:THR:HB	1:D:553:TYR:HB3	1.93	0.50
$2:K:109:TYR:C\overline{Z}$	3:L:53:LYS:HD2	2.46	0.50
1:C:651:HIS:CD2	1:C:653:LEU:HB2	2.46	0.50
1:C:661:ILE:O	1:C:664:MET:HG2	2.11	0.50
1:A:689:VAL:HG12	1:A:696:MET:HE1	1.94	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:432:ARG:HG2	3:H:96:TRP:CZ3	2.47	0.50
1:B:696:MET:HB2	1:B:756:VAL:CG2	2.42	0.50
2:I:206:ASN:ND2	2:I:217:ASP:OD1	2.42	0.50
3:L:58:LEU:HD21	3:L:66:PHE:O	2.12	0.50
1:B:661:ILE:HA	1:B:664:MET:SD	2.52	0.50
1:C:447:GLN:HE22	1:C:724:LEU:HG	1.76	0.50
1:D:472:GLU:OE1	1:D:490:ARG:NH1	2.45	0.50
1:D:492:TRP:CD2	1:D:664:MET:HB2	2.47	0.50
1:C:660:PRO:HD3	2:I:58:SER:HA	1.94	0.50
1:D:820:PRO:HG2	1:D:822:VAL:O	2.12	0.50
1:A:584:PHE:CE2	1:A:616:ILE:HG21	2.46	0.50
1:C:426:LEU:O	1:C:430:LYS:HG2	2.12	0.50
1:C:737:ALA:CB	1:C:738:LEU:HB2	2.35	0.50
1:D:808:ARG:HH22	1:D:840:GLN:HG3	1.77	0.50
1:D:837:THR:O	1:D:840:GLN:HB2	2.12	0.50
1:B:866:THR:O	1:B:870:ARG:HB2	2.12	0.49
2:I:162:LEU:HD12	2:I:207:VAL:HG22	1.94	0.49
1:C:812:LEU:HA	1:C:834:HIS:HE1	1.77	0.49
1:C:432:ARG:HH22	1:C:480:GLU:CD	2.15	0.49
1:D:590:LYS:O	1:D:594:SER:N	2.46	0.49
1:A:634:VAL:HG12	1:A:774:ILE:HD13	1.95	0.49
1:B:492:TRP:CE2	1:B:664:MET:HB2	2.48	0.49
1:D:519:TYR:CD2	1:D:867:VAL:HG13	2.37	0.49
1:A:820:PRO:HG2	1:A:822:VAL:O	2.12	0.49
1:A:839:ILE:O	1:A:842:ILE:HG22	2.13	0.49
1:B:384:ARG:O	1:B:388:ARG:HG3	2.12	0.49
1:B:757:LYS:HB3	1:B:759:GLN:NE2	2.27	0.49
2:E:129:PRO:HB3	2:E:155:TYR:HB3	1.95	0.49
1:C:526:PHE:HD2	1:C:844:LEU:HD21	1.77	0.49
2:I:77:ASN:O	2:I:79:GLN:HG3	2.13	0.49
3:J:121:ILE:HG22	3:J:211:LYS:HE2	1.95	0.49
1:A:397:ILE:HG23	1:A:761:ILE:HD11	1.94	0.49
1:D:768:VAL:O	1:D:772:LEU:HG	2.12	0.49
2:G:34:ILE:HG23	2:G:99:ARG:HD2	1.94	0.49
3:J:117:PRO:HG3	3:J:148:ILE:HD11	1.94	0.49
1:C:651:HIS:CD2	1:C:653:LEU:H	2.31	0.49
1:D:686:THR:O	1:D:690:SER:OG	2.28	0.49
1:A:490:ARG:NH2	1:A:722:PRO:HA	2.28	0.49
1:D:658:GLU:HG2	2:K:59:LYS:CG	2.42	0.49
1:A:808:ARG:NH2	1:A:840:GLN:HG3	2.28	0.48
2:K:198:TRP:CG	2:K:199:PRO:HA	2.48	0.48



