Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2016 – 11:14 AM EDT

PDB ID	:	5B3J
Title	:	Activation of NMDA receptors and the mechanism of inhibition by ifenprodil
Authors	:	Tajima, N.; Karakas, E.; Grant, T.; Simorowski, N.; Diaz-Avalos, R.; Grigorieff, N.; Furukawa, H.
Deposited on	:	2016-03-01
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

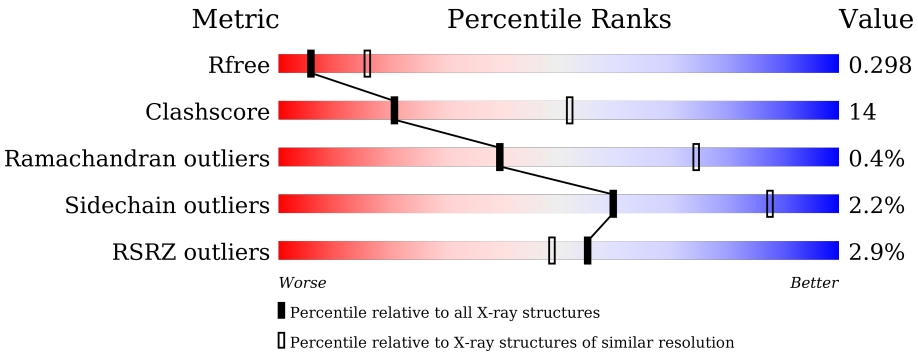
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027674

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	A	383	2% 64% 25% • 9%
1	B	383	4% 64% 23% • 12%
2	C	364	3% 65% 26% • 8%
2	D	364	6% 66% 23% • 10%
3	E	224	% 74% 20% • •
3	H	224	% 71% 23% • •

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Mol	Chain	Length	Quality of chain
4	F	213	
4	L	213	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NA	B	501	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15954 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NMDA glutamate receptor subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2491	1595	422	464	10			
1	B	338	Total	C	N	O	S	0	0	0
			2370	1516	396	448	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	engineered mutation	UNP Q91977
A	371	GLN	ASN	engineered mutation	UNP Q91977
B	61	GLN	ASN	engineered mutation	UNP Q91977
B	371	GLN	ASN	engineered mutation	UNP Q91977

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	335	Total	C	N	O	S	0	2	0
			2390	1536	390	450	14			
2	D	329	Total	C	N	O	S	0	0	0
			2315	1477	386	439	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	348	ASP	ASN	engineered mutation	UNP Q00960
D	348	ASP	ASN	engineered mutation	UNP Q00960

- Molecule 3 is a protein called Fab, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	215	Total	C	N	O	S	0	0	0
			1536	976	252	300	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	216	Total	C	N	O	S	0	0	0
			1551	983	254	306	8			

- Molecule 4 is a protein called Fab, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	211	Total	C	N	O	S	0	0	0
			1595	1001	269	319	6			
4	L	212	Total	C	N	O	S	0	0	0
			1598	1007	267	318	6			

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

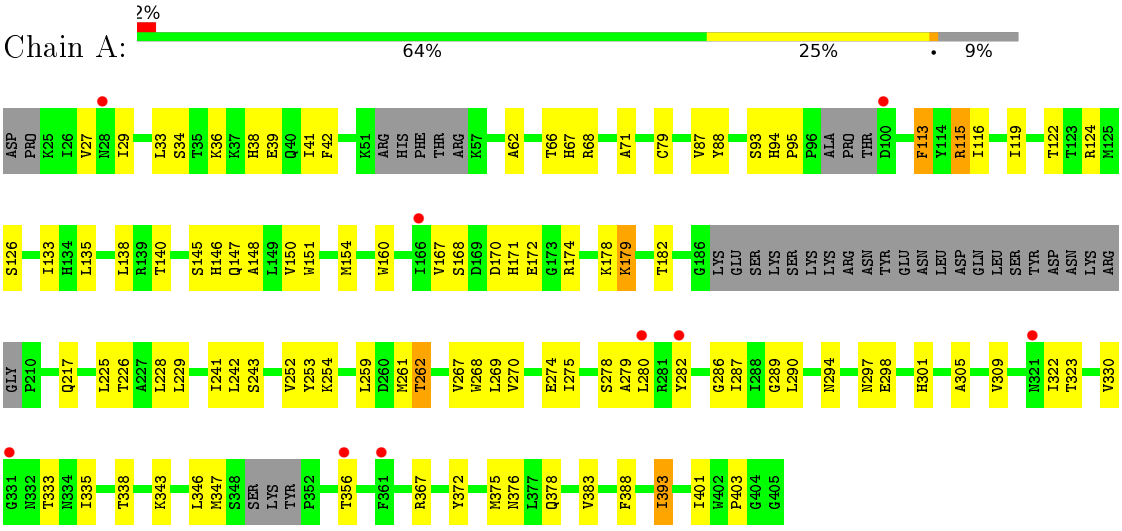
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	8	Total	O	0	0
			8	8		
6	C	11	Total	O	0	0
			11	11		
6	E	10	Total	O	0	0
			10	10		
6	D	10	Total	O	0	0
			10	10		
6	F	16	Total	O	0	0
			16	16		
6	H	21	Total	O	0	0
			21	21		
6	L	18	Total	O	0	0
			18	18		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

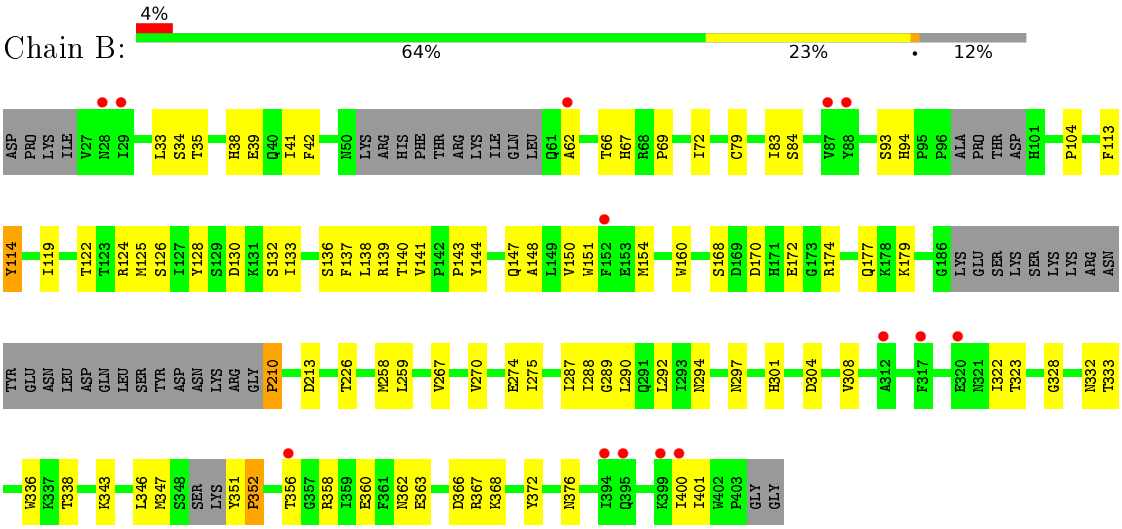
- Molecule 1: NMDA glutamate receptor subunit

Chain A:



