WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 04:51 AM BST

PDB ID	:	2RNR
Title	:	Solution structure of the complex between TFIIE alpha C-terminal acidic domain and TFIIH p62 PH domain
Authors	:	Okuda, M.; Nishimura, Y.
Deposited on	:	2008-01-31

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

|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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.
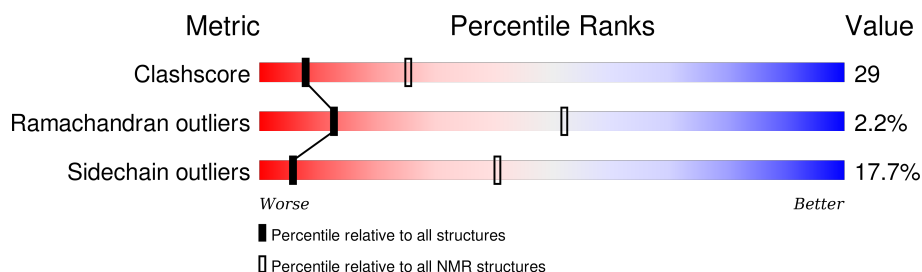
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	64	
2	B	110	

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy.*

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:382-A:436, B:7-B:104 (153)	0.61	18

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 3, 5, 6, 8, 10, 18
2	2, 4, 11, 12, 17, 19
3	7, 9, 13, 15, 20
4	14, 16

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2717 atoms, of which 1348 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	62	956	313	450	75	114	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	376	GLY	-	EXPRESSION TAG	UNP P29083
A	377	SER	-	EXPRESSION TAG	UNP P29083

- Molecule 2 is a protein called TFIIH basal transcription factor complex p62 subunit.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	108	1761	547	898	154	158	4	0

There are 2 discrepancies between the modelled and reference sequences:

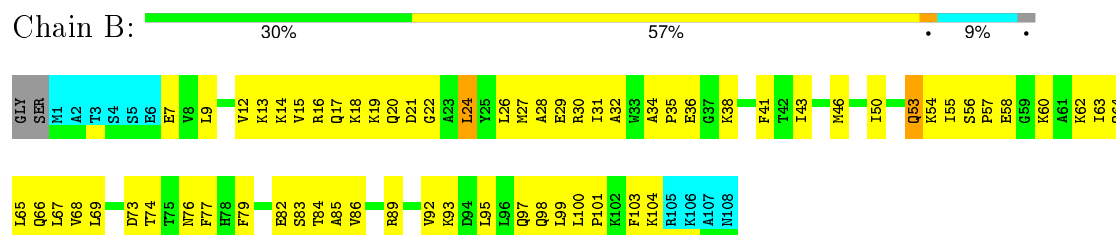| Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	EXPRESSION TAG	UNP P32780
B	0	SER	-	EXPRESSION TAG	UNP P32780

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A:

52%   31%   •   11%   •

GLY SER E378 E379 D380 E381 E382 E383 D384 D385 E386 F387 E388 E389 V390 A391 D392 D393 V396 S404 V408 E413 L414 V415 M418 K423 E424 M429 R432 D436 L437 F438 E439

- Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B:

30%   57%   •   9%   •

GLY SER M1 A2 T3 S4 S5 E6 E7 V8 L9 V12 K13 K14 V15 R16 Q17 K18 K19 Q20 D21 G22 A23 L24 Y25 L26 M27 A28 E29 R30 I31 A32 W33 A34 P35 E36 G37 K38 F41 T42 I43 M46 I50 Q53 K54 I55 S56 P57 E58 G59 K60 A61 K62 I63 Q64

L65 Q66 L67 V68 L69 D73 T74 T75 N76 F77 H78 F79 E82 S83 T84 A85 V86 R89 V92 K93 D94 L95 I96 Q97 Q98 L99 L100 P101 K102 F103 K104 R105 K106 A107 N108
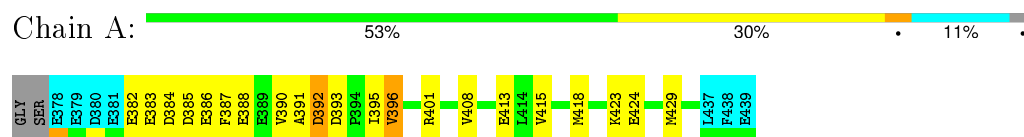
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A:

53%   30%   •   11%   •

GLY SER E378 E379 D380 E381 E382 E383 D384 D385 E386 F387 E388 E389 V390 A391 D392 D393 P394 I395 V396 R401 V408 E413 L414 V415 M418 K423 E424 M429 L437 F438 E439

- Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B:

27%   53%   9%   9%   •
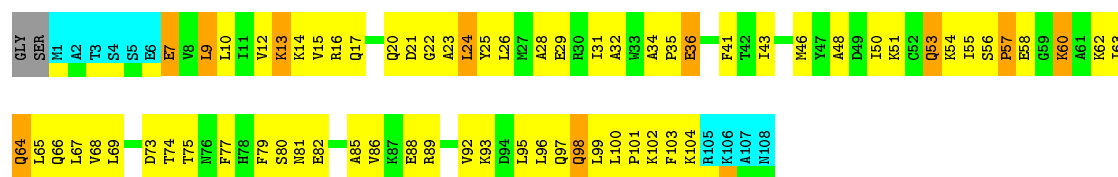
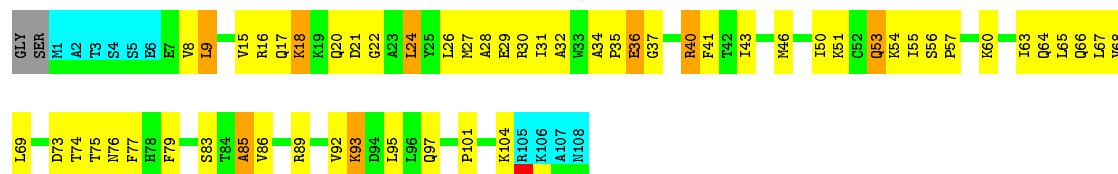### 4.2.2 Score per residue for model 2

• Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A: 52% 31% • 11% •

• Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B: 38% 44% 7% 9% •

4.2.3 Score per residue for model 3

• Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A: 50% 33% • 11% •

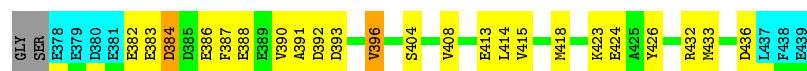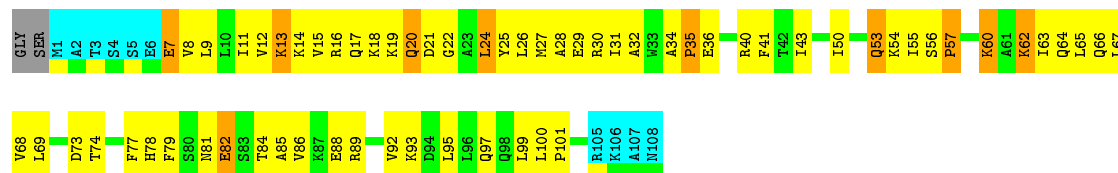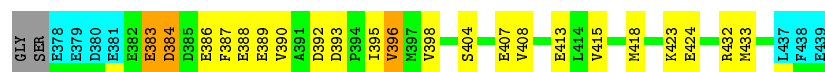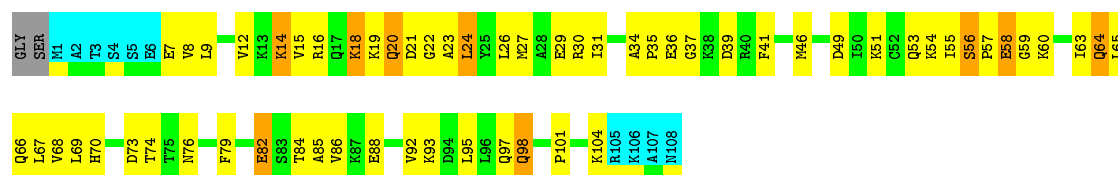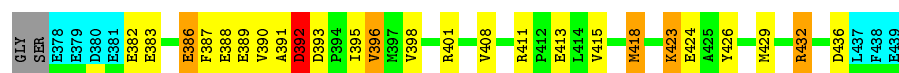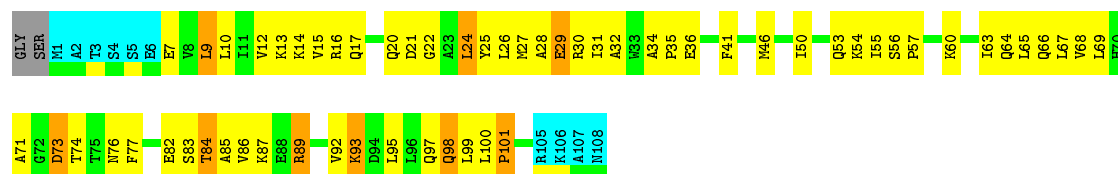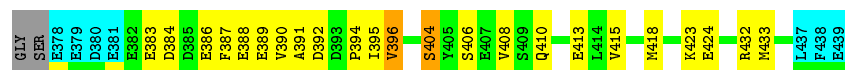• Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B: 31% 49% 9% 9% •