	, and pagetti	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:L:84:GLU:HA	3:L:110:ILE:CD1	2.43	0.48
1:C:757:LYS:HB3	1:C:759:GLN:NE2	2.27	0.48
1:D:496:TRP:CE2	1:D:668:ALA:HB2	2.48	0.48
1:A:389:ARG:NH2	1:A:396:ASP:OD2	2.28	0.48
1:A:581:THR:HG21	1:A:787:VAL:HG13	1.95	0.48
1:B:382:LEU:HB2	1:B:703:HIS:HB3	1.95	0.48
1:C:487:ILE:O	1:C:491:VAL:HG23	2.13	0.48
1:D:811:LEU:HD13	1:D:826:LYS:HE3	1.95	0.48
1:A:657:SER:HB2	1:A:658:GLU:C	2.34	0.48
1:B:413:TYR:CE1	1:B:769:LEU:HB3	2.49	0.48
1:C:811:LEU:HD22	1:C:826:LYS:HZ1	1.78	0.48
1:A:466:GLY:O	1:A:470:VAL:HG23	2.14	0.48
1:A:864:ILE:O	1:A:868:PRO:HD2	2.14	0.48
1:B:837:THR:O	1:B:840:GLN:HB2	2.13	0.48
1:D:780:LEU:HA	1:D:783:ILE:HD12	1.94	0.48
2:E:181:GLN:O	2:E:181:GLN:HG3	2.14	0.48
1:A:853:THR:O	1:A:856:SER:HB3	2.13	0.48
1:C:786:ALA:O	1:C:789:PHE:HB2	2.14	0.48
1:D:811:LEU:HD23	1:D:814:LYS:HD2	1.94	0.48
2:E:137:VAL:HG22	3:F:123:PRO:HD3	1.95	0.48
1:C:590:LYS:O	1:C:594:SER:N	2.47	0.48
1:D:447:GLN:HE21	1:D:712:MET:HB2	1.78	0.48
1:D:453:LEU:O	1:D:760:ARG:NH1	2.47	0.48
1:D:865:LEU:O	1:D:869:LEU:HB3	2.14	0.48
2:I:54:TRP:CH2	2:I:60:TYR:HD2	2.31	0.48
2:K:89:THR:HA	2:K:121:VAL:HB	1.95	0.48
1:A:520:THR:CG2	1:A:867:VAL:HG11	2.44	0.48
1:A:865:LEU:O	1:A:869:LEU:HB3	2.13	0.48
3:F:11:LEU:HG	3:F:13:VAL:HG23	1.95	0.48
2:I:37:GLY:HA3	2:I:52:HIS:CG	2.49	0.48
3:L:110:ILE:O	3:L:170:GLN:NE2	2.43	0.48
1:A:527:LEU:CD1	1:A:848:TRP:HD1	2.27	0.48
1:B:411:PHE:CD1	1:B:610:VAL:HG11	2.48	0.48
1:D:862:VAL:HA	1:D:865:LEU:HB3	1.95	0.48
3:J:214:ASN:HB2	3:J:217:GLU:HB3	1.96	0.48
1:A:737:ALA:CB	1:A:738:LEU:HB2	2.34	0.47
1:A:836:PHE:CD2	1:A:886:LEU:HD13	2.49	0.47
1:A:569:ASN:HD21	1:B:549:LEU:HD22	1.79	0.47
1:C:440:LEU:HD11	1:C:464:PHE:HB2	1.95	0.47
3:F:30:SER:HB3	3:F:35:SER:HA	1.95	0.47
1:A:757:LYS:HB3	1:A:759:GLN:HE22	1.79	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:847:LEU:HD21	1:A:863:LEU:HA	1.97	0.47
1:B:634:VAL:HG12	1:B:774:ILE:HD13	1.96	0.47
1:C:819:HIS:HA	1:C:826:LYS:HD2	1.97	0.47
2:G:109:TYR:CZ	3:H:53:LYS:HD2	2.50	0.47
2:K:129:PRO:HB3	2:K:155:TYR:HB3	1.95	0.47
1:A:544:PHE:CZ	1:A:572:LEU:HD23	2.49	0.47
1:D:808:ARG:HH21	1:D:837:THR:HA	1.79	0.47
2:E:109:TYR:CZ	3:F:53:LYS:HD2	2.50	0.47
1:B:657:SER:HB2	1:B:658:GLU:O	2.14	0.47
1:C:520:THR:HG22	1:C:867:VAL:CG1	2.44	0.47
1:A:519:TYR:CD2	1:A:867:VAL:HG13	2.47	0.47
1:B:479:CYS:HA	1:B:484:LEU:HD12	1.97	0.47
1:B:657:SER:HB2	1:B:658:GLU:C	2.35	0.47
4:B:1000:4KU:H11	4:B:1000:4KU:H7	1.43	0.47
1:C:777:GLU:HB3	1:C:778:PRO:HD3	1.96	0.47
1:D:390:TYR:O	1:D:393:TYR:HB3	2.15	0.47
1:D:733:THR:HG21	1:D:795:MET:HG2	1.97	0.47
1:D:878:PHE:HD2	1:D:882:GLU:HB3	1.79	0.47
3:J:112:ARG:HG2	3:J:113:ALA:N	2.30	0.47
1:A:588:LEU:HD12	1:A:609:GLY:HA2	1.96	0.47
1:B:404:GLN:HG2	1:B:738:LEU:H	1.80	0.47
1:B:865:LEU:O	1:B:869:LEU:HB3	2.15	0.47
1:C:519:TYR:CD2	1:C:867:VAL:HG13	2.47	0.47
3:F:116:ALA:HA	3:F:204:THR:HG21	1.97	0.47
2:I:92:THR:HG23	2:I:120:THR:HA	1.97	0.47
2:K:153:LYS:HG2	2:K:154:GLY:N	2.30	0.47
3:J:39:TRP:CZ3	3:J:92:CYS:HB3	2.49	0.47
1:C:597:PHE:HB3	1:C:602:ARG:HB2	1.95	0.47
2:K:41:GLN:HG3	2:K:46:GLY:O	2.15	0.47
1:B:812:LEU:HA	1:B:834:HIS:CE1	2.50	0.46
3:F:189:GLU:HA	3:F:192:ARG:HG3	1.97	0.46
1:A:443:SER:O	1:A:447:GLN:HB2	2.16	0.46
1:B:780:LEU:HA	1:B:783:ILE:HD12	1.97	0.46
1:C:630:GLN:HB3	1:C:785:LEU:HD12	1.97	0.46
1:A:678:ILE:HG12	1:A:725:SER:HB3	1.95	0.46
1:C:402:SER:HB2	1:C:405:VAL:HG23	1.98	0.46
1:C:432:ARG:O	1:C:433:ASN:HB2	2.15	0.46
1:C:485:GLU:OE2	1:C:655:LEU:HB2	2.14	0.46
3:H:40:TYR:HE2	3:H:93:GLN:HG2	1.80	0.46
3:J:112:ARG:NH1	3:J:174:ASP:HB2	2.26	0.46
1:B:538:SER:HA	1:B:541:ILE:HG22	1.98	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:715:VAL:O	1:D:719:PHE:HD1	1.97	0.46
2:I:131:VAL:HB	2:I:216:VAL:HG11	1.98	0.46
1:A:863:LEU:O	1:A:867:VAL:HG23	2.16	0.46
1:C:839:ILE:O	1:C:842:ILE:HG22	2.16	0.46
1:D:547:HIS:ND1	1:D:567:LEU:HA	2.30	0.46
2:E:77:ASN:O	2:E:79:GLN:HG3	2.16	0.46
2:G:179:VAL:HG21	3:H:165:ASN:O	2.15	0.46
2:I:5:GLN:O	2:I:22:CYS:HA	2.14	0.46
1:B:808:ARG:HH22	1:B:840:GLN:HG3	1.80	0.46
1:C:878:PHE:HD2	1:C:882:GLU:HB3	1.80	0.46
1:D:513:VAL:HG11	1:D:702:PHE:CE2	2.50	0.46
2:G:11:LYS:HB2	2:G:157:PRO:HG3	1.97	0.46
3:J:29:VAL:HG21	3:J:94:HIS:HB2	1.96	0.46
3:H:164:LEU:O	3:H:164:LEU:HD12	2.16	0.46
1:A:768:VAL:O	1:A:772:LEU:HG	2.16	0.46
1:D:487:ILE:HG13	1:D:650:ILE:HD13	1.98	0.46
2:G:102:TYR:CZ	2:G:106:GLY:HA2	2.51	0.46
1:B:862:VAL:HA	1:B:865:LEU:HB3	1.97	0.46
1:D:584:PHE:CE2	1:D:616:ILE:HG21	2.51	0.46
1:D:777:GLU:HB3	1:D:778:PRO:HD3	1.97	0.46
2:K:53:ILE:HD12	2:K:59:LYS:HE2	1.98	0.46
1:B:872:VAL:O	1:B:875:PRO:HD2	2.15	0.45
2:K:101:TYR:O	2:K:108:TYR:HA	2.16	0.45
1:A:812:LEU:HA	1:A:834:HIS:HE1	1.78	0.45
1:A:851:LYS:HA	1:A:856:SER:HB2	1.98	0.45
1:B:513:VAL:HG11	1:B:702:PHE:CE2	2.51	0.45
1:C:414:PHE:CE1	1:C:783:ILE:HD13	2.51	0.45
3:J:7:SER:HB2	3:J:8:PRO:HA	1.97	0.45
3:L:51:LEU:HA	3:L:62:VAL:HG21	1.98	0.45
1:A:440:LEU:HA	1:A:722:PRO:HG3	1.97	0.45
1:A:738:LEU:O	1:A:756:VAL:HB	2.16	0.45
1:A:873:LEU:O	1:A:876:LEU:HB3	2.17	0.45
1:B:768:VAL:O	1:B:772:LEU:HG	2.16	0.45
1:B:808:ARG:HH21	1:B:837:THR:HA	1.80	0.45
1:B:835:LEU:O	1:B:839:ILE:HG13	2.17	0.45
1:C:738:LEU:O	1:C:756:VAL:HB	2.15	0.45
1:D:419:PRO:O	1:D:423:PHE:HB2	2.15	0.45
2:E:4:LEU:HD13	2:E:24:PHE:HB3	1.98	0.45
3:L:93:GLN:HB3	3:L:102:PHE:CD2	2.51	0.45
1:A:845:ALA:O	1:A:849:VAL:HG23	2.17	0.45
1:B:757:LYS:HB3	1:B:759:GLN:HE22	1.80	0.45



