Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Sep 7, 2017 – 03:04 AM EDT

PDB ID	:	5WEM
EMDB ID:	:	EMD-8821
Title	:	GluA2 bound to GSG1L in digitonin, state 1
Authors	:	Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky, A.I.
Deposited on	:	unknown
Resolution	:	6.10 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

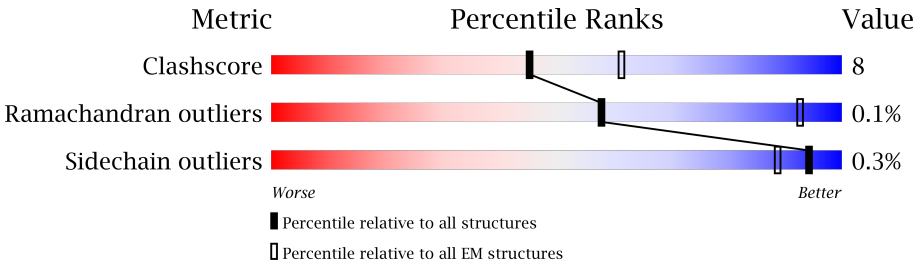
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.10 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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%

Mol	Chain	Length	Quality of chain
1	A	1057	71% 19% 9%
1	B	1057	57% 17% 26%
1	C	1057	71% 19% 9%
1	D	1057	58% 16% 26%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27360 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Chimera of Glutamate receptor 2,Germ cell-specific gene 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	962	Total	C	N	O	S	0	0
			7555	4864	1248	1401	42		
1	B	780	Total	C	N	O	S	0	0
			6125	3932	1011	1152	30		
1	C	962	Total	C	N	O	S	0	0
			7555	4864	1248	1401	42		
1	D	780	Total	C	N	O	S	0	0
			6125	3932	1011	1152	30		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	382	LEU	VAL	engineered mutation	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	engineered mutation	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
A	1151	LEU	VAL	engineered mutation	UNP D3Z7H4
B	241	GLU	ASN	engineered mutation	UNP P19491
B	382	LEU	VAL	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491

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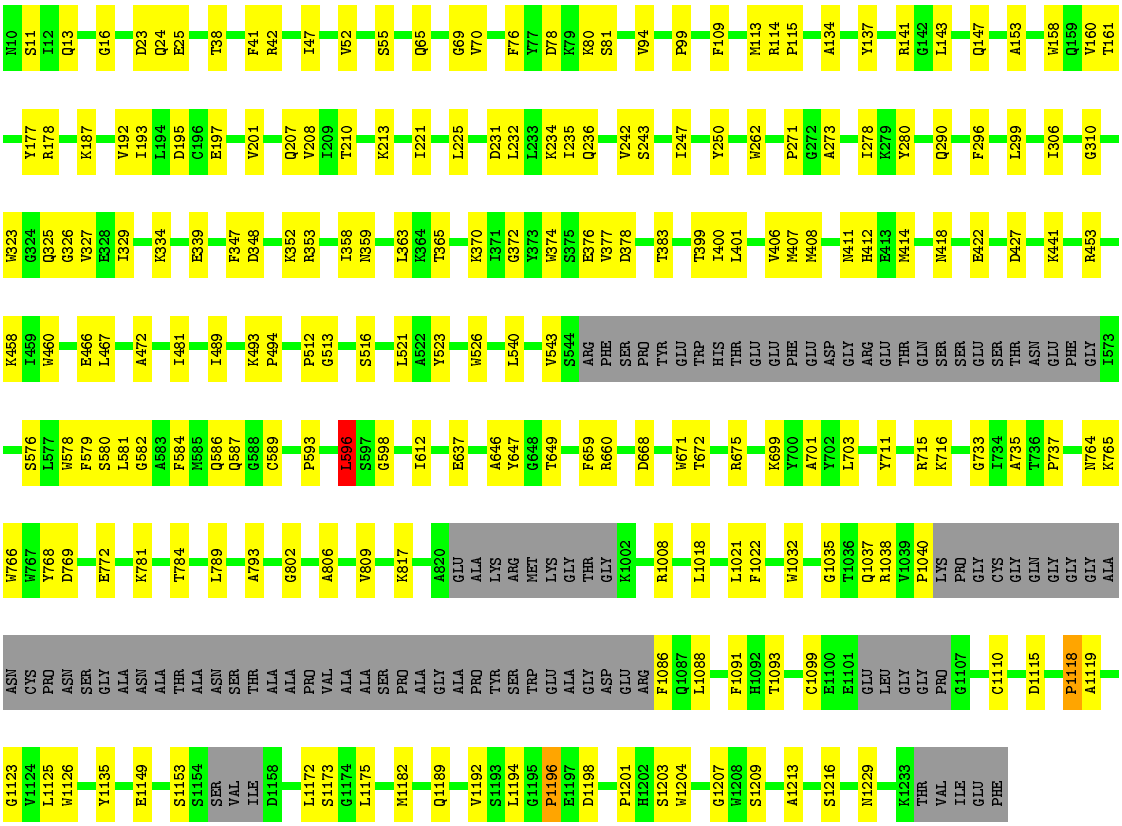
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	engineered mutation	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
B	1151	LEU	VAL	engineered mutation	UNP D3Z7H4
C	241	GLU	ASN	engineered mutation	UNP P19491
C	382	LEU	VAL	engineered mutation	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	engineered mutation	UNP P19491
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	engineered mutation	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
C	1151	LEU	VAL	engineered mutation	UNP D3Z7H4
D	241	GLU	ASN	engineered mutation	UNP P19491
D	382	LEU	VAL	engineered mutation	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	engineered mutation	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491
D	1151	LEU	VAL	engineered mutation	UNP D3Z7H4

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

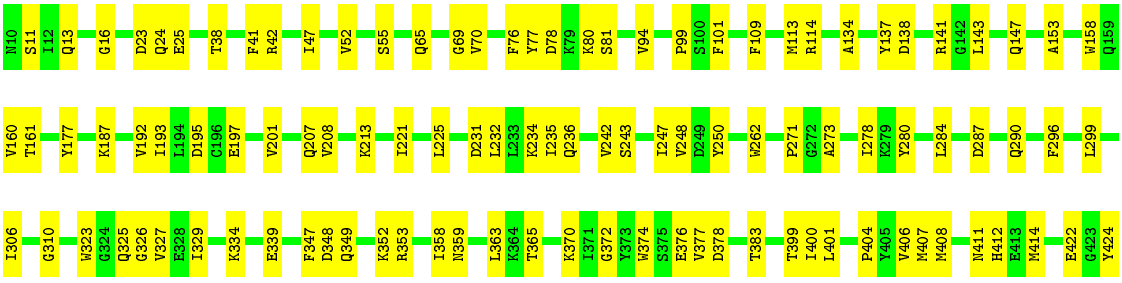
- Molecule 1: Chimera of Glutamate receptor 2,Germ cell-specific gene 1-like protein