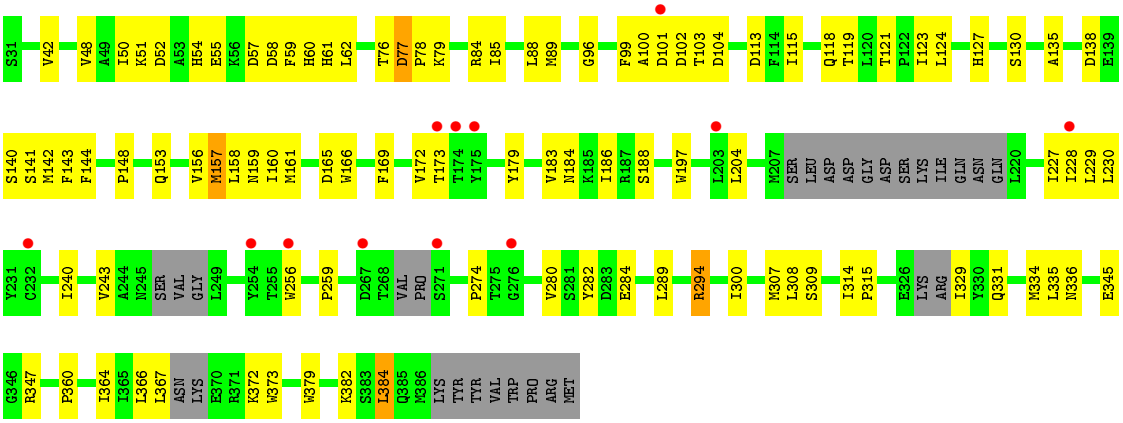
- Molecule 1: NMDA glutamate receptor subunit

Chain B:



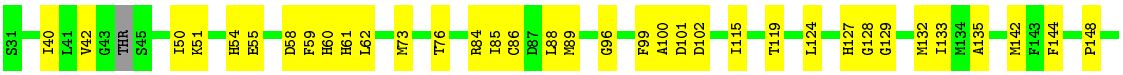
- Molecule 2: Glutamate receptor ionotropic, NMDA 2B

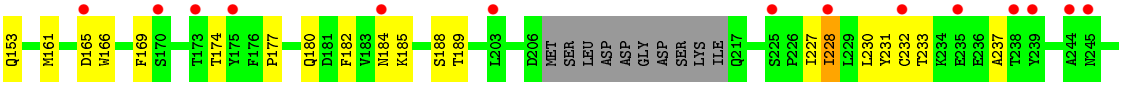
Chain C:

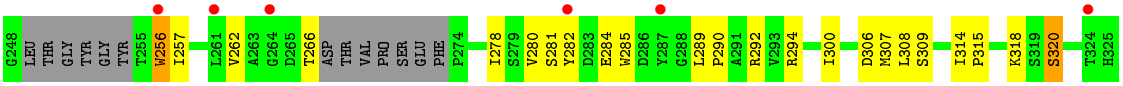


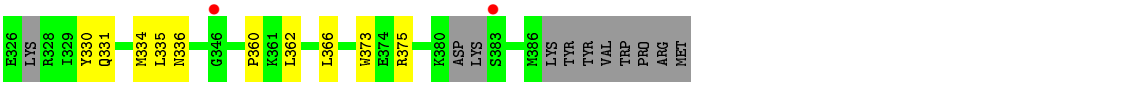
• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain D:



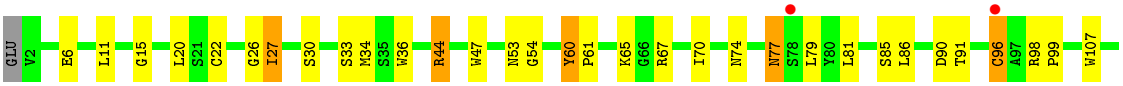






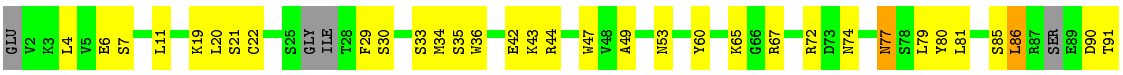
• Molecule 3: Fab, heavy chain

Chain E:



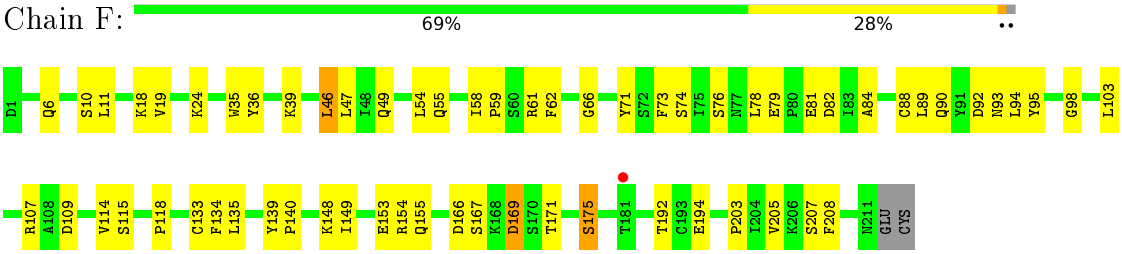
• Molecule 3: Fab, heavy chain

Chain H:



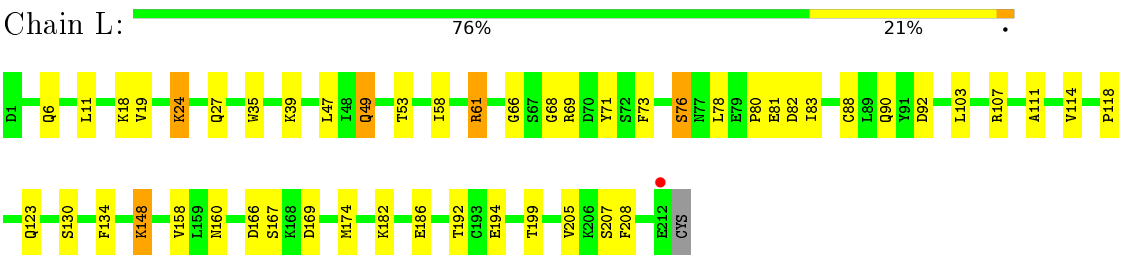
• Molecule 4: Fab, light chain

Chain F:



• Molecule 4: Fab, light chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	247.25Å 79.90Å 181.31Å 90.00° 127.09° 90.00°	Depositor
Resolution (Å)	29.93 – 2.90 47.80 – 2.78	Depositor EDS
% Data completeness (in resolution range)	84.1 (29.93-2.90) 77.5 (47.80-2.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.273 , 0.302 0.275 , 0.298	Depositor DCC
R_{free} test set	2565 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	15954	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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 23.79 % 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 4.3533e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.35	0/2539	0.59	2/3470 (0.1%)
1	B	0.43	1/2417 (0.0%)	0.58	0/3317
2	C	0.37	0/2440	0.63	2/3340 (0.1%)
2	D	0.42	2/2361 (0.1%)	0.64	2/3228 (0.1%)
3	E	0.33	0/1580	0.60	1/2175 (0.0%)
3	H	0.39	0/1593	0.67	1/2189 (0.0%)
4	F	0.47	0/1633	0.63	0/2225
4	L	0.36	0/1636	0.62	2/2230 (0.1%)
All	All	0.39	3/16199 (0.0%)	0.62	10/22174 (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	E	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	PRO	N-CD	-12.50	1.30	1.47
2	D	256	TRP	CB-CG	6.59	1.62	1.50
2	D	228	ILE	CG1-CD1	-5.60	1.11	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	148	LYS	CD-CE-NZ	-7.57	94.30	111.70
2	C	384	LEU	CB-CG-CD2	-7.38	98.45	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	228	ILE	CA-CB-CG1	-7.22	97.28	111.00
3	H	149	CYS	CA-CB-SG	6.46	125.62	114.00
3	E	149	CYS	CA-CB-SG	6.33	125.39	114.00
2	C	157	MET	CG-SD-CE	-5.97	90.65	100.20
2	D	320	SER	CB-CA-C	-5.92	98.86	110.10
1	A	225	LEU	CB-CG-CD2	-5.79	101.15	111.00
1	A	393	ILE	CG1-CB-CG2	-5.27	99.80	111.40
4	L	24	LYS	CD-CE-NZ	-5.05	100.09	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	26	GLY	Peptide
3	E	27	ILE	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	A	2491	0	2330	84	0
1	B	2370	0	2148	73	0
2	C	2390	0	2148	74	0
2	D	2315	0	2025	73	0
3	E	1536	0	1399	34	0
3	H	1551	0	1417	41	0
4	F	1595	0	1485	43	0
4	L	1598	0	1499	34	0
5	B	1	0	0	0	0
6	A	13	0	0	1	0
6	B	8	0	0	1	0
6	C	11	0	0	0	0
6	D	10	0	0	1	0
6	E	10	0	0	0	0
6	F	16	0	0	0	0
6	H	21	0	0	0	0
6	L	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15954	0	14451	438	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 (438) 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)
2:D:228:ILE:HD11	2:D:256:TRP:HA	1.47	0.93
1:B:210:PRO:HA	1:B:213:ASP:OD1	1.74	0.88
1:A:333:THR:HG1	2:C:76:THR:HG1	1.21	0.87
1:A:138:LEU:HD11	1:A:343:LYS:HG3	1.58	0.85
3:E:34:MET:HG2	3:E:98:ARG:HB2	1.59	0.84
3:H:60:TYR:HD2	3:H:65:LYS:HG3	1.44	0.83
2:D:51:LYS:O	2:D:55:GLU:HG3	1.79	0.82
2:C:113:ASP:OD2	2:C:143:PHE:HB3	1.79	0.82
1:A:174:ARG:NH2	1:A:217:GLN:OE1	2.13	0.81
3:H:147:LEU:HD13	3:H:202:VAL:HG21	1.60	0.81
3:E:98:ARG:HD3	3:E:111:VAL:HG21	1.63	0.81
4:F:18:LYS:NZ	4:F:74:SER:OG	2.15	0.79
1:A:38:HIS:HA	1:A:41:ILE:HD12	1.63	0.78
4:F:46:LEU:HD23	4:F:55:GLN:HG3	1.64	0.78
2:C:166:TRP:HB3	2:C:227:ILE:HG13	1.67	0.77
4:L:39:LYS:NZ	4:L:81:GLU:O	2.18	0.77
1:B:288:ILE:HD11	1:B:400:ILE:HD11	1.64	0.77
1:A:167:VAL:HG12	1:A:243:SER:HB3	1.65	0.77
3:H:67:ARG:NH2	3:H:90:ASP:OD2	2.17	0.76
4:F:61:ARG:NH1	4:F:79:GLU:OE1	2.19	0.75
1:B:38:HIS:HA	1:B:41:ILE:HD12	1.69	0.75
1:A:29:ILE:HD11	1:A:309:VAL:HG21	1.69	0.75
1:B:328:GLY:O	1:B:332:ASN:ND2	2.19	0.74
2:C:138:ASP:OD1	2:C:140:SER:OG	2.05	0.74
2:C:159:ASN:HD22	2:C:379:TRP:HZ3	1.33	0.73
1:A:270:VAL:HG13	1:A:274:GLU:HB2	1.70	0.73
1:A:94:HIS:HB3	1:A:122:THR:OG1	1.89	0.72
4:F:148:LYS:NZ	4:F:194:GLU:OE1	2.21	0.72
2:C:101:ASP:OD1	2:C:102:ASP:N	2.23	0.72
4:L:61:ARG:NH2	4:L:82:ASP:OD1	2.23	0.72
2:D:101:ASP:OD1	2:D:102:ASP:N	2.24	0.71
3:H:22:CYS:HB3	3:H:79:LEU:HB3	1.72	0.70
2:C:51:LYS:O	2:C:55:GLU:HG3	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:VAL:HG13	1:B:274:GLU:HB2	1.74	0.70
3:E:36:TRP:NE1	3:E:81:LEU:HB2	2.08	0.69
1:B:137:PHE:CE2	1:B:139:ARG:HG2	2.28	0.68
4:F:24:LYS:NZ	4:L:6:GLN:O	2.26	0.68
1:B:323:THR:HG22	1:B:338:THR:HG23	1.76	0.68
3:H:11:LEU:HB2	3:H:156:PRO:HG3	1.76	0.68
3:E:98:ARG:HD3	3:E:111:VAL:CG2	2.23	0.68
3:H:74:ASN:O	3:H:77:ASN:ND2	2.27	0.68
4:F:11:LEU:HD22	4:F:19:VAL:HB	1.75	0.67
2:C:153:GLN:NE2	2:C:259:PRO:HB3	2.09	0.67
4:F:47:LEU:HD23	4:F:58:ILE:HD12	1.77	0.67
1:A:146:HIS:HA	1:A:179:LYS:HE3	1.77	0.66
2:D:40:ILE:HD11	2:D:73:MET:HE2	1.76	0.66
1:A:42:PHE:CE2	1:A:62:ALA:HB1	2.30	0.66
2:D:180:GLN:O	2:D:184:ASN:ND2	2.28	0.66
1:B:351:TYR:N	1:B:352:PRO:HD3	2.11	0.66
1:A:113:PHE:CD2	2:C:78:PRO:HD3	2.31	0.66
2:C:160:ILE:HD11	2:C:364:ILE:HG12	1.78	0.65
2:C:85:ILE:O	2:C:89:MET:HG3	1.96	0.65
1:A:178:LYS:O	1:A:182:THR:HG23	1.97	0.65
1:A:170:ASP:OD1	1:A:171:HIS:N	2.30	0.65
3:E:74:ASN:O	3:E:77:ASN:ND2	2.30	0.65
2:D:42:VAL:CG2	2:D:101:ASP:HA	2.27	0.64
1:B:148:ALA:HB3	1:B:179:LYS:HG2	1.79	0.64
4:L:182:LYS:O	4:L:186:GLU:HG3	1.97	0.64
1:B:226:THR:HG23	1:B:259:LEU:HD11	1.79	0.64
1:B:83:ILE:HD13	1:B:114:TYR:HE2	1.62	0.64
4:L:192:THR:HG23	4:L:207:SER:HB3	1.79	0.63
4:L:24:LYS:NZ	4:L:69:ARG:HH21	1.96	0.63
1:B:376:ASN:HD22	1:B:400:ILE:HG13	1.63	0.62
3:H:72:ARG:HE	3:H:74:ASN:ND2	1.97	0.62
1:B:356:THR:OG1	1:B:367:ARG:NH2	2.31	0.62
2:D:174:THR:HG23	2:D:232:CYS:HB3	1.80	0.62
1:A:71:ALA:HB3	2:C:118:GLN:OE1	1.99	0.62
4:F:194:GLU:HG2	4:F:203:PRO:HB3	1.81	0.62
1:B:94:HIS:HB3	1:B:122:THR:HB	1.82	0.62
2:D:100:ALA:HB1	2:D:289:LEU:HD11	1.82	0.61
2:C:57:ASP:OD1	2:C:294:ARG:NH1	2.33	0.61