4.2.4 Score per residue for model 4

• Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A: 52% 30% 5% 11% •

GLY SER E378 E379 D380 E381 E382 E383 D384 D385 E386 F387 E388 E389 V390 A391 D392 D393 P394 I395 V396 M397 V398 S404 E407 V408 E413 L414 V415 M418 K423 E424 R432 M433 L437 F438 E439

• Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B: 35% 46% 8% 9% •

GLY SER M1 A2 T3 S4 S5 E6 E7 V8 L9 V12 K13 K14 V15 R16 Q17 K18 K19 Q20 D21 G22 A23 Y25 L26 M27 A28 E29 R30 I31 A34 P35 E36 G37 K38 D39 R40 F41 M46 D49 I50 K51 C52 Q53 K54 I55 S56 P57 E58 G59 K60 I63 Q64 L65

Q66 L67 V68 L69 H70 D73 T74 T75 N76 F79 E82 S83 T84 A85 V86 K87 E88 V92 K93 D94 L95 L96 Q97 Q98 P101 K104 R105 K106 A107 N108

4.2.5 Score per residue for model 5

• Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A: 47% 30% 8% • 11% •

GLY SER E378 E379 D380 E381 E382 E383 E386 F387 E388 E389 V390 A391 D392 D393 P394 I395 V396 M397 V398 R401 V408 R411 P412 E413 L414 V415 M418 K423 E424 A425 Y426 M429 R432 D436 L437 F438 E439

• Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B: 35% 46% 8% 9% •

GLY SER M1 A2 T3 S4 S5 E6 E7 V8 L9 L10 I11 V12 K13 K14 V15 R16 Q17 Q20 D21 G22 A23 L24 Y25 L26 M27 A28 E29 R30 I31 A32 W33 A34 P35 E36 F41 M46 I50 Q53 K54 I55 S56 P57 K60 I63 Q64 L65 Q66 L67 V68 L69 H70

A71 G72 D73 T74 T75 N76 F77 E82 S83 T84 A85 V86 K87 E88 R89 V92 K93 D94 L95 L96 Q97 Q98 L99 L100 P101 R105 K106 A107 N108

4.2.6 Score per residue for model 6

• Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A: 50% 33% • 11% •

GLY SER E378 E379 D380 E381 E382 E383 D384 D385 E386 F387 E388 E389 V390 A391 D392 D393 P394 I395 V396 S404 Y405 S406 E407 V408 S409 Q410 E413 L414 V415 M418 K423 E424 R432 M433 L437 F438 E439

• Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B: 32% 48% 9% 9% •

GLY SER M1 A2 T3 S4 S5 E6 E7 V8 L9 L10 I11 V12 K13 K14 V15 R16 K19 Q20 D21 G22 A23 L24 Y25 L26 M27 A28 E29 R30 I31 A34 P35 E36 G37 K38 F41 M46 Y47 A48 D49 I50 Q53 K54 I55 S56 P57 E58 G59 K60 I63 Q64 L65 Q66

L67 V68 L69 D73 T74 T75 N76 F79 S80 N81 E82 A85 V86 K87 E88 R89 V92 K93 D94 L95 L96 Q97 Q98 L99 L100 P101 K102 F103 K104 R105 K106 A107 N108

4.2.7 Score per residue for model 7

• Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A: 52%   28%   6%   11%   •