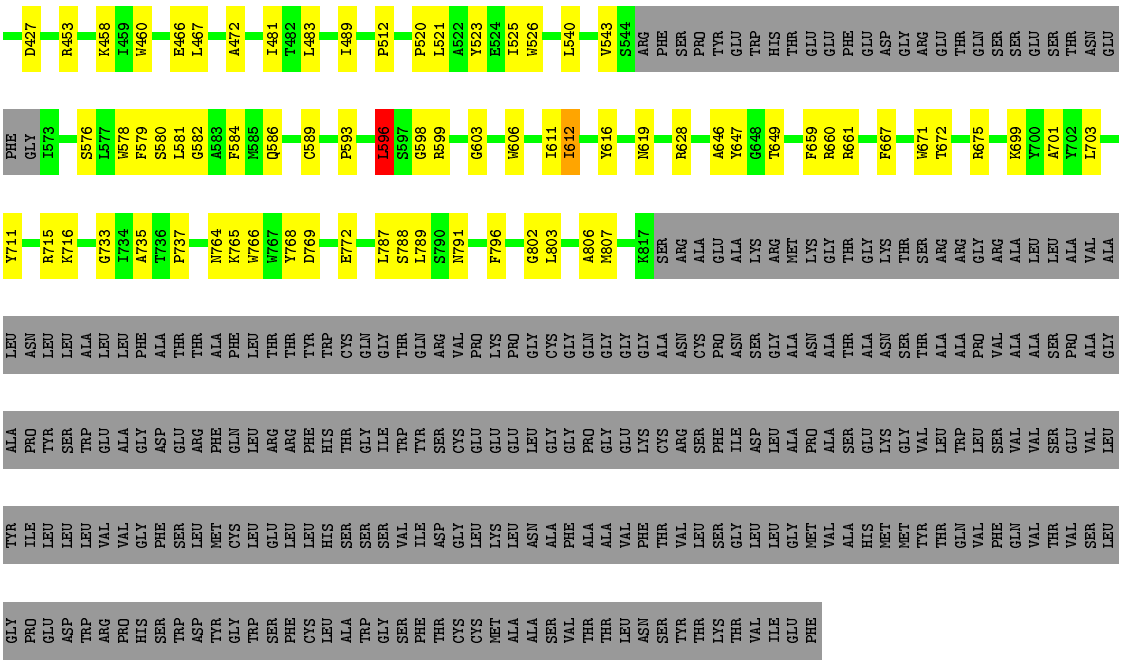
Chain A:



- Molecule 1: Chimera of Glutamate receptor 2,Germ cell-specific gene 1-like protein

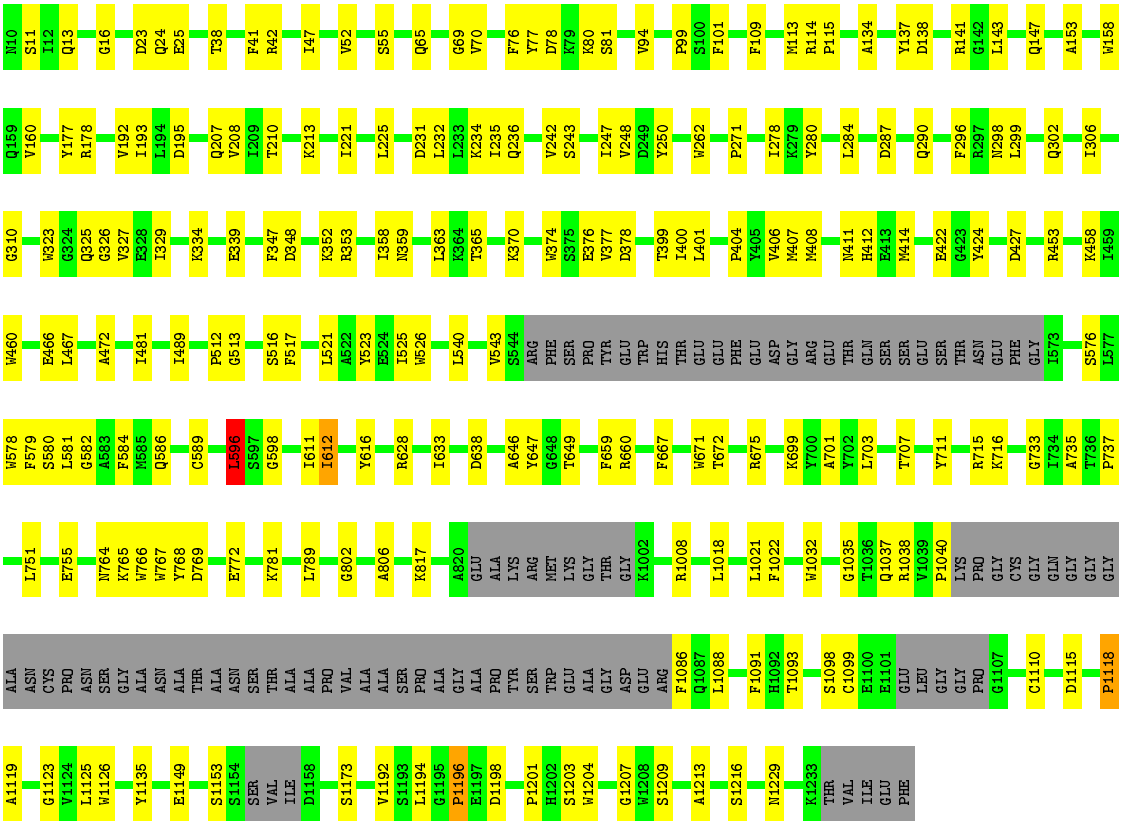
Chain B:





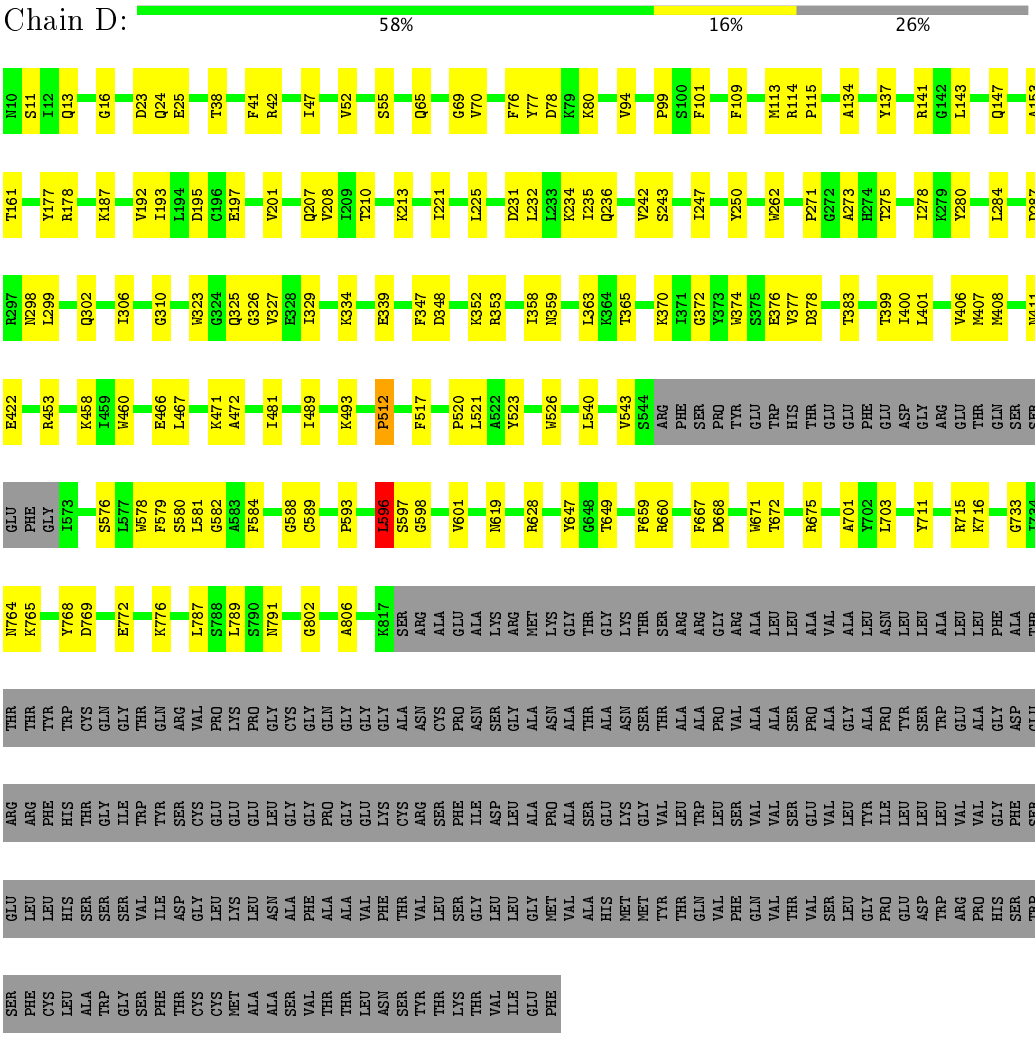
• Molecule 1: Chimera of Glutamate receptor 2,Germ cell-specific gene 1-like protein

Chain C:



• Molecule 1: Chimera of Glutamate receptor 2,Germ cell-specific gene 1-like protein

Chain D:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	20392	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	67	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.30	1/7718 (0.0%)	0.50	1/10438 (0.0%)
1	B	0.29	0/6253	0.50	1/8450 (0.0%)
1	C	0.30	1/7718 (0.0%)	0.50	1/10438 (0.0%)
1	D	0.30	0/6253	0.50	2/8450 (0.0%)
All	All	0.30	2/27942 (0.0%)	0.50	5/37776 (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
1	A	0	8
1	B	0	4
1	C	0	7
1	D	0	3
All	All	0	22

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	612	ILE	C-N	6.91	1.50	1.34
1	A	612	ILE	C-N	-6.54	1.19	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	596	LEU	CA-CB-CG	8.06	133.84	115.30
1	A	596	LEU	CA-CB-CG	8.03	133.78	115.30
1	D	596	LEU	CA-CB-CG	8.03	133.77	115.30
1	B	596	LEU	CA-CB-CG	8.02	133.74	115.30
1	D	512	PRO	C-N-CA	-5.72	110.30	122.30

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1118	PRO	Peptide
1	A	1196	PRO	Peptide
1	A	1203	SER	Peptide
1	A	1207	GLY	Peptide
1	A	378	ASP	Peptide
1	A	593	PRO	Peptide
1	A	781	LYS	Peptide
1	A	817	LYS	Mainchain
1	B	378	ASP	Peptide
1	B	512	PRO	Peptide
1	B	593	PRO	Peptide
1	B	612	ILE	Mainchain
1	C	1118	PRO	Peptide
1	C	1196	PRO	Peptide
1	C	1203	SER	Peptide
1	C	1207	GLY	Peptide
1	C	378	ASP	Peptide
1	C	781	LYS	Peptide
1	C	817	LYS	Mainchain
1	D	378	ASP	Peptide
1	D	512	PRO	Peptide
1	D	593	PRO	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	7555	0	7535	120	0
1	B	6125	0	6110	110	0
1	C	7555	0	7536	126	0
1	D	6125	0	6110	98	0
All	All	27360	0	27291	423	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 8.