1:B:140:THR:O	1:B:367:ARG:NH1	2.29	0.61
1:A:226:THR:HG23	1:A:259:LEU:HD11	1.82	0.61
1:A:270:VAL:CG1	1:A:274:GLU:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:HIS:O	1:B:122:THR:HG21	1.99	0.61
4:L:194:GLU:HG3	4:L:205:VAL:HG23	1.83	0.61
1:A:67:HIS:NE2	1:A:93:SER:O	2.30	0.61
2:D:282:TYR:HE1	2:D:360:PRO:HB2	1.66	0.61
3:E:11:LEU:HD22	3:E:156:PRO:HG3	1.83	0.61
1:B:270:VAL:CG1	1:B:274:GLU:HB2	2.31	0.60
2:C:184:ASN:O	2:C:188:SER:OG	2.14	0.60
2:C:84:ARG:O	2:C:88:LEU:HG	2.01	0.60
3:H:4:LEU:HD21	3:H:96:CYS:HB3	1.83	0.60
1:A:113:PHE:HD2	2:C:78:PRO:HD3	1.66	0.60
1:A:305:ALA:O	1:A:309:VAL:HG22	2.01	0.60
1:B:137:PHE:HE2	1:B:139:ARG:HG2	1.66	0.60
2:D:42:VAL:HG22	2:D:100:ALA:O	2.00	0.60
2:D:318:LYS:NZ	2:D:320:SER:O	2.34	0.60
2:D:84:ARG:O	2:D:88:LEU:HG	2.01	0.60
3:H:20:LEU:HD12	3:H:81:LEU:HD23	1.82	0.60
1:B:104:PRO:HG2	1:B:128:TYR:CE2	2.36	0.59
2:D:119:THR:HB	2:D:318:LYS:HE2	1.83	0.59
2:D:308:LEU:HB2	2:D:314:ILE:CG2	2.32	0.59
4:F:36:TYR:CZ	4:F:46:LEU:HD12	2.37	0.59
4:F:90:GLN:NE2	4:F:93:ASN:H	2.01	0.59
4:L:11:LEU:HD22	4:L:19:VAL:HB	1.85	0.59
4:L:123:GLN:HE22	4:L:130:SER:CB	2.15	0.59
3:E:67:ARG:NH2	3:E:90:ASP:OD2	2.36	0.59
4:L:80:PRO:O	4:L:83:ILE:HD12	2.03	0.59
1:B:270:VAL:HG21	1:B:287:ILE:HD11	1.84	0.59
4:F:18:LYS:HB2	4:F:76:SER:HA	1.85	0.59
2:C:59:PHE:O	2:C:62:LEU:HB2	2.03	0.58
3:H:42:GLU:O	3:H:44:ARG:N	2.35	0.58
1:B:133:ILE:HD11	2:D:135:ALA:O	2.03	0.58
1:A:242:LEU:HD11	1:A:252:VAL:HG21	1.86	0.58
2:D:40:ILE:HG23	2:D:99:PHE:HA	1.86	0.58
1:B:323:THR:HG23	1:B:336:TRP:HE1	1.68	0.57
2:C:274:PRO:O	2:C:367:LEU:HD23	2.04	0.57
1:A:270:VAL:HG21	1:A:287:ILE:HD11	1.87	0.57
1:B:69:PRO:HB3	4:F:153:GLU:OE2	2.04	0.57
1:B:35:THR:O	1:B:39:GLU:HG3	2.04	0.57
1:B:72:ILE:HD11	2:D:115:ILE:HD11	1.87	0.57
2:D:282:TYR:CE1	2:D:360:PRO:HB2	2.39	0.56
2:D:50:ILE:HD11	2:D:289:LEU:HD23	1.86	0.56
1:A:275:ILE:HD13	1:A:289:GLY:HA3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:308:LEU:HB2	2:D:314:ILE:HG23	1.88	0.56
2:C:366:LEU:O	2:C:373:TRP:HA	2.05	0.56
3:H:98:ARG:HD2	3:H:111:VAL:CG2	2.35	0.56
2:C:228:ILE:HG12	2:C:256:TRP:CD2	2.41	0.56
1:A:34:SER:OG	1:A:298:GLU:OE2	2.15	0.56
3:E:60:TYR:HD2	3:E:65:LYS:HG3	1.70	0.56
2:C:100:ALA:HB1	2:C:289:LEU:HD11	1.87	0.56
2:C:50:ILE:HD11	2:C:289:LEU:HD23	1.86	0.56
2:D:101:ASP:OD2	2:D:129:GLY:N	2.36	0.56
1:A:378:GLN:HG2	1:A:401:ILE:HD12	1.88	0.56
1:A:33:LEU:HD12	1:A:39:GLU:HA	1.88	0.56
3:E:30:SER:O	3:E:53:ASN:HB2	2.06	0.55
3:E:22:CYS:HB3	3:E:79:LEU:HB3	1.86	0.55
4:F:194:GLU:HG3	4:F:205:VAL:HG23	1.87	0.55
1:B:323:THR:HG23	1:B:336:TRP:NE1	2.22	0.55
1:A:388:PHE:CD1	1:A:393:ILE:HG22	2.42	0.55
2:C:331:GLN:H	2:C:331:GLN:CD	2.09	0.55
2:D:185:LYS:O	2:D:189:THR:HG23	2.06	0.55
2:C:42:VAL:HG22	2:C:100:ALA:O	2.07	0.55
1:A:330:VAL:HG23	2:C:79:LYS:HD3	1.89	0.55
1:A:229:LEU:HB3	1:A:261:MET:SD	2.47	0.55
2:C:282:TYR:O	2:C:284:GLU:HG2	2.06	0.55
2:D:228:ILE:HD11	2:D:256:TRP:CA	2.27	0.55
2:D:230:LEU:HD11	2:D:232:CYS:SG	2.47	0.55
2:D:228:ILE:HD12	2:D:256:TRP:CE3	2.42	0.54
1:B:290:LEU:HD22	1:B:372:TYR:CB	2.38	0.54
2:D:101:ASP:HB3	2:D:127:HIS:O	2.08	0.54
3:H:36:TRP:CH2	3:H:96:CYS:SG	3.01	0.54
1:A:115:ARG:CD	1:A:335:ILE:HD11	2.37	0.54
1:B:126:SER:N	1:B:172:GLU:OE1	2.39	0.54
3:E:172:VAL:HG12	3:E:190:VAL:HG23	1.90	0.53
4:L:35:TRP:CE2	4:L:73:PHE:HB2	2.43	0.53
2:D:230:LEU:HD12	2:D:262:VAL:HG21	1.90	0.53
2:D:228:ILE:CD1	2:D:256:TRP:HA	2.29	0.53
4:L:160:ASN:HD22	4:L:174:MET:CE	2.21	0.53
1:A:343:LYS:HA	1:A:346:LEU:HD12	1.90	0.53
1:B:376:ASN:ND2	1:B:400:ILE:HG13	2.22	0.53
1:B:124:ARG:HB2	1:B:144:TYR:CZ	2.44	0.53
1:B:333:THR:OG1	2:D:76:THR:HG23	2.09	0.53
2:D:86:CYS:HA	2:D:89:MET:HG3	1.91	0.53
4:F:78:LEU:HD22	4:F:103:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:119:THR:OG1	2:C:121:THR:OG1	2.14	0.53
2:C:172:VAL:HG13	2:C:230:LEU:HD13	1.91	0.53
1:A:27:VAL:HG13	1:A:88:TYR:CD1	2.44	0.53
2:C:58:ASP:HB2	3:E:53:ASN:OD1	2.08	0.53
3:E:36:TRP:CG	3:E:81:LEU:HD22	2.45	0.53
2:D:281:SER:HB3	6:D:408:HOH:O	2.08	0.52
1:A:147:GLN:HG2	1:A:372:TYR:HE2	1.75	0.52
1:B:150:VAL:O	1:B:154:MET:HG2	2.09	0.52
1:B:322:ILE:HA	1:B:338:THR:HG21	1.91	0.52
2:C:331:GLN:OE1	2:C:331:GLN:N	2.38	0.52
3:E:15:GLY:HA2	3:E:85:SER:HA	1.92	0.52
1:A:274:GLU:CD	1:A:274:GLU:H	2.10	0.52
1:B:258:MET:HG2	1:B:258:MET:O	2.10	0.52
2:C:153:GLN:HB3	2:C:280:VAL:HG11	1.91	0.52
2:D:60:HIS:O	2:D:61:HIS:HB2	2.09	0.52
2:D:166:TRP:HB3	2:D:227:ILE:HG13	1.92	0.52
2:C:54:HIS:HA	2:C:57:ASP:OD2	2.10	0.52
3:E:6:GLU:OE2	3:E:113:GLY:HA3	2.10	0.52
3:E:99:PRO:HB2	3:E:107:TRP:HB2	1.91	0.52
1:B:119:ILE:HD13	1:B:138:LEU:HB2	1.91	0.52
3:H:198:PRO:HG3	3:H:221:PRO:HG3	1.91	0.52
2:C:60:HIS:O	2:C:61:HIS:HB2	2.10	0.52
2:C:96:GLY:HA3	2:C:300:ILE:HD13	1.91	0.51
3:H:60:TYR:CD2	3:H:65:LYS:HG3	2.35	0.51
3:E:98:ARG:HH11	3:E:111:VAL:HG22	1.75	0.51
1:B:147:GLN:NE2	6:B:601:HOH:O	2.32	0.51
3:E:33:SER:O	3:E:34:MET:HG3	2.10	0.51
1:A:151:TRP:HA	1:A:154:MET:HG2	1.93	0.51
2:C:161:MET:O	2:C:165:ASP:N	2.43	0.51
1:B:362:ASN:OD1	1:B:363:GLU:N	2.44	0.51
2:C:307:MET:HE1	2:C:315:PRO:HG3	1.93	0.51
4:F:6:GLN:HE21	4:F:98:GLY:HA3	1.75	0.51
4:L:123:GLN:HE22	4:L:130:SER:HB2	1.76	0.50
4:F:39:LYS:HG2	4:F:84:ALA:HB2	1.93	0.50
2:C:345:GLU:C	2:C:347:ARG:H	2.15	0.50
2:D:59:PHE:O	2:D:62:LEU:HB2	2.12	0.50
1:A:274:GLU:OE1	1:A:274:GLU:N	2.35	0.50
2:C:77:ASP:HB2	2:C:78:PRO:HD2	1.92	0.50
4:F:192:THR:HG23	4:F:207:SER:HB3	1.93	0.50
3:H:72:ARG:HE	3:H:74:ASN:HD21	1.59	0.50