GLY SER E378 E379 D380 E381 E382 E383 D384 D385 E386 F387 E388 E389 V390 A391 D392 D393 P394 I395 V396 S404 E413 L414 V415 M418 K423 E424 M429 R432 M433 D436 L437 F438 E439

• Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B: 34%   46%   8%   •   9%   •

GLY SER M1 A2 T3 S4 S5 E6 E7 V8 L9 L10 V15 R16 Q17 K18 K19 Q20 D21 G22 A23 L24 Y25 L26 E29 R30 I31 A32 W33 A34 P35 E36 G37 K38 F41 T42 I43 M46 I50 Q53 K54 I55 S56 P57 E58 G59 K60 A61 K62 I63 Q64 L65 Q66 L67

V68 L69 H70 A71 G72 D73 T74 T75 N76 F77 H78 T84 A85 V86 K87 E88 R89 V92 K93 D94 L95 L96 Q97 Q98 L99 L100 P101 F103 K102 K104 R105 K106 A107 N108

4.2.8 Score per residue for model 8

• Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A: 50%   30%   6%   11%   •

GLY SER E378 E379 D380 E381 E382 E383 D384 D385 E386 F387 E388 E389 V390 A391 D392 D393 P394 I395 V396 S404 E407 V408 S409 Q410 R411 M418 K423 E424 R432 M433 F434 L437 F438 E439

• Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B: 35%   43%   12%   9%   •

GLY SER M1 A2 T3 S4 S5 E6 E7 V8 L9 L10 I11 V12 K13 K14 V15 R16 Q17 K18 K19 Q20 D21 G22 A23 L24 Y25 L26 M27 A28 E29 R30 I31 A32 P35 E36 I43 M46 Y47 I50 Q53 K54 I55 S56 P57 K60 A61 K62 I63 Q64 L65 Q66 L67 V68

L69 D73 T74 T75 N76 F77 H78 F79 S80 N81 E82 S83 T84 A85 V86 R89 V92 K93 D94 L95 L96 Q97 Q98 L99 F103 K104 R105 K106 A107 N108
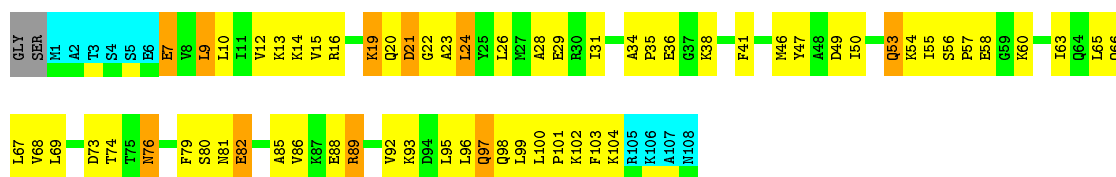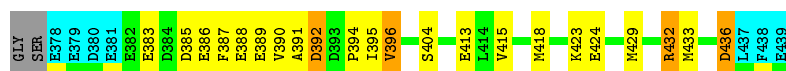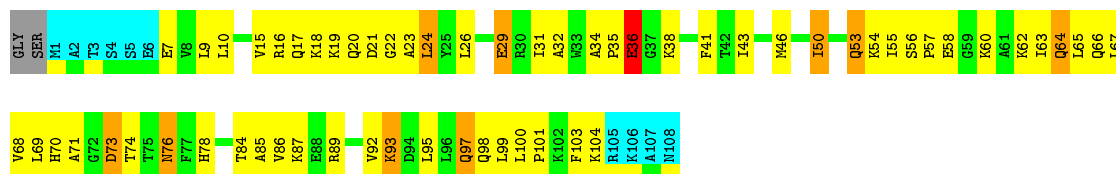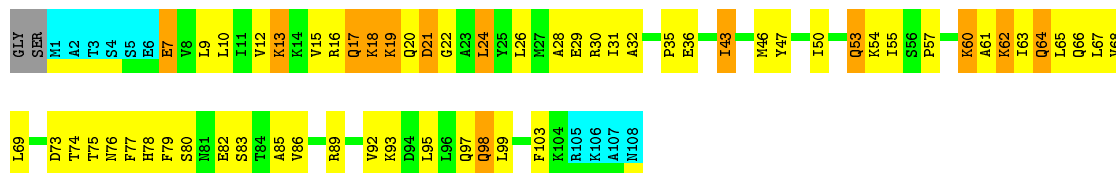
4.2.9 Score per residue for model 9