All (423) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:TRP:HZ2	1:C:586:GLN:H	1.27	0.78
1:D:596:LEU:HD22	1:D:598:GLY:H	1.55	0.71
1:C:596:LEU:HD22	1:C:598:GLY:H	1.55	0.71
1:A:596:LEU:HD22	1:A:598:GLY:H	1.55	0.70
1:B:596:LEU:HD22	1:B:598:GLY:H	1.55	0.70
1:A:806:ALA:HB2	1:D:601:VAL:HG21	1.74	0.69
1:A:512:PRO:HG2	1:A:516:SER:HB3	1.77	0.66
1:C:376:GLU:HG3	1:C:377:VAL:HG13	1.80	0.64
1:A:376:GLU:HG3	1:A:377:VAL:HG13	1.80	0.64
1:A:16:GLY:H	1:A:65:GLN:HE22	1.46	0.63
1:C:143:LEU:HD21	1:D:147:GLN:HE21	1.63	0.63
1:D:376:GLU:HG3	1:D:377:VAL:HG13	1.80	0.63
1:C:147:GLN:HE21	1:D:143:LEU:HD21	1.63	0.63
1:B:525:ILE:HG12	1:C:789:LEU:HD13	1.79	0.63
1:C:16:GLY:H	1:C:65:GLN:HE22	1.46	0.63
1:D:16:GLY:H	1:D:65:GLN:HE22	1.46	0.63
1:A:99:PRO:HA	1:A:113:MET:HB2	1.81	0.62
1:B:483:LEU:HD13	1:C:751:LEU:HB2	1.81	0.62
1:C:99:PRO:HA	1:C:113:MET:HB2	1.81	0.62
1:B:16:GLY:H	1:B:65:GLN:HE22	1.46	0.62
1:B:99:PRO:HA	1:B:113:MET:HB2	1.82	0.62
1:B:376:GLU:HG3	1:B:377:VAL:HG13	1.80	0.62
1:D:177:TYR:HD2	1:D:207:GLN:HG3	1.65	0.62
1:C:177:TYR:HD2	1:C:207:GLN:HG3	1.65	0.61
1:C:512:PRO:HG2	1:C:516:SER:HB3	1.81	0.61
1:C:1118:PRO:HD3	1:C:1194:LEU:HD21	1.83	0.61
1:B:579:PHE:HD1	1:B:589:CYS:HB2	1.66	0.61
1:B:177:TYR:HD2	1:B:207:GLN:HG3	1.65	0.60
1:D:99:PRO:HA	1:D:113:MET:HB2	1.81	0.60
1:A:1118:PRO:HD3	1:A:1194:LEU:HD21	1.83	0.60
1:A:177:TYR:HD2	1:A:207:GLN:HG3	1.65	0.60
1:C:579:PHE:HD1	1:C:589:CYS:HB2	1.66	0.60
1:A:193:ILE:HG12	1:A:221:ILE:HB	1.84	0.60
1:C:525:ILE:HG12	1:D:789:LEU:HD13	1.84	0.60
1:C:193:ILE:HG12	1:C:221:ILE:HB	1.84	0.59
1:B:520:PRO:O	1:B:619:ASN:ND2	2.36	0.59
1:B:193:ILE:HG12	1:B:221:ILE:HB	1.84	0.59
1:A:579:PHE:HD1	1:A:589:CYS:HB2	1.66	0.58
1:D:193:ILE:HG12	1:D:221:ILE:HB	1.84	0.58
1:D:579:PHE:HD1	1:D:589:CYS:HB2	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:TYR:HA	1:C:195:ASP:HB3	1.86	0.58
1:D:137:TYR:HA	1:D:195:ASP:HB3	1.86	0.58
1:C:581:LEU:HA	1:C:584:PHE:HB2	1.86	0.57
1:A:94:VAL:HG22	1:A:323:TRP:HE1	1.69	0.57
1:B:137:TYR:HA	1:B:195:ASP:HB3	1.86	0.57
1:C:94:VAL:HG22	1:C:323:TRP:HE1	1.70	0.57
1:A:137:TYR:HA	1:A:195:ASP:HB3	1.86	0.57
1:B:94:VAL:HG22	1:B:323:TRP:HE1	1.69	0.57
1:D:581:LEU:HA	1:D:584:PHE:HB2	1.86	0.57
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.87	0.56
1:B:69:GLY:HA3	1:B:310:GLY:HA2	1.88	0.56
1:A:1035:GLY:HA3	1:A:1091:PHE:HB2	1.88	0.56
1:B:578:TRP:O	1:B:582:GLY:N	2.38	0.56
1:D:134:ALA:HB3	1:D:192:VAL:HG22	1.87	0.56
1:A:578:TRP:O	1:A:582:GLY:N	2.38	0.56
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.87	0.56
1:A:581:LEU:HA	1:A:584:PHE:HB2	1.86	0.56
1:D:94:VAL:HG22	1:D:323:TRP:HE1	1.70	0.56
1:C:578:TRP:O	1:C:582:GLY:N	2.38	0.56
1:A:69:GLY:HA3	1:A:310:GLY:HA2	1.88	0.56
1:B:581:LEU:HA	1:B:584:PHE:HB2	1.86	0.56
1:A:134:ALA:HB3	1:A:192:VAL:HG22	1.87	0.55
1:A:1189:GLN:NE2	1:B:788:SER:OG	2.39	0.55
1:C:1035:GLY:HA3	1:C:1091:PHE:HB2	1.88	0.55
1:D:578:TRP:O	1:D:582:GLY:N	2.38	0.55
1:B:134:ALA:HB3	1:B:192:VAL:HG22	1.87	0.55
1:C:659:PHE:HB3	1:C:671:TRP:HB2	1.89	0.55
1:D:69:GLY:HA3	1:D:310:GLY:HA2	1.88	0.55
1:B:599:ARG:O	1:C:578:TRP:NE1	2.39	0.55
1:D:659:PHE:HB3	1:D:671:TRP:HB2	1.89	0.55
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.89	0.55
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.87	0.55
1:C:134:ALA:HB3	1:C:192:VAL:HG22	1.87	0.55
1:C:1037:GLN:NE2	1:C:1198:ASP:O	2.40	0.55
1:B:612:ILE:O	1:B:616:TYR:N	2.39	0.54
1:C:69:GLY:HA3	1:C:310:GLY:HA2	1.88	0.54
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.87	0.54
1:A:236:GLN:NE2	1:A:365:THR:O	2.41	0.54
1:B:236:GLN:NE2	1:B:365:THR:O	2.41	0.54
1:C:1099:CYS:HA	1:C:1110:CYS:HA	1.89	0.54
1:B:659:PHE:HB3	1:B:671:TRP:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:787:LEU:HD11	1:D:791:ASN:HD21	1.73	0.53
1:D:161:THR:OG1	1:D:187:LYS:NZ	2.41	0.53
1:A:1037:GLN:NE2	1:A:1198:ASP:O	2.40	0.53
1:B:787:LEU:HD11	1:B:791:ASN:HD21	1.73	0.53
1:C:236:GLN:NE2	1:C:365:THR:O	2.41	0.53
1:A:1099:CYS:HA	1:A:1110:CYS:HA	1.89	0.53
1:B:628:ARG:HH22	1:C:628:ARG:HD2	1.73	0.53
1:D:236:GLN:NE2	1:D:365:THR:O	2.41	0.53
1:C:1032:TRP:N	1:C:1093:THR:O	2.38	0.52
1:B:466:GLU:O	1:B:472:ALA:N	2.41	0.52
1:A:493:LYS:HD3	1:D:493:LYS:HD3	1.90	0.52
1:C:231:ASP:HB3	1:C:234:LYS:HE3	1.92	0.52
1:D:225:LEU:HD22	1:D:247:ILE:HB	1.92	0.52
1:D:231:ASP:HB3	1:D:234:LYS:HE3	1.92	0.52
1:A:231:ASP:HB3	1:A:234:LYS:HE3	1.92	0.52
1:B:231:ASP:HB3	1:B:234:LYS:HE3	1.92	0.52
1:B:225:LEU:HD22	1:B:247:ILE:HB	1.92	0.52
1:A:1018:LEU:HD23	1:A:1021:LEU:HD12	1.92	0.51
1:C:453:ARG:HE	1:C:458:LYS:HB3	1.76	0.51
1:A:809:VAL:HB	1:D:597:SER:HB3	1.93	0.51
1:B:453:ARG:HE	1:B:458:LYS:HB3	1.75	0.51
1:A:637:GLU:OE1	1:D:776:LYS:NZ	2.38	0.51