1:A:376:ASN:ND2	1:A:401:ILE:H	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ILE:HD13	1:B:114:TYR:CE2	2.45	0.50
1:A:119:ILE:HD13	1:A:138:LEU:HB2	1.94	0.50
1:B:124:ARG:HD2	1:B:141:VAL:HG12	1.93	0.50
1:B:139:ARG:HH12	1:B:143:PRO:HB3	1.77	0.50
1:B:351:TYR:CB	1:B:360:GLU:HG2	2.42	0.50
3:E:27:ILE:HG21	3:E:77:ASN:OD1	2.12	0.50
1:A:378:GLN:CD	1:A:383:VAL:HG21	2.31	0.49
1:B:275:ILE:HD13	1:B:289:GLY:HA3	1.94	0.49
4:F:35:TRP:CE2	4:F:73:PHE:HB2	2.47	0.49
2:C:308:LEU:HB2	2:C:314:ILE:CG2	2.42	0.49
4:F:89:LEU:HD11	4:F:95:TYR:HB3	1.93	0.49
4:L:47:LEU:HD23	4:L:58:ILE:HD12	1.94	0.49
1:A:356:THR:OG1	1:A:367:ARG:NH2	2.43	0.49
2:C:99:PHE:HD2	2:C:130:SER:HB3	1.77	0.49
2:D:119:THR:CB	2:D:318:LYS:HE2	2.42	0.49
2:D:282:TYR:HD1	2:D:362:LEU:HD23	1.78	0.49
3:H:19:LYS:HE2	3:H:80:TYR:CD1	2.47	0.49
1:B:160:TRP:CH2	1:B:267:VAL:HG11	2.48	0.49
3:H:98:ARG:HD2	3:H:111:VAL:HG21	1.94	0.49
2:C:367:LEU:HD12	2:C:372:LYS:H	1.78	0.49
4:F:18:LYS:HE2	4:F:76:SER:HB3	1.94	0.49
1:B:304:ASP:O	1:B:308:VAL:HG23	2.12	0.49
2:C:89:MET:HE1	2:C:119:THR:HB	1.95	0.49
2:D:228:ILE:CD1	2:D:256:TRP:CD2	2.96	0.49
3:E:77:ASN:N	3:E:77:ASN:HD22	2.10	0.49
4:F:61:ARG:NH2	4:F:82:ASP:OD1	2.46	0.49
3:H:35:SER:HB2	3:H:49:ALA:O	2.12	0.49
1:B:124:ARG:HB2	1:B:144:TYR:CE2	2.48	0.48
3:E:60:TYR:CD2	3:E:65:LYS:HG3	2.48	0.48
3:H:145:VAL:HG13	3:H:194:SER:OG	2.13	0.48
1:B:113:PHE:HD1	1:B:114:TYR:CD1	2.31	0.48
1:B:79:CYS:O	1:B:84:SER:OG	2.24	0.48
2:D:180:GLN:HB3	2:D:184:ASN:HD21	1.77	0.48
3:E:20:LEU:HD12	3:E:81:LEU:HD23	1.95	0.48
1:A:115:ARG:NH2	1:A:135:LEU:HD13	2.28	0.48
1:B:290:LEU:HD22	1:B:372:TYR:HB2	1.95	0.48
3:H:34:MET:HE2	3:H:98:ARG:HG3	1.94	0.48
2:C:169:PHE:HE2	2:C:197:TRP:CE3	2.32	0.48
1:B:67:HIS:NE2	1:B:93:SER:O	2.34	0.48
4:F:59:PRO:HB2	4:F:61:ARG:HG2	1.96	0.48
1:B:125:MET:O	1:B:139:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:THR:HG22	1:B:338:THR:CG2	2.44	0.48
1:A:133:ILE:HD11	2:C:135:ALA:O	2.14	0.48
1:A:115:ARG:HD3	1:A:335:ILE:HD11	1.95	0.48
3:H:208:HIS:CE1	3:H:210:ALA:HB3	2.49	0.48
2:C:282:TYR:HB3	2:C:284:GLU:OE2	2.13	0.47
2:C:379:TRP:HE3	2:C:384:LEU:CD2	2.26	0.47
1:A:322:ILE:HA	1:A:338:THR:HG21	1.95	0.47
2:D:228:ILE:H	2:D:228:ILE:HG12	1.49	0.47
1:A:36:LYS:HE3	1:A:36:LYS:HB2	1.66	0.47
3:H:91:THR:HA	3:H:118:VAL:O	2.13	0.47
2:C:157:MET:SD	2:C:229:LEU:HD22	2.54	0.47
2:C:315:PRO:HG2	2:C:335:LEU:HD22	1.97	0.47
3:H:47:TRP:NE1	3:H:49:ALA:O	2.47	0.47
1:B:362:ASN:CG	1:B:363:GLU:N	2.68	0.47
4:F:169:ASP:HB3	4:F:171:THR:HG23	1.95	0.47
3:H:85:SER:C	3:H:86:LEU:O	2.45	0.47
3:E:44:ARG:HB3	3:E:44:ARG:HE	1.54	0.47
3:H:98:ARG:HD2	3:H:111:VAL:HG22	1.97	0.47
1:A:274:GLU:CD	1:A:274:GLU:N	2.68	0.47
2:C:153:GLN:HE21	2:C:259:PRO:HB3	1.80	0.47
3:H:6:GLU:HG2	3:H:96:CYS:SG	2.55	0.47
1:A:148:ALA:HB3	1:A:179:LYS:HG2	1.97	0.46
1:A:148:ALA:HA	1:A:151:TRP:CE3	2.50	0.46
3:E:53:ASN:OD1	3:E:54:GLY:N	2.45	0.46
4:F:134:PHE:CE1	4:F:175:SER:HB2	2.50	0.46
4:L:66:GLY:HA3	4:L:71:TYR:HA	1.96	0.46
1:B:362:ASN:CG	1:B:363:GLU:H	2.19	0.46
4:F:90:GLN:HE21	4:F:93:ASN:H	1.63	0.46
1:A:68:ARG:HH21	4:L:194:GLU:CD	2.18	0.46
2:D:230:LEU:HD13	2:D:231:TYR:N	2.30	0.46
2:D:54:HIS:NE2	2:D:55:GLU:HG2	2.30	0.46
3:H:29:PHE:CD2	3:H:74:ASN:HA	2.51	0.46
4:L:78:LEU:HD22	4:L:103:LEU:HD21	1.96	0.46
1:A:147:GLN:HG2	1:A:372:TYR:CE2	2.49	0.46
1:A:150:VAL:O	1:A:154:MET:HG2	2.15	0.46
3:E:33:SER:O	3:E:99:PRO:HD2	2.16	0.46
4:L:49:GLN:NE2	4:L:53:THR:OG1	2.48	0.46
1:A:124:ARG:NH2	6:A:502:HOH:O	2.48	0.46
2:D:285:TRP:HB3	2:D:375:ARG:NH2	2.30	0.46
2:C:379:TRP:CH2	2:C:382:LYS:HA	2.50	0.46
3:H:72:ARG:NE	3:H:74:ASN:HD21	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:99:PRO:HB2	3:H:107:TRP:HB2	1.97	0.46
2:C:148:PRO:HB3	2:C:360:PRO:HG3	1.98	0.46
4:F:61:ARG:HG2	4:F:61:ARG:H	1.51	0.46
2:C:179:TYR:O	2:C:183:VAL:HG23	2.16	0.46
2:C:42:VAL:HG23	2:C:101:ASP:HA	1.97	0.46
3:H:213:THR:HG22	3:H:215:VAL:HG23	1.98	0.46
2:C:173:THR:O	2:C:204:LEU:HA	2.17	0.46
2:C:142:MET:HG2	2:C:336:ASN:HD21	1.81	0.46
2:D:233:THR:O	2:D:237:ALA:N	2.43	0.46
2:D:307:MET:HE1	2:D:315:PRO:HG3	1.98	0.46
2:D:161:MET:O	2:D:165:ASP:N	2.49	0.45
4:F:66:GLY:HA3	4:F:71:TYR:HA	1.98	0.45
4:L:19:VAL:HG13	4:L:78:LEU:HD11	1.98	0.45
1:B:174:ARG:HA	1:B:177:GLN:HB3	1.99	0.45
4:L:90:GLN:HG2	4:L:92:ASP:H	1.82	0.45
2:D:96:GLY:HA3	2:D:300:ILE:HD13	1.97	0.45
3:E:181:SER:HA	3:E:182:ASP:HA	1.62	0.45
4:F:90:GLN:HE21	4:F:92:ASP:N	2.15	0.45
3:H:42:GLU:H	3:H:42:GLU:CD	2.19	0.45
2:D:58:ASP:OD1	2:D:60:HIS:HB2	2.17	0.45
1:A:168:SER:O	1:A:170:ASP:N	2.49	0.45
1:B:294:ASN:O	1:B:301:HIS:NE2	2.48	0.45
1:B:297:ASN:O	1:B:301:HIS:HD2	2.00	0.45
1:B:33:LEU:HA	1:B:93:SER:OG	2.16	0.45
4:F:166:ASP:OD1	4:F:167:SER:N	2.50	0.45
1:A:148:ALA:HA	1:A:151:TRP:CD2	2.52	0.45
2:C:127:HIS:O	2:C:130:SER:OG	2.30	0.45
4:F:149:ILE:HD12	4:F:154:ARG:HG3	1.98	0.45
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.37	0.45
1:B:367:ARG:HG2	1:B:368:LYS:N	2.32	0.45
2:D:315:PRO:HB3	2:D:331:GLN:NE2	2.31	0.45
1:B:148:ALA:HA	1:B:151:TRP:CE3	2.52	0.45
2:D:42:VAL:O	2:D:42:VAL:HG23	2.17	0.45
4:L:114:VAL:HA	4:L:134:PHE:O	2.17	0.45
1:A:87:VAL:HG13	1:A:116:ILE:HG21	1.99	0.45
1:A:297:ASN:O	1:A:301:HIS:HD2	2.00	0.45
1:A:343:LYS:O	1:A:347:MET:HG3	2.16	0.45
2:C:113:ASP:OD2	2:C:141:SER:OG	2.30	0.45
2:C:142:MET:HG2	2:C:336:ASN:ND2	2.32	0.45
3:H:33:SER:O	3:H:99:PRO:HD2	2.16	0.45
1:B:141:VAL:HG13	1:B:292:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:LEU:HD22	1:B:372:TYR:HB3	1.99	0.44
2:C:42:VAL:CG2	2:C:101:ASP:HA	2.47	0.44
2:D:285:TRP:HB3	2:D:375:ARG:HH22	1.82	0.44