	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:C:657:SER:HB2	1:C:658:GLU:C	2.37	0.45
1:D:526:PHE:HD2	1:D:844:LEU:HD21	1.80	0.45
2:G:129:PRO:HB3	2:G:155:TYR:HB3	1.98	0.45
2:I:3:LYS:HA	2:I:3:LYS:HD3	1.79	0.45
3:J:129:LEU:O	3:J:187:LYS:HD2	2.16	0.45
1:A:412:ILE:HA	1:A:415:ALA:HB3	1.97	0.45
1:A:651:HIS:HA	1:A:652:PRO:HD2	1.82	0.45
1:B:438:SER:OG	1:B:639:LYS:O	2.33	0.45
1:A:439:GLU:OE2	1:A:640:VAL:HG13	2.17	0.45
1:A:596:TYR:O	1:A:602:ARG:HD2	2.17	0.45
1:B:485:GLU:OE2	1:B:655:LEU:HB2	2.17	0.45
1:C:849:VAL:O	1:C:852:SER:HB3	2.17	0.45
1:D:384:ARG:O	1:D:388:ARG:HG3	2.15	0.45
3:J:51:LEU:HA	3:J:62:VAL:HG21	1.99	0.45
3:L:164:LEU:HD12	3:L:164:LEU:O	2.17	0.45
1:B:715:VAL:O	1:B:719:PHE:HD1	2.00	0.45
1:C:439:GLU:OE2	1:C:640:VAL:HG13	2.17	0.45
1:D:657:SER:HB2	1:D:658:GLU:C	2.37	0.45
3:J:2:ILE:HD12	3:J:94:HIS:CE1	2.52	0.45
1:A:849:VAL:O	1:A:852:SER:HB3	2.17	0.45
1:B:432:ARG:HH22	1:B:480:GLU:CD	2.20	0.45
1:B:822:VAL:O	1:B:825:VAL:HG22	2.16	0.45
1:C:629:THR:HB	1:C:631:LYS:HE2	1.99	0.45
1:C:695:LYS:HB3	1:C:755:GLU:HA	1.98	0.45
1:C:845:ALA:O	1:C:849:VAL:HG23	2.16	0.45
1:D:468:LEU:O	1:D:472:GLU:HG2	2.17	0.45
1:D:842:ILE:O	1:D:846:VAL:HG23	2.17	0.45
4:D:1000:4KU:H7	4:D:1000:4KU:H11	1.45	0.45
2:I:69:LEU:CD2	2:I:84:ILE:HG12	2.47	0.45
1:A:733:THR:HG21	1:A:795:MET:HG2	1.99	0.45
1:B:482:ASN:HB3	2:G:56:SER:OG	2.17	0.45
1:B:839:ILE:O	1:B:842:ILE:HG22	2.17	0.45
1:B:877:ILE:HD13	1:B:877:ILE:HA	1.81	0.45
1:C:870:ARG:O	1:C:874:LEU:N	2.50	0.45
2:I:162:LEU:HA	2:I:206:ASN:O	2.16	0.45
1:A:878:PHE:HD2	1:A:882:GLU:HB3	1.82	0.44
1:C:696:MET:HB2	1:C:756:VAL:HG22	1.97	0.44
1:D:487:ILE:O	1:D:491:VAL:HG23	2.16	0.44
2:I:38:TRP:CD1	2:I:82:LEU:HB2	2.52	0.44
3:L:39:TRP:HB2	3:L:52:ILE:HB	1.99	0.44
1:D:765:LEU:O	1:D:769:LEU:HB2	2.17	0.44



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:J:119:VAL:HA	3:J:139:PHE:O	2.18	0.44
3:J:191:GLU:HA	3:J:215:ARG:CD	2.47	0.44
1:A:658:GLU:HG2	2:E:59:LYS:CG	2.47	0.44
1:A:808:ARG:HH21	1:A:837:THR:HA	1.83	0.44
3:H:116:ALA:HA	3:H:204:THR:HG21	1.98	0.44
1:A:389:ARG:HA	1:A:389:ARG:HD2	1.74	0.44
1:A:551:LYS:HB3	1:A:551:LYS:HE2	1.65	0.44
1:B:583:PHE:HD2	1:B:584:PHE:HD1	1.64	0.44
1:B:727:THR:HG21	1:B:730:ARG:NH2	2.32	0.44
1:C:524:PHE:CZ	1:C:528:ILE:HD11	2.52	0.44
1:D:494:GLY:O	1:D:498:ILE:HG13	2.16	0.44
1:A:382:LEU:HA	1:A:703:HIS:ND1	2.32	0.44
1:A:455:GLY:O	1:A:760:ARG:NH1	2.50	0.44
1:A:777:GLU:HB3	1:A:778:PRO:HD3	1.98	0.44
1:A:780:LEU:HA	1:A:783:ILE:HD12	2.00	0.44
1:D:404:GLN:HG2	1:D:738:LEU:H	1.82	0.44
1:D:443:SER:HB2	1:D:721:MET:HB3	1.99	0.44
1:D:651:HIS:CD2	1:D:653:LEU:HB2	2.52	0.44
2:E:69:LEU:HD22	2:E:82:LEU:HD11	2.00	0.44
3:F:121:ILE:HG22	3:F:211:LYS:HE2	2.00	0.44
2:G:29:LEU:O	2:G:55:TRP:HB2	2.18	0.44
1:B:458:PRO:HB3	1:B:760:ARG:HD3	2.00	0.44
2:G:41:GLN:HG3	2:G:46:GLY:O	2.17	0.44
2:K:11:LYS:HB3	2:K:157:PRO:HG3	1.98	0.44
2:K:109:TYR:HB3	3:L:38:ASN:ND2	2.32	0.44
2:K:153:LYS:HG2	2:K:154:GLY:H	1.82	0.44
1:B:695:LYS:HG2	1:B:755:GLU:HA	2.00	0.44
1:B:777:GLU:HB3	1:B:778:PRO:HD3	1.99	0.44
1:B:849:VAL:O	1:B:852:SER:HB3	2.18	0.44
1:B:853:THR:HB	1:B:855:ALA:HB3	2.00	0.44
1:C:551:LYS:HB3	1:C:551:LYS:HE2	1.67	0.44
1:C:740:VAL:HB	1:C:754:GLN:HB3	2.00	0.44
1:D:634:VAL:HG12	1:D:774:ILE:HD13	1.99	0.44
1:D:691:LYS:HE2	1:D:694:ARG:HE	1.82	0.44
2:K:13:GLN:HB2	2:K:16:GLN:CD	2.38	0.44
1:C:877:ILE:HD13	1:C:877:ILE:HA	1.82	0.44
1:D:822:VAL:O	1:D:825:VAL:HG22	2.17	0.44
2:G:198:TRP:CG	2:G:199:PRO:HA	2.52	0.44
2:K:105:TYR:HB2	3:L:54:TYR:CE1	2.53	0.44
1:A:414:PHE:CE1	1:A:783:ILE:HD13	2.52	0.44
1:A:818:TYR:C	1:A:826:LYS:HZ3	2.16	0.44