1:A:13:GLN:HB3	1:A:70:VAL:HG12	1.93	0.51
1:B:13:GLN:HB3	1:B:70:VAL:HG12	1.93	0.51
1:A:453:ARG:HE	1:A:458:LYS:HB3	1.76	0.51
1:B:481:ILE:HD11	1:B:733:GLY:HA3	1.93	0.51
1:C:225:LEU:HD22	1:C:247:ILE:HB	1.92	0.51
1:A:481:ILE:HD11	1:A:733:GLY:HA3	1.93	0.51
1:A:784:THR:HB	1:D:628:ARG:HH11	1.75	0.51
1:B:25:GLU:HG2	1:B:76:PHE:HZ	1.76	0.51
1:C:25:GLU:HG2	1:C:76:PHE:HZ	1.76	0.51
1:C:13:GLN:HB3	1:C:70:VAL:HG12	1.93	0.51
1:A:225:LEU:HD22	1:A:247:ILE:HB	1.92	0.51
1:C:1018:LEU:HD23	1:C:1021:LEU:HD12	1.92	0.51
1:C:290:GLN:NE2	1:C:339:GLU:O	2.45	0.50
1:B:611:ILE:HG21	1:C:517:PHE:HE1	1.75	0.50
1:D:290:GLN:NE2	1:D:339:GLU:O	2.45	0.50
1:A:153:ALA:HA	1:A:158:TRP:HB2	1.93	0.50
1:A:25:GLU:HG2	1:A:76:PHE:HZ	1.76	0.50
1:B:407:MET:N	1:B:422:GLU:O	2.39	0.50
1:D:453:ARG:HE	1:D:458:LYS:HB3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLN:NE2	1:A:339:GLU:O	2.45	0.50
1:A:348:ASP:OD1	1:A:352:LYS:N	2.45	0.50
1:D:25:GLU:HG2	1:D:76:PHE:HZ	1.76	0.50
1:D:407:MET:N	1:D:422:GLU:O	2.39	0.50
1:C:466:GLU:O	1:C:472:ALA:N	2.41	0.50
1:C:481:ILE:HD11	1:C:733:GLY:HA3	1.93	0.50
1:D:466:GLU:O	1:D:472:ALA:N	2.41	0.50
1:D:13:GLN:HB3	1:D:70:VAL:HG12	1.93	0.50
1:C:153:ALA:HA	1:C:158:TRP:HB2	1.93	0.49
1:D:481:ILE:HD11	1:D:733:GLY:HA3	1.93	0.49
1:D:153:ALA:HA	1:D:158:TRP:HB2	1.93	0.49
1:A:407:MET:N	1:A:422:GLU:O	2.39	0.49
1:A:789:LEU:O	1:A:793:ALA:N	2.44	0.49
1:C:348:ASP:OD1	1:C:352:LYS:N	2.45	0.49
1:A:306:ILE:HA	1:A:325:GLN:HG2	1.95	0.49
1:B:290:GLN:NE2	1:B:339:GLU:O	2.45	0.49
1:A:1192:VAL:HA	1:A:1196:PRO:HD3	1.95	0.49
1:C:1123:GLY:HA2	1:C:1126:TRP:HD1	1.78	0.49
1:B:306:ILE:HA	1:B:325:GLN:HG2	1.95	0.49
1:B:161:THR:OG1	1:B:187:LYS:NZ	2.41	0.49
1:B:348:ASP:OD1	1:B:352:LYS:N	2.45	0.49
1:A:1123:GLY:HA2	1:A:1126:TRP:HD1	1.78	0.49
1:C:306:ILE:HA	1:C:325:GLN:HG2	1.95	0.49
1:A:466:GLU:O	1:A:472:ALA:N	2.41	0.49
1:C:1135:TYR:O	1:C:1173:SER:OG	2.31	0.49
1:C:1192:VAL:HA	1:C:1196:PRO:HD3	1.95	0.49
1:B:153:ALA:HA	1:B:158:TRP:HB2	1.94	0.48
1:A:1182:MET:HE2	1:B:796:PHE:HE2	1.78	0.48
1:D:348:ASP:OD1	1:D:352:LYS:N	2.45	0.48
1:A:1032:TRP:N	1:A:1093:THR:O	2.38	0.48
1:A:141:ARG:NH2	1:A:195:ASP:OD1	2.42	0.48
1:A:489:ILE:HD12	1:A:735:ALA:HB1	1.96	0.48
1:B:489:ILE:HD12	1:B:735:ALA:HB1	1.96	0.48
1:D:306:ILE:HA	1:D:325:GLN:HG2	1.95	0.48
1:B:250:TYR:OH	1:B:278:ILE:O	2.32	0.48
1:A:326:GLY:HA2	1:A:329:ILE:HD12	1.96	0.47
1:D:411:ASN:HB2	1:D:414:MET:HB2	1.96	0.47
1:B:326:GLY:HA2	1:B:329:ILE:HD12	1.96	0.47
1:A:1209:SER:O	1:A:1213:ALA:N	2.42	0.47
1:C:299:LEU:HD21	1:C:329:ILE:HG12	1.97	0.47
1:C:543:VAL:HG22	1:C:596:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ASN:HB2	1:B:414:MET:HB2	1.96	0.47
1:C:407:MET:N	1:C:422:GLU:O	2.39	0.47
1:B:141:ARG:NH2	1:B:195:ASP:OD1	2.42	0.47
1:C:672:THR:HG23	1:C:675:ARG:HH11	1.79	0.47
1:B:347:PHE:HE1	1:B:353:ARG:HG2	1.79	0.47
1:C:1209:SER:O	1:C:1213:ALA:N	2.43	0.47
1:C:1022:PHE:HB2	1:C:1216:SER:HB3	1.96	0.47
1:D:250:TYR:OH	1:D:278:ILE:O	2.32	0.47
1:D:347:PHE:HE1	1:D:353:ARG:HG2	1.79	0.47
1:A:250:TYR:OH	1:A:278:ILE:O	2.32	0.47
1:A:347:PHE:HE1	1:A:353:ARG:HG2	1.79	0.47
1:C:347:PHE:HE1	1:C:353:ARG:HG2	1.79	0.47
1:C:489:ILE:HD12	1:C:735:ALA:HB1	1.96	0.47
1:D:326:GLY:HA2	1:D:329:ILE:HD12	1.96	0.47
1:D:489:ILE:HD12	1:D:735:ALA:HB1	1.96	0.47
1:D:672:THR:HG23	1:D:675:ARG:HH11	1.79	0.47
1:A:765:LYS:HA	1:A:769:ASP:HB2	1.97	0.47
1:B:543:VAL:HG22	1:B:596:LEU:HD21	1.97	0.47
1:B:672:THR:HG23	1:B:675:ARG:HH11	1.80	0.47
1:C:427:ASP:OD2	1:C:766:TRP:NE1	2.44	0.47
1:C:716:LYS:HG3	1:C:772:GLU:HB3	1.97	0.47
1:A:334:LYS:HA	1:A:347:PHE:HD2	1.81	0.46
1:A:672:THR:HG23	1:A:675:ARG:HH11	1.79	0.46
1:C:765:LYS:HA	1:C:769:ASP:HB2	1.97	0.46
1:A:299:LEU:HD21	1:A:329:ILE:HG12	1.97	0.46
1:B:521:LEU:O	1:B:526:TRP:NE1	2.49	0.46
1:B:661:ARG:HH22	1:C:755:GLU:HB3	1.81	0.46
1:C:326:GLY:HA2	1:C:329:ILE:HD12	1.96	0.46
1:D:523:TYR:HA	1:D:526:TRP:HD1	1.81	0.46
1:A:716:LYS:HG3	1:A:772:GLU:HB3	1.97	0.46
1:D:299:LEU:HD21	1:D:329:ILE:HG12	1.97	0.46
1:D:765:LYS:HA	1:D:769:ASP:HB2	1.97	0.46
1:B:401:LEU:HD23	1:B:406:VAL:HG12	1.98	0.46
1:B:765:LYS:HA	1:B:769:ASP:HB2	1.97	0.46
1:C:1035:GLY:HA2	1:C:1201:PRO:HB3	1.97	0.46
1:C:141:ARG:NH2	1:C:195:ASP:OD1	2.42	0.46
1:C:250:TYR:OH	1:C:278:ILE:O	2.32	0.46
1:C:334:LYS:HA	1:C:347:PHE:HD2	1.81	0.46
1:C:411:ASN:HB2	1:C:414:MET:HB2	1.96	0.46
1:D:401:LEU:HD23	1:D:406:VAL:HG12	1.98	0.46
1:D:716:LYS:HG3	1:D:772:GLU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:LYS:HA	1:B:347:PHE:HD2	1.81	0.46
1:A:1035:GLY:HA2	1:A:1201:PRO:HB3	1.97	0.46
1:A:1149:GLU:O	1:A:1153:SER:N	2.46	0.46
1:A:1008:ARG:HH22	1:A:1229:ASN:HD22	1.64	0.46
1:A:543:VAL:HG22	1:A:596:LEU:HD21	1.97	0.46
1:C:1038:ARG:HA	1:C:1088:LEU:HA	1.98	0.46