4:F:194:GLU:HG3	4:F:205:VAL:CG2	2.47	0.44
2:C:334:MET:HE2	2:C:334:MET:HB3	1.77	0.44
2:D:153:GLN:HB3	2:D:280:VAL:HG11	2.00	0.44
3:H:147:LEU:CD1	3:H:202:VAL:HG21	2.39	0.44
2:C:158:LEU:HD11	2:C:186:ILE:HG23	1.99	0.44
1:B:130:ASP:OD1	1:B:132:SER:OG	2.32	0.44
1:B:33:LEU:HD12	1:B:39:GLU:HA	1.99	0.44
3:H:131:TYR:CE2	4:L:123:GLN:HG3	2.53	0.44
2:C:329:ILE:N	2:C:331:GLN:NE2	2.65	0.44
1:A:323:THR:H	1:A:338:THR:HG21	1.83	0.44
2:C:103:THR:HG22	2:C:104:ASP:H	1.83	0.44
3:E:161:VAL:HG22	3:E:206:VAL:HG22	1.99	0.44
1:A:148:ALA:HB3	1:A:179:LYS:CG	2.48	0.43
2:D:85:ILE:O	2:D:89:MET:HG3	2.18	0.43
3:H:181:SER:HA	3:H:182:ASP:HA	1.65	0.43
1:A:113:PHE:CE2	2:C:77:ASP:HA	2.53	0.43
4:F:139:TYR:CD1	4:F:140:PRO:HA	2.53	0.43
4:F:153:GLU:OE1	4:F:155:GLN:NE2	2.51	0.43
1:B:124:ARG:HD2	1:B:141:VAL:CG1	2.48	0.43
4:F:47:LEU:CD2	4:F:58:ILE:HD12	2.45	0.43
2:D:284:GLU:HG2	2:D:292:ARG:HH12	1.84	0.43
3:H:72:ARG:NE	3:H:74:ASN:ND2	2.66	0.43
4:F:118:PRO:HB3	4:F:208:PHE:CE2	2.54	0.43
1:A:393:ILE:HG21	1:A:393:ILE:HD13	1.70	0.43
2:C:367:LEU:CD1	2:C:372:LYS:H	2.32	0.43
2:C:169:PHE:HA	2:C:227:ILE:O	2.19	0.43
2:D:129:GLY:HA2	2:D:132:MET:HG3	2.01	0.43
2:D:307:MET:HE2	2:D:335:LEU:HD13	2.01	0.43
4:L:166:ASP:OD1	4:L:167:SER:N	2.52	0.43
4:L:24:LYS:HZ1	4:L:69:ARG:HH21	1.66	0.43
1:A:146:HIS:HA	1:A:179:LYS:CE	2.45	0.42
1:A:254:LYS:NZ	1:A:282:TYR:CD2	2.87	0.42
1:B:34:SER:O	1:B:66:THR:HG23	2.18	0.42
2:D:228:ILE:CD1	2:D:256:TRP:CG	3.01	0.42
4:F:39:LYS:NZ	4:F:81:GLU:O	2.28	0.42
4:L:18:LYS:HB2	4:L:76:SER:HA	2.01	0.42
1:B:168:SER:O	1:B:170:ASP:N	2.53	0.42
4:F:114:VAL:HG22	4:F:135:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:61:ARG:NH2	4:F:82:ASP:OD2	2.52	0.42
1:A:151:TRP:HA	1:A:154:MET:CG	2.48	0.42
1:A:376:ASN:O	1:A:383:VAL:HG22	2.19	0.42
4:L:27:GLN:C	4:L:69:ARG:HG2	2.40	0.42
1:A:286:GLY:O	1:A:403:PRO:HD3	2.19	0.42
1:A:294:ASN:O	1:A:301:HIS:NE2	2.49	0.42
1:A:94:HIS:HB3	1:A:122:THR:HG1	1.79	0.42
2:C:115:ILE:HG22	2:C:123:ILE:HD11	2.00	0.42
1:A:160:TRP:CH2	1:A:267:VAL:HG11	2.54	0.42
1:B:139:ARG:HD2	1:B:366:ASP:OD1	2.19	0.42
2:C:294:ARG:HH11	2:C:294:ARG:HD2	1.73	0.42
3:E:208:HIS:CE1	3:E:210:ALA:HB3	2.54	0.42
1:A:262:THR:HA	1:A:268:TRP:HE1	1.84	0.42
2:D:42:VAL:HG23	2:D:101:ASP:HA	1.99	0.42
1:A:145:SER:O	1:A:179:LYS:HD2	2.20	0.42
3:E:91:THR:HA	3:E:118:VAL:O	2.20	0.42
1:A:119:ILE:HD13	1:A:138:LEU:HD13	2.02	0.42
3:E:213:THR:HG22	3:E:215:VAL:HG23	2.02	0.42
4:F:109:ASP:OD2	4:F:140:PRO:HD3	2.19	0.42
1:B:119:ILE:HD11	1:B:346:LEU:HD13	2.02	0.42
2:C:48:VAL:O	2:C:52:ASP:OD1	2.38	0.42
2:D:257:ILE:HA	2:D:278:ILE:O	2.19	0.42
3:H:172:VAL:HG22	3:H:190:VAL:HG23	2.00	0.42
1:A:253:TYR:HE2	1:A:279:ALA:HB1	1.85	0.41
1:B:376:ASN:ND2	1:B:401:ILE:H	2.18	0.41
2:D:289:LEU:N	2:D:290:PRO:HD2	2.35	0.41
3:E:60:TYR:HE1	3:E:70:ILE:HG22	1.85	0.41
4:F:94:LEU:HD23	4:F:94:LEU:HA	1.89	0.41
4:L:111:ALA:HA	4:L:199:THR:HG21	2.00	0.41
2:C:124:LEU:HA	2:C:144:PHE:O	2.20	0.41
2:C:156:VAL:HG22	2:C:379:TRP:CD2	2.55	0.41
1:A:343:LYS:HE3	1:A:343:LYS:HB3	1.83	0.41
2:D:182:PHE:CG	2:D:231:TYR:CD2	3.08	0.41
2:D:266:THR:HB	2:D:373:TRP:CD1	2.55	0.41
3:H:7:SER:HB2	3:H:21:SER:HB2	2.01	0.41
3:H:86:LEU:HD23	3:H:86:LEU:HA	1.92	0.41
2:C:240:ILE:O	2:C:243:VAL:HG22	2.21	0.41
3:E:79:LEU:HD23	3:E:96:CYS:SG	2.60	0.41
4:L:6:GLN:HE22	4:L:88:CYS:H	1.67	0.41
1:A:126:SER:N	1:A:172:GLU:OE1	2.43	0.41
2:D:133:ILE:HG13	2:D:148:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:142:MET:HG2	2:D:336:ASN:ND2	2.36	0.41
4:F:35:TRP:CH2	4:F:88:CYS:HB3	2.56	0.41
1:A:375:MET:HA	1:A:383:VAL:O	2.21	0.41
1:A:378:GLN:OE1	1:A:383:VAL:HG11	2.19	0.41
4:F:54:LEU:HD21	4:F:62:PHE:O	2.21	0.41
4:L:194:GLU:HG3	4:L:205:VAL:CG2	2.50	0.41
1:B:290:LEU:HA	1:B:290:LEU:HD23	1.80	0.41
1:B:343:LYS:O	1:B:347:MET:HG3	2.20	0.41
2:D:315:PRO:HA	2:D:331:GLN:OE1	2.19	0.41
3:E:47:TRP:O	3:E:61:PRO:HG3	2.21	0.41
4:L:118:PRO:HB3	4:L:208:PHE:CE2	2.56	0.41
2:D:169:PHE:HA	2:D:227:ILE:O	2.21	0.41
3:H:30:SER:O	3:H:53:ASN:HB2	2.21	0.41
1:A:66:THR:CG2	4:L:148:LYS:NZ	2.84	0.41
4:L:68:GLY:O	4:L:71:TYR:OH	2.25	0.41
1:A:140:THR:O	1:A:367:ARG:HD3	2.21	0.40
1:A:290:LEU:HD22	1:A:372:TYR:CB	2.51	0.40
2:C:228:ILE:HD11	2:C:256:TRP:HB3	2.04	0.40
1:A:79:CYS:SG	2:C:79:LYS:HB2	2.61	0.40
2:D:142:MET:HG2	2:D:336:ASN:HD21	1.86	0.40
3:H:77:ASN:HD22	3:H:77:ASN:N	2.18	0.40
2:D:124:LEU:HA	2:D:144:PHE:O	2.21	0.40
2:D:278:ILE:HG12	2:D:366:LEU:HD13	2.02	0.40
2:D:40:ILE:HD11	2:D:73:MET:CE	2.46	0.40
4:L:24:LYS:HA	4:L:69:ARG:O	2.22	0.40
1:A:174:ARG:HH22	1:A:217:GLN:CD	2.22	0.40
1:B:132:SER:N	2:D:177:PRO:HG2	2.37	0.40
2:D:184:ASN:O	2:D:188:SER:OG	2.22	0.40
1:A:241:ILE:HA	1:A:269:LEU:O	2.21	0.40
1:A:94:HIS:HA	1:A:95:PRO:HD3	1.83	0.40
1:B:42:PHE:CE2	1:B:62:ALA:HB1	2.56	0.40
2:D:334:MET:HE2	2:D:334:MET:HB3	1.82	0.40
4:F:115:SER:O	4:F:133:CYS:HA	2.21	0.40
4:L:158:VAL:HG12	4:L:160:ASN:OD1	2.21	0.40
2:D:101:ASP:HB3	2:D:128:GLY:HA3	2.04	0.40
3:E:86:LEU:H	3:E:86:LEU:HD22	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	337/383 (88%)	312 (93%)	25 (7%)	0	100	100
1	B	328/383 (86%)	307 (94%)	18 (6%)	3 (1%)	21	57
2	C	325/364 (89%)	294 (90%)	31 (10%)	0	100	100
2	D	315/364 (86%)	291 (92%)	24 (8%)	0	100	100
3	E	211/224 (94%)	194 (92%)	15 (7%)	2 (1%)	21	57
3	H	208/224 (93%)	192 (92%)	12 (6%)	4 (2%)	10	35
4	F	209/213 (98%)	198 (95%)	11 (5%)	0	100	100
4	L	210/213 (99%)	198 (94%)	12 (6%)	0	100	100
All	All	2143/2368 (90%)	1986 (93%)	148 (7%)	9 (0%)	39	74