	to do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:678:ILE:HG12	1:C:725:SER:HB3	1.99	0.44
1:D:551:LYS:O	1:D:552:THR:OG1	2.26	0.44
3:F:165:ASN:HA	3:F:180:SER:O	2.18	0.44
3:F:190:TYR:CZ	3:F:215:ARG:HG3	2.53	0.44
2:I:41:GLN:HG3	2:I:46:GLY:O	2.17	0.44
1:D:389:ARG:HG3	1:D:760:ARG:NH2	2.33	0.43
1:D:839:ILE:O	1:D:842:ILE:HG22	2.18	0.43
3:J:116:ALA:HA	3:J:204:THR:HG21	2.00	0.43
1:A:686:THR:O	1:A:690:SER:OG	2.33	0.43
1:B:447:GLN:HE21	1:B:712:MET:HB2	1.83	0.43
1:B:552:THR:HB	1:B:553:TYR:HB3	1.99	0.43
2:G:153:LYS:HG2	2:G:154:GLY:N	2.33	0.43
3:J:13:VAL:CG1	3:J:17:GLN:HB3	2.48	0.43
3:J:29:VAL:CG2	3:J:96:TRP:HB2	2.45	0.43
1:B:487:ILE:O	1:B:491:VAL:HG23	2.17	0.43
1:A:581:THR:OG1	1:A:617:MET:HG3	2.18	0.43
1:A:660:PRO:HD3	2:E:58:SER:HA	1.99	0.43
1:C:416:ALA:HA	1:C:730:ARG:HD3	2.00	0.43
1:A:487:ILE:O	1:A:491:VAL:HG23	2.18	0.43
1:D:551:LYS:HE2	1:D:551:LYS:HB3	1.64	0.43
1:A:820:PRO:HD3	1:A:826:LYS:CD	2.46	0.43
1:B:510:SER:O	1:B:513:VAL:HB	2.18	0.43
1:C:658:GLU:HG2	2:I:59:LYS:HD2	2.00	0.43
1:D:443:SER:O	1:D:447:GLN:HB2	2.19	0.43
2:E:34:ILE:CG2	2:E:99:ARG:HD2	2.49	0.43
2:E:109:TYR:HB3	3:F:38:ASN:ND2	2.33	0.43
2:E:158:GLU:HG3	2:E:159:PRO:CA	2.49	0.43
3:F:129:LEU:O	3:F:187:LYS:HD2	2.19	0.43
2:K:181:GLN:O	2:K:181:GLN:HG3	2.19	0.43
1:A:429:GLU:OE2	3:F:32:SER:HB3	2.18	0.43
1:A:547:HIS:ND1	1:A:567:LEU:HA	2.34	0.43
1:C:753:ILE:HD12	1:C:753:ILE:N	2.33	0.43
2:G:18:LEU:HD13	2:G:119:LEU:HD13	2.01	0.43
2:I:137:VAL:HG22	3:J:123:PRO:HD3	2.00	0.43
2:K:29:LEU:O	2:K:55:TRP:HB2	2.19	0.43
1:A:715:VAL:O	1:A:718:LEU:HB3	2.19	0.43
1:B:389:ARG:HG3	1:B:760:ARG:NH2	2.34	0.43
3:F:40:TYR:HE2	3:F:93:GLN:CG	2.31	0.43
2:G:89:THR:HA	2:G:121:VAL:HB	2.00	0.43
3:H:153:LYS:HB2	3:H:197:THR:HB	2.01	0.43
1:A:837:THR:O	1:A:840:GLN:HB2	2.19	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:853:THR:HB	1:A:855:ALA:HB3	2.00	0.43
1:B:851:LYS:HB2	1:B:859:LEU:HD13	2.01	0.43
1:C:806:PHE:HA	1:C:809:ILE:HD12	2.00	0.43
1:D:413:TYR:CE1	1:D:769:LEU:HB3	2.54	0.43
1:D:740:VAL:HB	1:D:754:GLN:HB3	2.01	0.43
2:G:153:LYS:HG2	2:G:154:GLY:H	1.84	0.43
3:H:117:PRO:HG3	3:H:148:ILE:HD11	2.01	0.43
1:B:429:GLU:OE1	3:H:31:THR:HB	2.19	0.43
1:A:484:LEU:HD13	1:A:663:MET:HG2	2.01	0.42
1:B:496:TRP:CE2	1:B:668:ALA:HB2	2.54	0.42
2:E:198:TRP:CG	2:E:199:PRO:HA	2.53	0.42
3:F:20:THR:HG22	3:F:78:ASN:OD1	2.18	0.42
3:F:191:GLU:HA	3:F:215:ARG:CD	2.49	0.42
2:I:198:TRP:CG	2:I:199:PRO:HA	2.53	0.42
3:L:40:TYR:CE2	3:L:93:GLN:HG2	2.51	0.42
1:A:812:LEU:HD22	1:A:834:HIS:ND1	2.34	0.42
1:B:487:ILE:HD11	1:B:720:GLY:HA2	2.00	0.42
1:D:526:PHE:CE1	1:D:800:LEU:HD11	2.54	0.42
3:L:112:ARG:HG3	3:L:113:ALA:N	2.34	0.42
1:B:754:GLN:HG3	1:B:755:GLU:OE1	2.19	0.42
3:F:62:VAL:HA	3:F:63:PRO:HD3	1.84	0.42
2:I:6:GLU:OE2	2:I:114:GLY:HA3	2.19	0.42
2:I:60:TYR:CD2	3:J:98:ILE:HG12	2.53	0.42
2:I:209:HIS:CE1	2:I:211:ALA:HB3	2.53	0.42
1:A:432:ARG:HG2	3:F:96:TRP:CZ3	2.54	0.42
1:A:482:ASN:HB3	2:E:56:SER:HG	1.82	0.42
1:C:405:VAL:HG22	1:C:759:GLN:NE2	2.34	0.42
2:E:22:CYS:HB2	2:E:38:TRP:CZ2	2.55	0.42
2:G:109:TYR:HB3	3:H:38:ASN:ND2	2.34	0.42
1:D:440:LEU:HD11	1:D:464:PHE:HB2	2.00	0.42
1:D:597:PHE:HB3	1:D:602:ARG:HB2	2.01	0.42
1:D:651:HIS:NE2	1:D:653:LEU:HB2	2.35	0.42
3:F:43:LYS:HE2	3:F:85:GLU:O	2.18	0.42
1:A:678:ILE:HG21	1:A:710:VAL:HG22	2.01	0.42
1:B:812:LEU:HD22	1:B:834:HIS:ND1	2.35	0.42
1:C:660:PRO:HG3	2:I:58:SER:HB2	2.02	0.42
2:I:13:GLN:HB2	2:I:16:GLN:CD	2.40	0.42
2:I:113:TRP:CE3	3:J:48:PRO:HD2	2.55	0.42
1:A:487:ILE:HD11	1:A:720:GLY:HA2	2.02	0.42
1:A:862:VAL:HA	1:A:865:LEU:HB3	2.01	0.42
1:B:494:GLY:O	1:B:498:ILE:HG13	2.19	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:622:PHE:HD1	1:B:623:PHE:CD1	2.38	0.42
2:K:18:LEU:HD13	2:K:119:LEU:HD13	2.01	0.42
2:K:37:GLY:HA3	2:K:52:HIS:CG	2.55	0.42
1:A:458:PRO:HB3	1:A:760:ARG:HD3	2.02	0.42
1:B:432:ARG:HG2	3:H:96:TRP:CH2	2.54	0.42
1:C:510:SER:O	1:C:513:VAL:HB	2.20	0.42
1:D:629:THR:HB	1:D:631:LYS:HE2	2.01	0.42
3:H:52:ILE:HD13	3:H:58:LEU:HA	2.02	0.42
1:A:665:PHE:HD1	1:A:665:PHE:HA	1.71	0.42
1:C:510:SER:HG	1:C:703:HIS:HE2	1.67	0.42
1:C:820:PRO:HD3	1:C:826:LYS:CD	2.48	0.42
3:F:93:GLN:HE21	3:F:93:GLN:HB2	1.61	0.42
3:J:40:TYR:CE2	3:J:93:GLN:HG2	2.50	0.42
1:A:485:GLU:OE2	1:A:655:LEU:HB2	2.19	0.42
1:A:616:ILE:O	1:A:620:VAL:HG23	2.20	0.42
1:B:804:GLN:HG2	1:B:808:ARG:HH11	1.85	0.42
1:C:432:ARG:HG2	3:J:96:TRP:CH2	2.55	0.42
1:C:678:ILE:HG21	1:C:710:VAL:HG22	2.00	0.42
1:D:389:ARG:HD2	1:D:389:ARG:HA	1.72	0.42
1:D:870:ARG:O	1:D:874:LEU:N	2.53	0.42
3:F:93:GLN:HB3	3:F:102:PHE:CD2	2.55	0.42
2:I:157:PRO:HD2	2:I:211:ALA:CB	2.50	0.42
2:I:221:GLU:HA	2:I:222:PRO:HD3	1.92	0.42
3:L:214:ASN:HB2	3:L:217:GLU:HB3	2.02	0.42
1:A:382:LEU:HB2	1:A:703:HIS:HB3	2.02	0.41
1:B:870:ARG:O	1:B:874:LEU:N	2.53	0.41
1:B:382:LEU:HA	1:B:703:HIS:ND1	2.35	0.41
1:C:466:GLY:O	1:C:470:VAL:HG23	2.20	0.41
1:C:510:SER:HG	1:C:703:HIS:CD2	2.37	0.41
1:C:836:PHE:CD2	1:C:886:LEU:HD13	2.55	0.41
2:I:181:GLN:O	2:I:181:GLN:HG3	2.20	0.41
3:L:24:ARG:HA	3:L:73:THR:O	2.20	0.41
1:A:450:LEU:HD23	1:A:450:LEU:HA	1.86	0.41
2:G:126:THR:HG22	2:G:157:PRO:HD3	2.02	0.41
1:C:520:THR:CG2	1:C:867:VAL:HG11	2.49	0.41
2:I:153:LYS:NZ	3:J:184:THR:HG21	2.35	0.41
1:B:492:TRP:CD2	1:B:664:MET:HB2	2.55	0.41
1:B:678:ILE:HG21	1:B:710:VAL:HG22	2.02	0.41
1:C:810:LEU:HB3	1:C:814:LYS:HE2	2.01	0.41
1:D:584:PHE:HE2	1:D:616:ILE:HG21	1.85	0.41
1:D:851:LYS:HE2	4:D:1000:4KU:H2	1.73	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:L:116:ALA:HA	3:L:204:THR:HG21	2.02	0.41
1:A:413:TYR:CE1	1:A:769:LEU:HB3	2.56	0.41
1:A:653:LEU:HA	1:A:653:LEU:HD13	1.66	0.41
1:B:487:ILE:HG13	1:B:650:ILE:HD13	2.03	0.41
1:B:524:PHE:CZ	1:B:528:ILE:HD11	2.55	0.41
1:B:851:LYS:HE2	4:B:1000:4KU:H2	1.77	0.41
3:H:40:TYR:HE2	3:H:93:GLN:CG	2.33	0.41
3:H:93:GLN:HB3	3:H:102:PHE:CD2	2.56	0.41
1:B:526:PHE:CE1	1:B:800:LEU:HD11	2.55	0.41
1:C:457:GLN:HG3	1:C:460:LEU:HG	2.02	0.41
1:D:583:PHE:HD2	1:D:584:PHE:HD1	1.67	0.41
2:I:105:TYR:HD2	3:J:54:TYR:CE2	2.39	0.41
2:I:109:TYR:CZ	3:J:53:LYS:HD2	2.56	0.41
1:A:870:ARG:O	1:A:874:LEU:N	2.53	0.41
1:B:390:TYR:O	1:B:393:TYR:HB3	2.21	0.41
1:B:765:LEU:O	1:B:769:LEU:HB2	2.21	0.41
1:B:820:PRO:HD3	1:B:826:LYS:CD	2.49	0.41
1:C:583:PHE:HD2	1:C:584:PHE:HD1	1.68	0.41
1:C:808:ARG:HH21	1:C:837:THR:HA	1.86	0.41
1:D:393:TYR:HD1	1:D:760:ARG:NE	2.18	0.41
1:D:439:GLU:OE2	1:D:640:VAL:HG13	2.19	0.41
2:E:105:TYR:HB2	3:F:54:TYR:CE1	2.56	0.41
1:C:715:VAL:O	1:C:718:LEU:HB3	2.21	0.41
1:D:432:ARG:NH2	1:D:480:GLU:OE1	2.53	0.41
1:D:518:ARG:HB3	1:D:887:ASP:HB2	2.03	0.41
1:D:661:ILE:HA	1:D:664:MET:SD	2.61	0.41
1:D:812:LEU:HD22	1:D:834:HIS:ND1	2.36	0.41
1:D:849:VAL:O	1:D:852:SER:HB3	2.21	0.41
3:J:16:GLY:HA2	3:J:81:PRO:HB2	2.03	0.41
2:K:22:CYS:HB2	2:K:38:TRP:CZ2	2.56	0.41
1:A:583:PHE:HD2	1:A:584:PHE:HD1	1.68	0.41
1:B:389:ARG:HD2	1:B:389:ARG:HA	1.73	0.41
1:B:463:GLY:HA2	1:B:724:LEU:HD13	2.02	0.41
1:B:691:LYS:HE2	1:B:694:ARG:HE	1.86	0.41
1:C:807:ASP:O	1:C:811:LEU:HG	2.20	0.41
4:C:1000:4KU:SAG	4:C:1000:4KU:H6	2.61	0.41
1:D:494:GLY:O	1:D:497:LEU:HB2	2.21	0.41
1:D:524:PHE:CZ	1:D:528:ILE:HD11	2.56	0.41
1:A:675:PHE:HD2	1:A:676:ILE:HD13	1.85	0.40
4:C:1000:4KU:H11	4:C:1000:4KU:H7	1.49	0.40
2:E:18:LEU:HD23	2:E:84:ILE:HD12	2.03	0.40