1:C:523:TYR:HA	1:C:526:TRP:HD1	1.81	0.46
1:C:611:ILE:HG21	1:D:517:PHE:HE1	1.81	0.46
1:A:523:TYR:HA	1:A:526:TRP:HD1	1.81	0.46
1:A:1022:PHE:HB2	1:A:1216:SER:HB3	1.96	0.46
1:A:411:ASN:HB2	1:A:414:MET:HB2	1.96	0.46
1:C:521:LEU:O	1:C:526:TRP:NE1	2.49	0.46
1:D:208:VAL:HG13	1:D:213:LYS:HB2	1.98	0.46
1:A:1038:ARG:HA	1:A:1088:LEU:HA	1.98	0.45
1:A:1172:LEU:HD11	1:B:807:MET:HE2	1.99	0.45
1:D:197:GLU:O	1:D:201:VAL:N	2.41	0.45
1:A:1040:PRO:O	1:A:1086:PHE:N	2.49	0.45
1:A:401:LEU:HD23	1:A:406:VAL:HG12	1.98	0.45
1:B:467:LEU:HD22	1:B:737:PRO:HD3	1.99	0.45
1:C:208:VAL:HG13	1:C:213:LYS:HB2	1.98	0.45
1:D:235:ILE:HD13	1:D:242:VAL:HG21	1.99	0.45
1:D:647:TYR:HB3	1:D:701:ALA:HB3	1.99	0.45
1:B:77:TYR:OH	1:B:101:PHE:O	2.22	0.45
1:B:523:TYR:HA	1:B:526:TRP:HD1	1.81	0.45
1:B:716:LYS:HG3	1:B:772:GLU:HB3	1.97	0.45
1:D:467:LEU:HD22	1:D:737:PRO:HD3	1.99	0.45
1:A:38:THR:HG23	1:A:41:PHE:H	1.82	0.45
1:C:1008:ARG:HH22	1:C:1229:ASN:HD22	1.64	0.45
1:C:401:LEU:HD23	1:C:406:VAL:HG12	1.98	0.45
1:C:633:ILE:HG23	1:C:638:ASP:HB2	1.99	0.45
1:D:334:LYS:HA	1:D:347:PHE:HD2	1.80	0.45
1:B:299:LEU:HD21	1:B:329:ILE:HG12	1.97	0.45
1:D:543:VAL:HG22	1:D:596:LEU:HD21	1.97	0.45
1:B:235:ILE:HD13	1:B:242:VAL:HG21	1.99	0.45
1:C:1040:PRO:O	1:C:1086:PHE:N	2.49	0.45
1:D:232:LEU:HD23	1:D:363:LEU:HD13	1.99	0.45
1:D:521:LEU:O	1:D:526:TRP:NE1	2.49	0.45
1:A:161:THR:OG1	1:A:187:LYS:NZ	2.41	0.45
1:A:208:VAL:HG13	1:A:213:LYS:HB2	1.98	0.45
1:A:521:LEU:O	1:A:526:TRP:NE1	2.49	0.45
1:A:235:ILE:HD13	1:A:242:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LEU:HD23	1:B:363:LEU:HD13	1.99	0.45
1:B:38:THR:HG23	1:B:41:PHE:H	1.82	0.45
1:C:38:THR:HG23	1:C:41:PHE:H	1.82	0.45
1:A:647:TYR:HB3	1:A:701:ALA:HB3	1.99	0.45
1:B:52:VAL:HG13	1:B:78:ASP:HB2	1.99	0.45
1:C:221:ILE:HG12	1:C:243:SER:HB2	1.99	0.45
1:C:647:TYR:HB3	1:C:701:ALA:HB3	1.99	0.45
1:A:147:GLN:HE21	1:B:143:LEU:HD21	1.82	0.44
1:A:467:LEU:HD22	1:A:737:PRO:HD3	1.99	0.44
1:C:1115:ASP:HA	1:C:1125:LEU:HD13	1.99	0.44
1:C:52:VAL:HG13	1:C:78:ASP:HB2	1.99	0.44
1:D:221:ILE:HG12	1:D:243:SER:HB2	1.99	0.44
1:A:1035:GLY:N	1:A:1091:PHE:O	2.44	0.44
1:A:221:ILE:HG12	1:A:243:SER:HB2	1.99	0.44
1:A:1115:ASP:HA	1:A:1125:LEU:HD13	2.00	0.44
1:A:764:ASN:HA	1:A:768:TYR:HD2	1.82	0.44
1:B:208:VAL:HG13	1:B:213:LYS:HB2	1.98	0.44
1:C:467:LEU:HD22	1:C:737:PRO:HD3	1.99	0.44
1:C:232:LEU:HD23	1:C:363:LEU:HD13	1.99	0.44
1:C:764:ASN:HA	1:C:768:TYR:HD2	1.82	0.44
1:D:38:THR:HG23	1:D:41:PHE:H	1.82	0.44
1:D:764:ASN:HA	1:D:768:TYR:HD2	1.82	0.44
1:B:221:ILE:HG12	1:B:243:SER:HB2	1.99	0.44
1:C:235:ILE:HD13	1:C:242:VAL:HG21	1.99	0.44
1:A:232:LEU:HD23	1:A:363:LEU:HD13	1.99	0.44
1:C:77:TYR:OH	1:C:101:PHE:O	2.22	0.44
1:D:358:ILE:HB	1:D:374:TRP:HB3	2.00	0.44
1:B:358:ILE:HB	1:B:374:TRP:HB3	2.00	0.44
1:C:1035:GLY:N	1:C:1091:PHE:O	2.44	0.44
1:A:23:ASP:HB3	1:A:271:PRO:HG2	2.00	0.44
1:B:764:ASN:HA	1:B:768:TYR:HD2	1.82	0.44
1:B:603:GLY:HA3	1:C:581:LEU:HD21	2.00	0.44
1:D:52:VAL:HG13	1:D:78:ASP:HB2	1.99	0.44
1:A:143:LEU:HD21	1:B:147:GLN:HE21	1.82	0.43
1:A:586:GLN:HE22	1:B:586:GLN:HG3	1.83	0.43
1:B:23:ASP:HB3	1:B:271:PRO:HG2	2.00	0.43
1:B:647:TYR:HB3	1:B:701:ALA:HB3	1.99	0.43
1:C:23:ASP:HB3	1:C:271:PRO:HG2	2.00	0.43
1:D:141:ARG:NH2	1:D:195:ASP:OD1	2.42	0.43
1:D:298:ASN:O	1:D:302:GLN:N	2.43	0.43
1:B:716:LYS:N	1:B:772:GLU:OE1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ASP:HB3	1:D:271:PRO:HG2	2.00	0.43
1:A:109:PHE:HZ	1:A:327:VAL:HG22	1.84	0.43
1:A:668:ASP:O	1:A:672:THR:N	2.46	0.43
1:B:158:TRP:HB3	1:B:160:VAL:HG23	2.00	0.43
1:C:1149:GLU:O	1:C:1153:SER:N	2.46	0.43
1:A:1135:TYR:O	1:A:1173:SER:OG	2.31	0.43
1:A:802:GLY:O	1:A:806:ALA:N	2.50	0.43
1:B:628:ARG:HH22	1:C:628:ARG:HB3	1.84	0.43
1:D:296:PHE:HA	1:D:299:LEU:HB2	2.01	0.43
1:A:158:TRP:HB3	1:A:160:VAL:HG23	2.00	0.43
1:A:52:VAL:HG13	1:A:78:ASP:HB2	1.99	0.43
1:B:197:GLU:O	1:B:201:VAL:N	2.41	0.43
1:D:109:PHE:HZ	1:D:327:VAL:HG22	1.84	0.43
1:D:158:TRP:HB3	1:D:160:VAL:HG23	2.00	0.43
1:A:358:ILE:HB	1:A:374:TRP:HB3	2.00	0.43
1:C:716:LYS:N	1:C:772:GLU:OE1	2.50	0.43
1:D:802:GLY:O	1:D:806:ALA:N	2.50	0.43
1:A:513:GLY:O	1:A:516:SER:OG	2.35	0.43
1:A:55:SER:OG	1:A:80:LYS:O	2.37	0.43
1:A:646:ALA:N	1:A:699:LYS:O	2.50	0.43
1:B:296:PHE:HA	1:B:299:LEU:HB2	2.01	0.43
1:C:296:PHE:HA	1:C:299:LEU:HB2	2.01	0.43
1:D:262:TRP:HE1	1:D:275:THR:HG1	1.67	0.43
1:D:716:LYS:N	1:D:772:GLU:OE1	2.50	0.43
1:C:109:PHE:HZ	1:C:327:VAL:HG22	1.84	0.43
1:C:399:THR:OG1	1:C:400:ILE:N	2.52	0.43
1:C:802:GLY:O	1:C:806:ALA:N	2.50	0.43
1:D:236:GLN:HA	1:D:363:LEU:HD21	2.01	0.43
1:D:55:SER:OG	1:D:80:LYS:O	2.37	0.43
1:C:358:ILE:HB	1:C:374:TRP:HB3	2.00	0.42
1:C:55:SER:OG	1:C:80:LYS:O	2.37	0.42
1:A:236:GLN:HA	1:A:363:LEU:HD21	2.01	0.42