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	TYR
3	H	43	LYS
3	E	181	SER
3	H	181	SER
3	H	221	PRO
3	E	199	SER
1	B	358	ARG
3	H	86	LEU
1	B	352	PRO

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	238/329 (72%)	232 (98%)	6 (2%)	55 85
1	B	219/329 (67%)	218 (100%)	1 (0%)	92 98
2	C	227/327 (69%)	224 (99%)	3 (1%)	76 94
2	D	213/327 (65%)	209 (98%)	4 (2%)	65 89
3	E	159/191 (83%)	153 (96%)	6 (4%)	40 76
3	H	163/191 (85%)	160 (98%)	3 (2%)	66 90
4	F	171/190 (90%)	165 (96%)	6 (4%)	43 78
4	L	172/190 (90%)	167 (97%)	5 (3%)	50 83
All	All	1562/2074 (75%)	1528 (98%)	34 (2%)	60 88

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	PHE
1	A	115	ARG
1	A	179	LYS
1	A	228	LEU
1	A	262	THR
1	A	278	SER
1	B	136	SER
2	C	77	ASP
2	C	294	ARG
2	C	309	SER
3	E	44	ARG
3	E	60	TYR
3	E	77	ASN
3	E	96	CYS
3	E	187	SER
3	E	204	CYS
2	D	294	ARG
2	D	306	ASP
2	D	309	SER
2	D	330	TYR
4	F	10	SER
4	F	46	LEU
4	F	49	GLN
4	F	107	ARG
4	F	169	ASP