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:F:40:TYR:CE2	3:F:93:GLN:HG2	2.56	0.40
2:K:77:ASN:O	2:K:79:GLN:HG3	2.21	0.40
1:A:635:PRO:HG2	1:A:774:ILE:HD11	2.03	0.40
1:C:393:TYR:HD1	1:C:760:ARG:NE	2.19	0.40
1:C:811:LEU:HD22	1:C:826:LYS:NZ	2.37	0.40
1:D:808:ARG:HH22	1:D:840:GLN:NE2	2.19	0.40
1:A:683:GLN:OE1	1:A:702:PHE:HD2	2.05	0.40
1:A:695:LYS:HB3	1:A:755:GLU:HA	2.03	0.40
1:B:740:VAL:HB	1:B:754:GLN:HB3	2.03	0.40
1:C:527:LEU:HD11	1:C:848:TRP:HD1	1.86	0.40
1:D:815:PRO:HG2	1:D:818:TYR:HD2	1.86	0.40
2:K:122:SER:HG	2:K:156:PHE:HE1	1.67	0.40
1:A:696:MET:HB2	1:A:756:VAL:HG22	2.02	0.40
1:C:468:LEU:O	1:C:472:GLU:HG2	2.20	0.40
1:D:393:TYR:HD1	1:D:760:ARG:CZ	2.34	0.40
1:D:539:LYS:O	1:D:542:LYS:HB3	2.22	0.40
2:E:3:LYS:HB2	2:E:25:SER:OG	2.22	0.40
1:A:447:GLN:HE21	1:A:712:MET:HB2	1.87	0.40
1:A:484:LEU:HD21	2:E:56:SER:HB3	2.03	0.40
1:B:651:HIS:HA	1:B:652:PRO:HD2	1.94	0.40
1:B:734:HIS:CE1	1:B:762:SER:HG	2.38	0.40
1:C:634:VAL:HG12	1:C:774:ILE:HD13	2.03	0.40
1:D:628:TYR:OH	1:D:630:GLN:HG2	2.21	0.40
1:D:874:LEU:HD23	1:D:874:LEU:HA	1.92	0.40
2:E:29:LEU:O	2:E:55:TRP:HB2	2.22	0.40
2:E:221:GLU:HA	2:E:222:PRO:HD3	1.86	0.40
2:G:99:ARG:HG3	2:G:100:ALA:N	2.36	0.40
3:H:121:ILE:HG22	3:H:211:LYS:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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



41 Δ Γ	4	Y	ZF
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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	467/911~(51%)	435~(93%)	31 (7%)	1 (0%)	47	81
1	В	467/911~(51%)	436~(93%)	30~(6%)	1 (0%)	47	81
1	С	467/911~(51%)	436 (93%)	30 (6%)	1 (0%)	47	81
1	D	467/911 (51%)	436 (93%)	30 (6%)	1 (0%)	47	81
2	Е	221/223~(99%)	211 (96%)	7 (3%)	3 (1%)	11	46
2	G	221/223~(99%)	214 (97%)	7(3%)	0	100	100
2	Ι	221/223~(99%)	212 (96%)	6 (3%)	3 (1%)	11	46
2	Κ	221/223~(99%)	213~(96%)	8 (4%)	0	100	100
3	F	216/218~(99%)	208~(96%)	8 (4%)	0	100	100
3	Н	216/218~(99%)	209~(97%)	7 (3%)	0	100	100
3	J	216/218~(99%)	209~(97%)	7 (3%)	0	100	100
3	L	216/218~(99%)	211 (98%)	5 (2%)	0	100	100
All	All	3616/5408~(67%)	3430 (95%)	176 (5%)	10 (0%)	41	75

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Ε	166	SER
2	Ι	166	SER
2	Ε	159	PRO
2	Ι	159	PRO
2	Ε	210	PRO
2	Ι	210	PRO
1	В	598	PRO
1	С	598	PRO
1	А	598	PRO
1	D	598	PRO