1:A:408:MET:HE3	1:A:412:HIS:HB2	2.01	0.42
1:B:408:MET:HE3	1:B:412:HIS:HB2	2.01	0.42
1:C:612:ILE:O	1:C:616:TYR:N	2.45	0.42
1:A:427:ASP:OD2	1:A:766:TRP:NE1	2.44	0.42
1:D:453:ARG:HB2	1:D:460:TRP:CE2	2.54	0.42
1:A:296:PHE:HA	1:A:299:LEU:HB2	2.01	0.42
1:A:453:ARG:HB2	1:A:460:TRP:CE2	2.54	0.42
1:C:158:TRP:HB3	1:C:160:VAL:HG23	2.00	0.42
1:A:24:GLN:HE21	1:A:262:TRP:HZ2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:THR:OG1	1:A:400:ILE:N	2.52	0.42
1:B:24:GLN:HE21	1:B:262:TRP:HZ2	1.68	0.42
1:C:114:ARG:HD3	1:C:280:TYR:HE2	1.84	0.42
1:D:668:ASP:O	1:D:672:THR:N	2.46	0.42
1:B:236:GLN:HA	1:B:363:LEU:HD21	2.01	0.42
1:C:711:TYR:CZ	1:C:715:ARG:HD3	2.55	0.42
1:B:109:PHE:HZ	1:B:327:VAL:HG22	1.84	0.42
1:B:453:ARG:HB2	1:B:460:TRP:CE2	2.54	0.42
1:D:77:TYR:OH	1:D:101:PHE:O	2.22	0.42
1:A:587:GLN:OE1	1:D:588:GLY:HA2	2.20	0.42
1:B:114:ARG:HD3	1:B:280:TYR:HE2	1.84	0.42
1:B:55:SER:OG	1:B:80:LYS:O	2.37	0.42
1:C:453:ARG:HB2	1:C:460:TRP:CE2	2.54	0.42
1:D:24:GLN:HE21	1:D:262:TRP:HZ2	1.68	0.42
1:D:359:ASN:HB3	1:D:370:LYS:HE2	2.02	0.42
1:A:540:LEU:HD11	1:A:580:SER:HB3	2.02	0.42
1:B:427:ASP:OD2	1:B:766:TRP:NE1	2.44	0.42
1:C:178:ARG:HH21	1:C:210:THR:HG21	1.85	0.42
1:C:236:GLN:HA	1:C:363:LEU:HD21	2.01	0.42
1:A:114:ARG:HD3	1:A:280:TYR:HE2	1.84	0.41
1:B:11:SER:HA	1:B:42:ARG:HB2	2.02	0.41
1:C:513:GLY:O	1:C:516:SER:OG	2.36	0.41
1:C:540:LEU:HD11	1:C:580:SER:HB3	2.02	0.41
1:A:711:TYR:CZ	1:A:715:ARG:HD3	2.55	0.41
1:B:399:THR:OG1	1:B:400:ILE:N	2.52	0.41
1:B:78:ASP:N	1:B:81:SER:OG	2.54	0.41
1:C:359:ASN:HB3	1:C:370:LYS:HE2	2.02	0.41
1:B:628:ARG:HH12	1:C:628:ARG:HD2	1.84	0.41
1:D:114:ARG:HD3	1:D:280:TYR:HE2	1.84	0.41
1:D:16:GLY:HA3	1:D:47:ILE:HA	2.03	0.41
1:A:178:ARG:HH21	1:A:210:THR:HG21	1.85	0.41
1:B:628:ARG:HH12	1:C:628:ARG:HH11	1.69	0.41
1:D:115:PRO:HG3	1:D:353:ARG:HD3	2.03	0.41
1:A:115:PRO:HG3	1:A:353:ARG:HD3	2.03	0.41
1:B:284:LEU:HA	1:B:287:ASP:HB2	2.03	0.41
1:B:659:PHE:HD1	1:B:667:PHE:HB3	1.86	0.41
1:A:1172:LEU:HD21	1:B:807:MET:HG3	2.02	0.41
1:C:11:SER:HA	1:C:42:ARG:HB2	2.02	0.41
1:D:178:ARG:HH21	1:D:210:THR:HG21	1.85	0.41
1:B:16:GLY:HA3	1:B:47:ILE:HA	2.03	0.41
1:C:646:ALA:N	1:C:699:LYS:O	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1213:ALA:O	1:A:1216:SER:OG	2.33	0.41
1:A:493:LYS:HA	1:A:494:PRO:HD3	1.95	0.41
1:B:404:PRO:O	1:B:424:TYR:N	2.46	0.41
1:D:284:LEU:HA	1:D:287:ASP:HB2	2.03	0.41
1:D:408:MET:HE3	1:D:412:HIS:HB2	2.01	0.41
1:D:711:TYR:CZ	1:D:715:ARG:HD3	2.55	0.41
1:A:11:SER:HA	1:A:42:ARG:HB2	2.02	0.41
1:B:711:TYR:CZ	1:B:715:ARG:HD3	2.55	0.41
1:B:802:GLY:O	1:B:806:ALA:N	2.50	0.41
1:D:399:THR:OG1	1:D:400:ILE:N	2.52	0.41
1:D:659:PHE:HD1	1:D:667:PHE:HB3	1.86	0.41
1:B:372:GLY:HA2	1:B:383:THR:H	1.86	0.41
1:C:284:LEU:HA	1:C:287:ASP:HB2	2.03	0.41
1:D:372:GLY:HA2	1:D:383:THR:H	1.86	0.41
1:A:576:SER:HA	1:A:579:PHE:HD2	1.86	0.41
1:B:334:LYS:NZ	1:B:349:GLN:O	2.47	0.41
1:C:358:ILE:O	1:C:374:TRP:N	2.44	0.41
1:C:659:PHE:HD1	1:C:667:PHE:HB3	1.86	0.41
1:C:78:ASP:N	1:C:81:SER:OG	2.54	0.41
1:A:1175:LEU:HD22	1:B:803:LEU:HD13	2.03	0.41
1:C:16:GLY:HA3	1:C:47:ILE:HA	2.02	0.41
1:C:576:SER:HA	1:C:579:PHE:HD2	1.86	0.41
1:B:586:GLN:HE22	1:C:586:GLN:HE21	1.69	0.41
1:D:11:SER:HA	1:D:42:ARG:HB2	2.02	0.41
1:D:540:LEU:HD11	1:D:580:SER:HB3	2.02	0.41
1:D:576:SER:HA	1:D:579:PHE:HD2	1.86	0.41
1:A:262:TRP:CZ2	1:A:273:ALA:HA	2.56	0.41
1:B:359:ASN:HB3	1:B:370:LYS:HE2	2.02	0.41
1:B:576:SER:HA	1:B:579:PHE:HD2	1.86	0.41
1:C:298:ASN:O	1:C:302:GLN:N	2.43	0.41
1:C:404:PRO:O	1:C:424:TYR:N	2.46	0.41
1:A:372:GLY:HA2	1:A:383:THR:H	1.86	0.40
1:A:78:ASP:N	1:A:81:SER:OG	2.54	0.40
1:C:24:GLN:HE21	1:C:262:TRP:HZ2	1.68	0.40
1:A:1189:GLN:HE22	1:B:789:LEU:H	1.69	0.40
1:A:16:GLY:HA3	1:A:47:ILE:HA	2.02	0.40
1:A:359:ASN:HB3	1:A:370:LYS:HE2	2.02	0.40
1:B:138:ASP:N	1:B:195:ASP:O	2.49	0.40
1:B:540:LEU:HD11	1:B:580:SER:HB3	2.02	0.40
1:C:115:PRO:HG3	1:C:353:ARG:HD3	2.03	0.40
1:D:262:TRP:CZ2	1:D:273:ALA:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ASN:HD21	1:A:441:LYS:HA	1.87	0.40
1:C:408:MET:HE3	1:C:412:HIS:HB2	2.02	0.40
1:D:358:ILE:O	1:D:374:TRP:N	2.44	0.40
1:D:520:PRO:O	1:D:619:ASN:ND2	2.54	0.40
1:B:262:TRP:CZ2	1:B:273:ALA:HA	2.56	0.40
1:B:646:ALA:N	1:B:699:LYS:O	2.50	0.40
1:C:138:ASP:N	1:C:195:ASP:O	2.49	0.40
1:C:707:THR:O	1:C:767:TRP:NE1	2.50	0.40
1:C:711:TYR:O	1:C:715:ARG:HG2	2.22	0.40
1:A:197:GLU:O	1:A:201:VAL:N	2.41	0.40
1:B:247:ILE:HG23	1:B:248:VAL:HG23	2.04	0.40
1:C:1093:THR:HA	1:C:1098:SER:HA	2.04	0.40
1:C:247:ILE:HG23	1:C:248:VAL:HG23	2.04	0.40
1:D:466:GLU:HA	1:D:471:LYS:HB2	2.04	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 PDB entries followed by that with respect to all EM entries.