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Mol	Chain	Res	Type
4	F	175	SER
3	H	77	ASN
3	H	98	ARG
3	H	204	CYS
4	L	49	GLN
4	L	61	ARG
4	L	76	SER
4	L	107	ARG
4	L	169	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	86	GLN
1	B	311	GLN
2	C	153	GLN
2	D	184	ASN
4	F	6	GLN
4	F	90	GLN
4	F	155	GLN
3	H	74	ASN
3	H	77	ASN
4	L	6	GLN
4	L	49	GLN
4	L	123	GLN
4	L	160	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	347/383 (90%)	0.32	9 (2%)	59	54	36, 48, 68, 88	0
1	B	338/383 (88%)	0.35	14 (4%)	41	34	38, 53, 72, 86	0
2	C	335/364 (92%)	0.39	12 (3%)	46	38	27, 48, 79, 123	0
2	D	329/364 (90%)	0.50	22 (6%)	21	15	28, 53, 92, 140	0
3	E	215/224 (95%)	0.13	2 (0%)	85	84	27, 42, 58, 69	0
3	H	216/224 (96%)	0.21	2 (0%)	85	84	28, 40, 52, 66	0
4	F	211/213 (99%)	0.01	1 (0%)	91	90	23, 32, 50, 67	0
4	L	212/213 (99%)	0.09	1 (0%)	91	90	24, 32, 47, 82	0
All	All	2203/2368 (93%)	0.28	63 (2%)	55	49	23, 45, 74, 140	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	239	TYR	7.6
1	B	87	VAL	4.5
2	D	244	ALA	4.0
2	D	245	ASN	3.8
2	D	264	GLY	3.5
1	B	399	LYS	3.5
1	B	62	ALA	3.5
2	D	203	LEU	3.3
1	A	356	THR	3.2
2	C	101	ASP	3.2
2	C	254	TYR	3.1
2	D	346	GLY	3.1
2	C	267	ASP	3.0
2	D	232	CYS	2.9
2	D	228	ILE	2.8
2	D	170	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	175	TYR	2.8
1	A	28	ASN	2.8
1	B	88	TYR	2.7
2	D	287	TYR	2.7
2	D	184	ASN	2.7
1	B	152	PHE	2.7
1	A	361	PHE	2.6
1	B	395	GLN	2.6
2	D	383	SER	2.6
1	B	28	ASN	2.6
1	A	282	TYR	2.6
3	H	223	ASP	2.5
2	D	173	THR	2.5
2	D	282	TYR	2.5
4	F	181	THR	2.5
2	C	174	THR	2.4
2	D	238	THR	2.4
1	A	331	GLY	2.4
2	C	173	THR	2.4
2	C	203	LEU	2.3
3	H	96	CYS	2.3
1	B	320	GLU	2.3
2	C	228	ILE	2.3
1	B	356	THR	2.3
2	D	261	LEU	2.3
1	B	400	ILE	2.3
2	C	271	SER	2.3
1	A	166	ILE	2.3
2	C	232	CYS	2.2
1	B	317	PHE	2.2
2	C	276	GLY	2.2
1	B	29	ILE	2.2
3	E	78	SER	2.2
2	C	256	TRP	2.2
3	E	96	CYS	2.2
2	D	256	TRP	2.2
1	A	100	ASP	2.2
2	D	225	SER	2.2
1	A	280	LEU	2.2
4	L	212	GLU	2.2
1	B	312	ALA	2.1
2	D	324	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	321	ASN	2.1
2	D	235	GLU	2.0
2	D	165	ASP	2.0
1	B	394	ILE	2.0
2	D	175	TYR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
5	NA	B	501	1/1	0.85	0.49	13.90	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.