5.3.2 Protein sidechains (i)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles	
1	А	417/786~(53%)	411 (99%)	6 (1%)	67	85	
1	В	417/786~(53%)	413 (99%)	4 (1%)	76	88	
1	С	417/786~(53%)	412 (99%)	5 (1%)	71	87	
1	D	417/786~(53%)	413 (99%)	4 (1%)	76	88	
2	Ε	190/190~(100%)	188~(99%)	2(1%)	73	88	
2	G	190/190~(100%)	188~(99%)	2(1%)	73	88	
2	Ι	190/190~(100%)	187~(98%)	3~(2%)	62	83	
2	Κ	190/190~(100%)	189~(100%)	1 (0%)	88	94	
3	F	193/193~(100%)	191~(99%)	2(1%)	76	88	
3	Н	193/193~(100%)	191~(99%)	2(1%)	76	88	
3	J	193/193~(100%)	191~(99%)	2(1%)	76	88	
3	L	193/193~(100%)	190~(98%)	3~(2%)	62	83	
All	All	3200/4676~(68%)	3164 (99%)	$3\overline{6} (1\%)$	73	88	

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	382	LEU
1	А	544	PHE
1	А	581	THR
1	А	588	LEU
1	А	597	PHE
1	А	723	TRP
1	В	382	LEU
1	В	544	PHE
1	В	597	PHE
1	В	607	ASP
1	С	382	LEU
1	С	544	PHE
1	С	597	PHE
1	С	607	ASP
1	С	723	TRP
1	D	382	LEU
1	D	544	PHE
1	D	597	PHE
1	D	723	TRP



Mol	Chain	Res	Type
2	Е	63	THR
2	Е	222	PRO
3	F	93	GLN
3	F	168	THR
2	G	63	THR
2	G	126	THR
3	Н	93	GLN
3	Н	168	THR
2	Ι	54	TRP
2	Ι	199	PRO
2	Ι	222	PRO
3	J	93	GLN
3	J	168	THR
2	К	63	THR
3	L	58	LEU
3	L	93	GLN
3	L	168	THR

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such side chains are listed below:

Mol	Chain	Res	Type
1	А	457	GLN
1	А	651	HIS
1	А	834	HIS
1	В	569	ASN
1	С	447	GLN
1	С	651	HIS
1	С	834	HIS
1	D	840	GLN
3	Н	80	HIS
3	L	80	HIS

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)

4 ligands 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	Tiple	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	4KU	В	1000	1	27,29,29	1.74	4 (14%)	36,42,42	2.77	13 (36%)
4	4KU	D	1000	1	27,29,29	1.76	3 (11%)	36,42,42	2.54	12 (33%)
4	4KU	А	1000	1	27,29,29	1.77	3 (11%)	36,42,42	<mark>3.29</mark>	15 (41%)
4	4KU	С	1000	1	27,29,29	1.73	2 (7%)	36,42,42	2.72	12 (33%)

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
4	4KU	В	1000	1	-	7/21/23/23	0/2/2/2
4	4KU	D	1000	1	-	6/21/23/23	0/2/2/2
4	4KU	А	1000	1	-	2/21/23/23	0/2/2/2
4	4KU	С	1000	1	-	6/21/23/23	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
4	А	1000	4KU	CAI-SAG	-6.20	1.66	1.81
4	D	1000	4KU	CAI-SAG	-6.04	1.66	1.81
4	С	1000	4KU	CAI-SAG	-5.92	1.66	1.81
4	В	1000	4KU	CAI-SAG	-5.84	1.67	1.81
4	D	1000	4KU	CAJ-SAH	-5.82	1.67	1.81
4	В	1000	4KU	CAJ-SAH	-5.69	1.67	1.81



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	С	1000	4KU	CAJ-SAH	-5.68	1.67	1.81
4	А	1000	4KU	CAJ-SAH	-5.49	1.67	1.81
4	D	1000	4KU	CAV-NAT	2.12	1.44	1.38
4	В	1000	4KU	CAV-NAT	2.12	1.44	1.38
4	В	1000	4KU	CAU-NAS	2.06	1.44	1.38
4	А	1000	4KU	CAU-NAS	2.05	1.44	1.38

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	1000	4KU	CAR-CAX-CAZ	-9.08	115.58	125.29
4	А	1000	4KU	CAR-CAQ-CAW	-7.93	99.98	112.81
4	В	1000	4KU	CAR-CAX-CAZ	-7.11	117.69	125.29
4	С	1000	4KU	CAR-CAX-CAZ	-6.95	117.86	125.29
4	D	1000	4KU	CAR-CAX-CAZ	-6.79	118.03	125.29
4	А	1000	4KU	OAB-SBA-CAY	6.61	117.69	106.51
4	А	1000	4KU	OAD-SBB-CAZ	6.31	117.18	106.51
4	С	1000	4KU	CAQ-CAW-CAY	-6.05	118.82	125.29
4	А	1000	4KU	CAO-CAY-CAW	-5.83	117.80	121.75
4	В	1000	4KU	OAB-SBA-CAY	5.60	115.97	106.51
4	В	1000	4KU	CAQ-CAW-CAY	-5.52	119.39	125.29
4	С	1000	4KU	OAD-SBB-CAZ	5.23	115.36	106.51
4	В	1000	4KU	CAO-CAY-CAW	-5.16	118.25	121.75
4	В	1000	4KU	OAF-SBB-CAZ	5.06	115.06	106.51
4	D	1000	4KU	OAA-SBA-CAY	4.98	114.93	106.51
4	С	1000	4KU	OAB-SBA-CAY	4.88	114.77	106.51
4	D	1000	4KU	OAB-SBA-CAY	4.86	114.73	106.51
4	В	1000	4KU	OAA-SBA-CAY	4.78	114.60	106.51
4	D	1000	4KU	CAQ-CAW-CAY	-4.65	120.32	125.29
4	С	1000	4KU	CAR-CAQ-CAW	-4.59	105.39	112.81
4	D	1000	4KU	OAF-SBB-CAZ	4.56	114.21	106.51
4	С	1000	4KU	CAO-CAY-CAW	-4.53	118.68	121.75
4	А	1000	4KU	CAP-CAZ-CAX	-4.38	118.78	121.75
4	В	1000	4KU	CAR-CAQ-CAW	-4.31	105.83	112.81
4	D	1000	4KU	CAR-CAQ-CAW	-4.25	105.94	112.81
4	А	1000	4KU	CAQ-CAW-CAY	-3.88	121.14	125.29
4	D	1000	4KU	CAO-CAY-CAW	-3.85	119.14	121.75
4	D	1000	4KU	OAD-SBB-CAZ	3.66	112.70	106.51
4	A	1000	4KU	OAF-SBB-CAZ	3.63	112.65	106.51
4	А	1000	4KU	CAN-CAX-CAZ	3.58	121.79	116.37
4	С	1000	4KU	OAA-SBA-CAY	3.56	112.54	106.51
4	С	1000	4KU	OAF-SBB-CAZ	3.44	112.33	106.51