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	950/1057 (90%)	888 (94%)	60 (6%)	2 (0%)	51 84
1	B	776/1057 (73%)	728 (94%)	48 (6%)	0	100 100
1	C	950/1057 (90%)	886 (93%)	62 (6%)	2 (0%)	51 84
1	D	776/1057 (73%)	729 (94%)	47 (6%)	0	100 100
All	All	3452/4228 (82%)	3231 (94%)	217 (6%)	4 (0%)	58 89

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1204	TRP

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Mol	Chain	Res	Type
1	C	1204	TRP
1	A	1119	ALA
1	C	1119	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	816/888 (92%)	814 (100%)	2 (0%)	94	97
1	B	662/888 (74%)	660 (100%)	2 (0%)	94	96
1	C	816/888 (92%)	814 (100%)	2 (0%)	94	97
1	D	662/888 (74%)	660 (100%)	2 (0%)	94	96
All	All	2956/3552 (83%)	2948 (100%)	8 (0%)	94	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	596	LEU
1	A	660	ARG
1	B	596	LEU
1	B	660	ARG
1	C	596	LEU
1	C	660	ARG
1	D	596	LEU
1	D	660	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	83	ASN
1	A	586	GLN
1	A	1189	GLN
1	B	65	GLN

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Mol	Chain	Res	Type
1	B	619	ASN
1	C	24	GLN
1	C	65	GLN
1	C	147	GLN
1	C	412	HIS
1	C	586	GLN
1	C	642	GLN
1	D	65	GLN
1	D	83	ASN
1	D	147	GLN
1	D	392	GLN
1	D	586	GLN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	612:ILE	C	613:ILE	N	1.19