• Molecule 1: Transcription initiation factor IIE subunit alpha
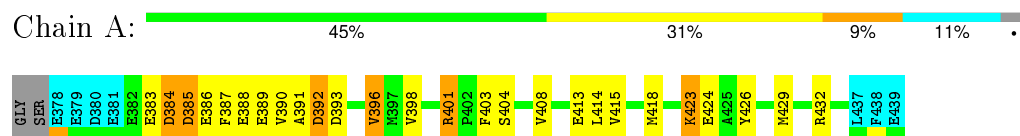
Chain A:

45% 31% 9% 11%

• Molecule 2: TFIIH basal transcription factor complex p62 subunit
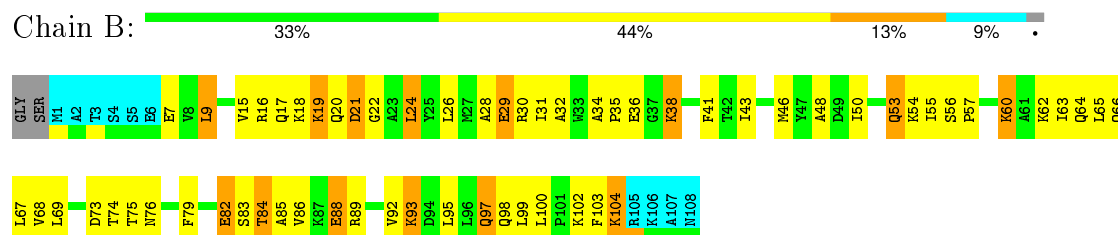
Chain B:

33% 44% 13% 9%

4.2.10 Score per residue for model 10

• Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A:

52% 28% 6% 11%

• Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B:

23% 57% 9% 9%

4.2.11 Score per residue for model 11

• Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A:

53% 25% 8% 11%

• Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B:

36% 44% 9% 9%

4.2.12 Score per residue for model 12

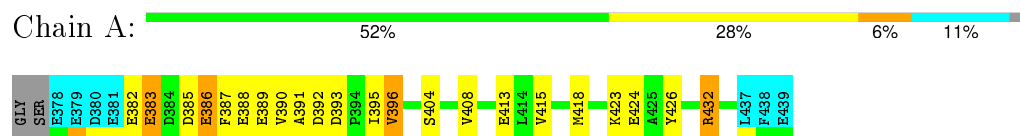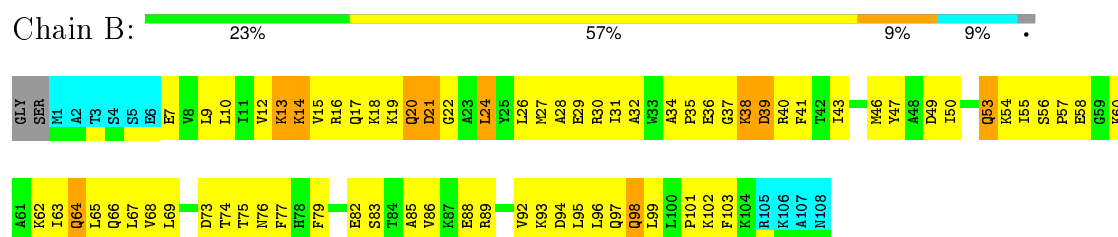• Molecule 1: Transcription initiation factor IIE subunit alpha