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	С	1000	4KU	CAP-CAZ-CAX	-3.43	119.42	121.75
4	В	1000	4KU	OAD-SBB-CAZ	3.24	111.98	106.51
4	С	1000	4KU	CAN-CAX-CAZ	3.14	121.12	116.37
4	В	1000	4KU	CAP-CAZ-CAX	-3.06	119.68	121.75
4	С	1000	4KU	CAM-CAW-CAY	2.95	120.83	116.37
4	В	1000	4KU	CAN-CAX-CAZ	2.93	120.80	116.37
4	А	1000	4KU	CAU-CAO-CAY	2.87	122.20	119.27
4	А	1000	4KU	OAA-SBA-CAY	2.76	111.17	106.51
4	D	1000	4KU	CAN-CAX-CAZ	2.72	120.48	116.37
4	В	1000	4KU	CAM-CAW-CAY	2.72	120.48	116.37
4	А	1000	4KU	CAL-CAN-CAX	-2.71	117.82	121.39
4	D	1000	4KU	CAP-CAZ-CAX	-2.69	119.93	121.75
4	А	1000	4KU	CAM-CAW-CAY	2.48	120.13	116.37
4	С	1000	4KU	CAL-CAN-CAX	-2.42	118.21	121.39
4	В	1000	4KU	CAL-CAN-CAX	-2.36	118.28	121.39
4	D	1000	4KU	CAL-CAN-CAX	-2.33	118.31	121.39
4	А	1000	4KU	CAW-CAY-SBA	2.22	123.19	121.24
4	D	1000	4KU	CAM-CAW-CAY	2.20	119.69	116.37
4	А	1000	4KU	CAQ-CAR-CAX	2.18	116.33	112.81
4	В	1000	4KU	CAU-CAO-CAY	2.12	121.44	119.27

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
4	D	1000	4KU	CAW-CAQ-CAR-CAX
4	В	1000	4KU	CAW-CAQ-CAR-CAX
4	А	1000	4KU	CAR-CAQ-CAW-CAY
4	В	1000	4KU	CAQ-CAR-CAX-CAZ
4	С	1000	4KU	CAR-CAQ-CAW-CAY
4	D	1000	4KU	CAQ-CAR-CAX-CAZ
4	В	1000	4KU	CAL-CAV-NAT-CAJ
4	С	1000	4KU	CAW-CAQ-CAR-CAX
4	А	1000	4KU	CAR-CAQ-CAW-CAM
4	В	1000	4KU	CAQ-CAR-CAX-CAN
4	С	1000	4KU	CAQ-CAR-CAX-CAZ
4	С	1000	4KU	CAQ-CAR-CAX-CAN
4	D	1000	4KU	CAQ-CAR-CAX-CAN
4	В	1000	4KU	CAO-CAU-NAS-CAI
4	D	1000	4KU	CAL-CAV-NAT-CAJ
4	C	1000	4KU	CAR-CAQ-CAW-CAM
4	В	1000	4KU	CAP-CAV-NAT-CAJ



Mol	Chain	Res	Type	Atoms
4	В	1000	4KU	CAK-CAU-NAS-CAI
4	D	1000	4KU	CAP-CAV-NAT-CAJ
4	С	1000	4KU	CAL-CAV-NAT-CAJ
4	D	1000	4KU	CAO-CAU-NAS-CAI

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	1000	4KU	2	0
4	D	1000	4KU	2	0
4	А	1000	4KU	1	0
4	С	1000	4KU	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

















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	475/911~(52%)	-0.21	13 (2%) 54 4	8	71,103,169,208	0
1	В	475/911~(52%)	-0.02	29 (6%) 21 1	9	90, 142, 202, 249	0
1	С	475/911~(52%)	-0.17	12 (2%) 57 5	1	79,114,184,226	0
1	D	475/911~(52%)	-0.01	26 (5%) 25 2	2	103,151,219,259	0
2	Е	223/223~(100%)	0.24	20 (8%) 9 10	0	79,105,150,177	0
2	G	223/223~(100%)	0.28	21 (9%) 8 9		124, 152, 211, 250	0
2	Ι	223/223~(100%)	1.07	41 (18%) 1	1	79,112,310,355	0
2	K	223/223~(100%)	0.33	19 (8%) 10 1	.1	126, 152, 209, 248	0
3	F	218/218~(100%)	0.11	17 (7%) 13 1	3	81, 111, 141, 179	0
3	Н	218/218~(100%)	0.82	46 (21%) 1	1	125, 181, 255, 268	0
3	J	218/218~(100%)	0.80	44 (20%) 1	1	90, 164, 292, 310	0
3	L	218/218~(100%)	0.50	27 (12%) 4	5	127, 169, 242, 253	0
All	All	3664/5408~(67%)	0.20	315 (8%) 10 1	11	71, 139, 238, 355	0

All (315) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Ι	143	GLY	20.1
2	Ι	135	ALA	17.3
2	Ι	144	SER	13.7
2	Ι	195	SER	12.6
2	Κ	141	THR	10.3
3	F	194	ASN	9.8
3	Н	216	ASN	9.2
2	Ι	194	THR	9.1
2	Ι	167	GLY	8.8
2	Κ	140	ASP	8.8
3	J	135	SER	8.5



Mol	Chain	Res	Type	RSRZ
3	J	136	VAL	8.3
2	Ι	163	THR	8.1
2	Ι	140	ASP	8.0
3	L	216	ASN	7.9
3	J	184	THR	7.7
2	Ι	145	SER	7.2
2	Ι	170	SER	6.9
3	J	175	SER	6.9
2	G	139	GLY	6.7
2	Ι	161	THR	6.5
3	J	162	GLY	6.4
1	А	819	HIS	6.0
2	G	140	ASP	5.9
2	К	139	GLY	5.9
2	G	200	SER	5.9
3	Н	218	CYS	5.8
2	Ι	148	LEU	5.8
2	Ι	168	SER	5.7
2	Ι	139	GLY	5.6
3	L	218	CYS	5.5
2	Ι	193	VAL	5.5
2	Ι	196	SER	5.5
2	Ι	166	SER	5.3
2	G	137	VAL	5.3
3	Н	174	ASP	5.2
2	Ι	147	THR	5.2
2	Ι	162	LEU	5.2
3	Н	213	PHE	5.2
2	G	141	THR	5.1
1	А	831	TRP	5.1
3	F	193	HIS	5.0
3	L	146	LYS	5.0
1	D	874	LEU	5.0
2	G	148	LEU	5.0
1	D	700	SER	4.9
3	J	128	GLN	4.9
3	J	193	HIS	4.9
1	C	818	TYR	4.9
3	J	183	LEU	4.8
2	Ι	141	THR	4.8
3	Н	112	ARG	4.8
3	L	131	SER	4.7



Mol	Chain	Res	Type	RSRZ
2	Κ	183	ASP	4.7
3	L	155	ASP	4.6
3	J	134	ALA	4.6
2	Ι	187	LEU	4.6
2	Е	195	SER	4.6
2	G	138	CYS	4.5
3	J	173	LYS	4.5
2	Ι	223	ARG	4.5
2	Ι	136	PRO	4.5
1	С	398	THR	4.5
2	Κ	142	THR	4.5
3	L	132	GLY	4.4
3	J	137	VAL	4.4
1	С	819	HIS	4.4
1	В	818	TYR	4.4
2	Ι	142	THR	4.3
3	Н	212	SER	4.3
2	G	136	PRO	4.2
3	Н	191	GLU	4.2
1	D	866	THR	4.2
3	L	129	LEU	4.2
3	J	124	PRO	4.2
1	А	398	THR	4.2
1	А	830	THR	4.2
3	Н	210	VAL	4.1
2	G	174	HIS	4.1
3	F	206	THR	4.1
1	В	653	LEU	4.1
1	В	649	VAL	4.1
2	G	222	PRO	4.1
3	Н	176	THR	4.1
2	K	31	THR	4.0
3	J	160	GLN	4.0
2	Ι	138	CYS	4.0
2	Ι	169	LEU	4.0
3	Н	121	ILE	3.9
1	D	870	ARG	3.9
3	L	124	PRO	3.9
2	Е	196	SER	3.8
3	Н	214	ASN	3.8
3	L	217	GLU	3.8
1	А	832	ARG	3.8