• Molecule 2: TFIIH basal transcription factor complex p62 subunit

4.2.13 Score per residue for model 13

• Molecule 1: Transcription initiation factor IIE subunit alpha

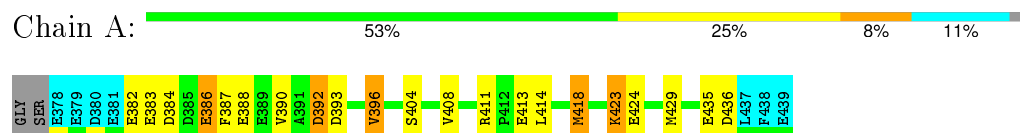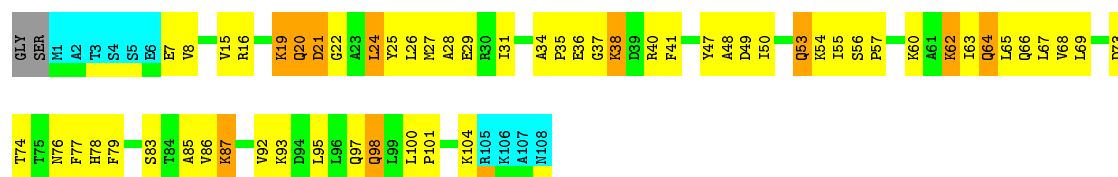• Molecule 2: TFIIH basal transcription factor complex p62 subunit
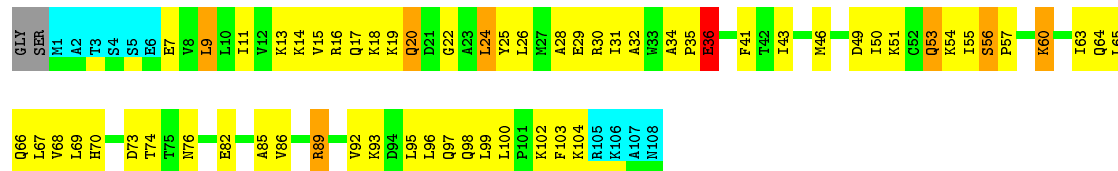
4.2.14 Score per residue for model 14

• Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A:

- Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B:

4.2.15 Score per residue for model 15

- Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A:

- Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B:
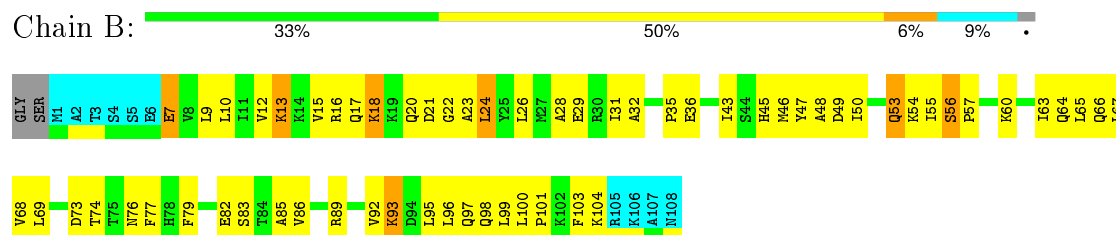
4.2.16 Score per residue for model 16

- Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A:

- Molecule 2: TFIIH basal transcription factor complex p62 subunit
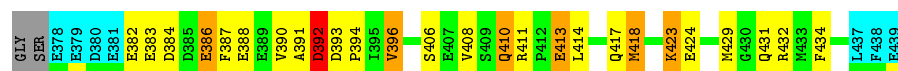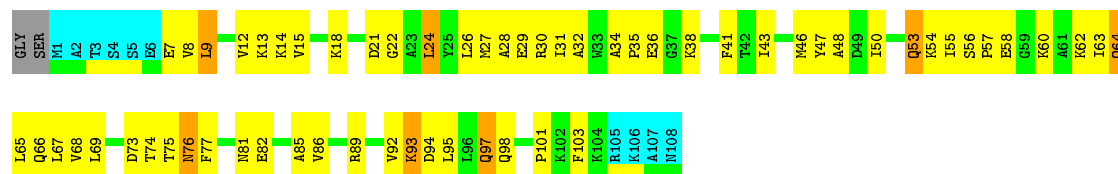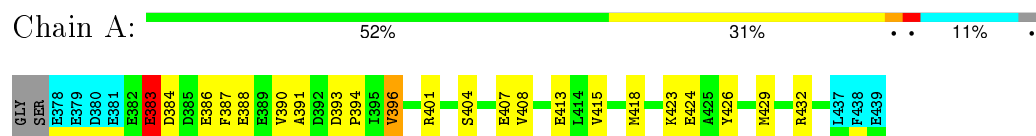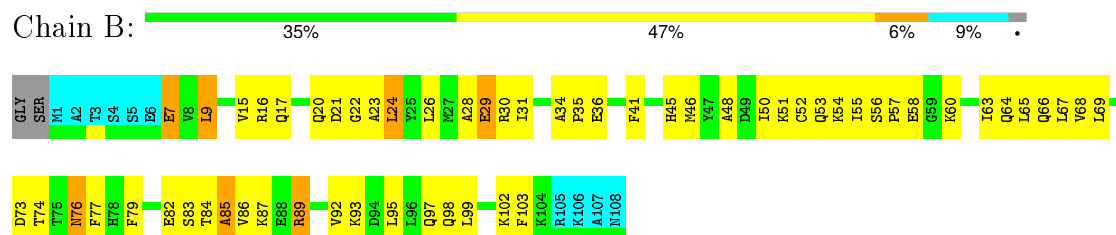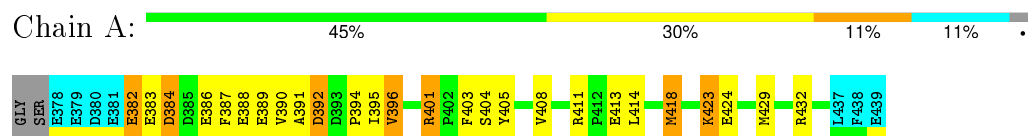
Chain B:

GLY SER M1 A2 T3 S4 S5 E6 E7 V8 L9 V15 R16 Q17 Q20 D21 G22 A23 L24 Y25 L26 M27 A28 E29 R30 I31 A34 P35 E36 D39 R40 F41 M46 Y47 A48 D49 I50 Q53 K54 I55 S56 P57 K60 I63 Q64 L65 Q66 L67 V68 L69 D73

T74 T75 N76 F79 E82 S83 T84 A85 V86 K87 E88 V92 K93 D94 L95 L96 Q97 Q98 L99 L100 P101 K102 F103 K104 R105 K106 A107 N108
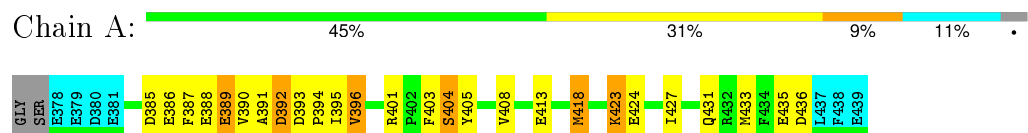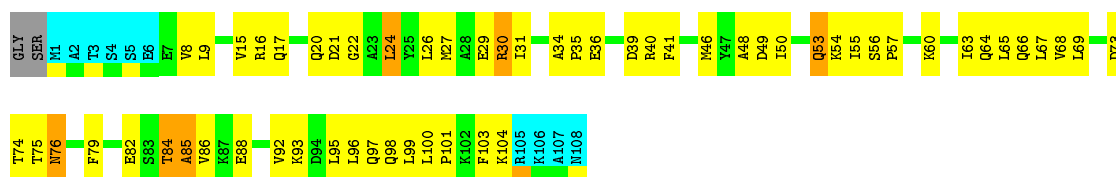
4.2.17 Score per residue for model 17

• Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A: 47%　　30%　　8% • 11% •

GLY SER E378 E379 D380 E381 E382 E383 D384 D385 E386 F387 E388 E389 V390 A391 D392 D393 P394 I395 V396 S404 Y405 V408 R411 P412 E413 M418 K423 E424 M429 G430 Q431 R432 M433 F434 E435 D436 L437 F438 E439

• Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B: 32%　　50%　　6% • 9% •

GLY SER M1 A2 T3 S4 S5 E6 E7 V8 L9 V12 K13 K14 V15 R16 Q17 K18 K19 Q20 D21 G22 A23 L24 Y25 L26 M27 A28 E29 R30 I31 A34 P35 E36 R40 F41 M46 Y47 A48 D49 I50 Q53 K54 I55 S56 P57 E58 G59 K60 A61 K62 I63 Q64 L65 Q66