Mol	Chain	Res	Type	RSRZ
1	В	821	ASP	3.8
2	G	221	GLU	3.8
2	K	170	SER	3.7
3	Н	36	TYR	3.7
3	Н	187	LYS	3.7
3	J	194	ASN	3.7
1	В	695	LYS	3.7
3	Н	173	LYS	3.7
3	J	121	ILE	3.7
3	J	172	SER	3.7
2	Е	144	SER	3.6
2	Ι	146	VAL	3.6
1	D	834	HIS	3.6
2	Ι	208	ALA	3.6
3	J	131	SER	3.6
3	Н	142	ASN	3.6
3	Н	190	TYR	3.6
1	D	398	THR	3.6
1	В	754	GLN	3.5
1	А	553	TYR	3.5
3	L	37	MET	3.5
1	В	875	PRO	3.5
3	Н	211	LYS	3.5
2	Е	220	ILE	3.5
1	В	650	ILE	3.5
2	Е	107	GLY	3.5
2	Ι	186	THR	3.4
1	В	639	LYS	3.4
2	Ι	206	ASN	3.4
2	Е	108	TYR	3.4
1	В	755	GLU	3.4
3	Н	133	GLY	3.4
2	Κ	71	ILE	3.3
3	L	154	ILE	3.3
2	К	148	LEU	3.3
3	J	161	ASN	3.3
2	Ι	165	ASN	3.3
3	F	19	ALA	3.3
1	В	820	PRO	3.3
2	G	202	SER	3.3
3	Н	35	SER	3.3
3	Н	119	VAL	3.3



Mol	Chain	Res	Type	RSRZ
3	J	185	LEU	3.3
1	В	870	ARG	3.2
1	С	821	ASP	3.2
2	Ι	215	LYS	3.2
2	Ι	197	THR	3.2
3	Н	39	TRP	3.2
3	J	112	ARG	3.2
3	L	55	ALA	3.2
1	С	817	LYS	3.2
3	J	81	PRO	3.2
1	В	654	GLY	3.2
3	F	215	ARG	3.2
3	F	217	GLU	3.2
3	J	11	LEU	3.1
3	L	39	TRP	3.1
2	Ι	201	GLN	3.1
3	Н	129	LEU	3.1
1	А	817	LYS	3.1
1	В	874	LEU	3.0
1	В	652	PRO	3.0
3	Н	60	SER	3.0
3	F	203	LYS	3.0
3	L	165	ASN	3.0
1	D	519	TYR	3.0
2	Ε	154	GLY	3.0
1	А	816	PRO	3.0
3	Н	63	PRO	3.0
1	D	652	PRO	3.0
1	В	651	HIS	3.0
1	С	831	TRP	3.0
2	G	219	LYS	3.0
3	J	12	ALA	3.0
3	F	214	ASN	3.0
1	D	819	HIS	3.0
3	L	36	TYR	3.0
1	D	650	ILE	2.9
3	J	170	GLN	2.9
3	L	133	GLY	2.9
2	Ι	207	VAL	2.9
3	H	134	ALA	2.9
3	H	215	ARG	2.9
2	Е	194	THR	2.9



Mol	Chain	Res	Type	RSRZ
3	J	125	SER	2.9
2	Е	122	SER	2.9
3	Н	66	PHE	2.9
3	Н	207	SER	2.8
3	J	122	PHE	2.8
1	D	387	ARG	2.8
2	K	179	VAL	2.8
3	J	191	GLU	2.8
2	Е	221	GLU	2.8
3	J	210	VAL	2.8
3	Н	204	THR	2.8
3	Н	55	ALA	2.8
3	F	216	ASN	2.8
1	D	869	LEU	2.8
2	Е	183	ASP	2.8
3	L	130	THR	2.8
3	Н	196	TYR	2.7
2	Е	143	GLY	2.7
1	В	601	LEU	2.7
3	J	120	SER	2.7
3	F	207	SER	2.6
3	L	4	MET	2.6
1	В	819	HIS	2.6
1	С	835	LEU	2.6
2	K	138	CYS	2.6
1	В	638	PHE	2.6
1	В	872	VAL	2.6
2	G	122	SER	2.6
2	G	220	ILE	2.6
3	H	205	SER	2.6
3	F	189	GLU	2.6
1	D	835	LEU	2.6
2	Ι	217	ASP	2.6
2	K	181	GLN	2.6
1	D	693	GLU	2.5
3	L	196	TYR	2.5
2	K	137	VAL	2.5
3	J	83	GLU	2.5
3	J	85	GLU	2.5
3	J	84	GLU	2.5
1	D	821	ASP	2.5
1	D	876	LEU	2.5



Mol	Chain	Res	Type	RSRZ
2	Е	14	PRO	2.4
3	Н	132	GLY	2.4
1	В	398	THR	2.4
2	Е	145	SER	2.4
1	А	834	HIS	2.4
2	Е	180	LEU	2.4
3	J	139	PHE	2.4
1	В	871	ARG	2.4
2	G	142	THR	2.4
3	Н	171	ASP	2.4
2	G	109	TYR	2.4
1	D	651	HIS	2.4
2	Е	181	GLN	2.4
1	В	637	GLY	2.4
2	G	135	ALA	2.4
3	F	18	ARG	2.4
3	L	63	PRO	2.4
1	С	625	GLN	2.4
3	F	192	ARG	2.4
3	Н	124	PRO	2.4
2	Ι	192	THR	2.4
1	А	829	LYS	2.4
3	J	207	SER	2.4
3	Н	131	SER	2.4
1	D	873	LEU	2.3
3	J	97	GLU	2.3
2	G	201	GLN	2.3
3	L	203	LYS	2.3
3	J	215	ARG	2.3
1	В	394	LEU	2.3
3	L	147	ASP	2.3
1	В	886	LEU	2.3
3	F	79	ILE	2.3
1	В	839	ILE	2.3
3	L	128	GLN	2.3
3	L	114	ASP	2.3
3	Н	194	ASN	2.3
3	J	43	LYS	2.3
1	В	640	VAL	2.3
3	J	123	PRO	2.3
2	E	1	$GL\overline{U}$	2.3
1	D	839	ILE	2.2



|--|

Mol	Chain	Res	Type	RSRZ
1	A	826	LYS	2.2
1	С	834	HIS	2.2
1	D	837	THR	2.2
3	J	119	VAL	2.2
2	Ι	134	LEU	2.2
3	J	216	ASN	2.2
3	Н	68	GLY	2.2
3	Н	114	ASP	2.2
3	L	161	ASN	2.2
2	Κ	52	HIS	2.2
2	Κ	108	TYR	2.2
1	В	463	GLY	2.2
1	С	397	ILE	2.2
1	С	601	LEU	2.1
2	Ι	179	VAL	2.1
3	F	208	PRO	2.1
3	Н	130	THR	2.1
1	D	654	GLY	2.1
1	D	414	PHE	2.1
3	L	62	VAL	2.1
2	Κ	220	ILE	2.1
2	Ι	164	TRP	2.1
1	С	816	PRO	2.1
3	Н	54	TYR	2.1
1	D	463	GLY	2.1
3	Н	115	ALA	2.1
3	J	154	ILE	2.1
1	D	755	GLU	2.1
1	В	866	THR	2.1
3	J	163	VAL	2.1
3	J	171	ASP	2.1
2	K	109	TYR	2.1
2	Κ	124	ALA	2.1
1	D	649	VAL	2.1
2	Е	133	PRO	2.1
2	G	59	LYS	2.0
3	L	190	TYR	2.0
2	G	149	GLY	2.0
3	F	51	LEU	2.0
3	F	17	GLN	2.0
2	Ι	171	SER	2.0
2	Κ	123	SER	2.0



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Mol	Chain	Res	Type	RSRZ
3	Н	64	ALA	2.0
3	J	67	SER	2.0
2	Е	123	SER	2.0
1	А	818	TYR	2.0
3	Н	185	LEU	2.0
2	Е	141	THR	2.0
1	А	835	LEU	2.0
1	D	653	LEU	2.0
3	Н	203	LYS	2.0
3	Н	175	SER	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	4KU	С	1000	28/28	0.74	0.33	113,118,123,125	0
4	4KU	А	1000	28/28	0.78	0.29	105,108,112,114	0
4	4KU	В	1000	28/28	0.79	0.27	143,146,152,155	0
4	4KU	D	1000	28/28	0.82	0.24	148,152,159,163	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.











6.5 Other polymers (i)

There are no such residues in this entry.