L67 V68 L69 D73 T74 T75 N76 F77 H78 N81 E82 S83 T84 V86 R89 V92 K93 D94 L95 L96 Q97 Q98 P101 K102 F103 K104 R105 K106 A107 N108
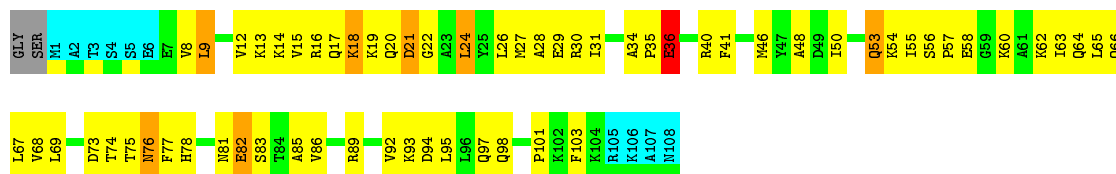
4.2.18 Score per residue for model 18 (medoid)

• Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A: 61%　　17%　　5% • 11% •

GLY SER E378 E379 D380 E381 E382 E383 D384 D385 E386 F387 E388 E389 V390 A391 D392 V396 S404 V408 E413 M418 K423 E424 D436 L437 F438 E439

• Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B: 35%　　41%　　12% • 9% •

GLY SER M1 A2 T3 S4 S5 E6 E7 V8 L9 V15 R16 Q17 K18 K19 Q20 D21 G22 A23 L24 Y25 L26 M27 A28 E29 R30 I31 A32 P35 E36 D39 R40 I43 M46 Y47 A48 D49 I50 Q53 K54 I55 S56 P57 E58 G59 K60 A61 K62 I63 Q64 L65 Q66 L67

V68 L69 D73 T74 T75 N76 F77 H78 F79 E82 S83 T84 A85 V86 K87 E88 V92 K93 D94 L95 L96 Q97 Q98 L99 L100 P101 K102 F103 K104 R105 K106 A107 N108

4.2.19 Score per residue for model 19

• Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A: 45% 36% 5% 11% •

GLY SER E378 E379 D380 E381 E382 E383 D384 D385 E386 F387 E388 E389 V390 A391 D392 D393 V396 R401 P402 F403 S404 V408 E413 L414 M418 K423 E424 A425 Y426 M429 R432 M433 D436 L437 F438 E439

• Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B: 38% 45% 5% 9% •

GLY SER M1 A2 T3 S4 S5 E6 E7 V8 V12 K13 K14 V15 R16 Q17 K18 K19 Q20 D21 G22 A23 L24 Y25 L26 M27 A28 E29 R30 I31 A34 P35 E36 G37 K38 D39 R40 F41 Y47 A48 D49 I50 Q53 K54 I55 S56 P57 E58 G59 K60 A61 K62 I63 Q64 L65 Q66

L67 V68 L69 D73 T74 H78 S83 T84 A85 V86 V92 K93 D94 L95 L96 Q97 Q98 L99 L100 P101 K102 F103 R105 K104 K106 A107 N108

4.2.20 Score per residue for model 20

• Molecule 1: Transcription initiation factor IIE subunit alpha

Chain A: 45% 33% 5% • 11% •

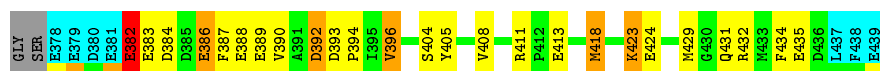GLY SER E378 E379 D380 E381 E382 E383 D384 D385 E386 F387 E388 E389 V390 A391 D392 D393 P394 I395 V396 R401 S404 V408 R411 V415 M418 K423 E424 M429 G430 Q431 R432 M433 F434 E435 D436 L437 F438 E439

• Molecule 2: TFIIH basal transcription factor complex p62 subunit

Chain B: 30% 51% 8% 9% •

GLY SER M1 A2 T3 S4 S5 E6 E7 V8 L9 L10 K14 V15 R16 Q17 K18 K19 Q20 D21 G22 A23 L24 Y25 L26 M27 A28 E29 R30 I31 A32 W33 A34 P35 K38 D39 R40 F41 T42 I43 M46 Y47 I50 Q53 K54 I55 S56 P57 K60 I63 Q64 L65 Q66

L67 V68 L69 D73 T74 T75 N76 F77 H78 F79 S80 N81 E82 A85 V86 R89 V92 K93 D94 L95 L96 Q97 Q98 L99 L100 P101 K102 R105 K106 A107 N108

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DGSA-distance geometry simulated annealing, simulated annealing.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	442	402	402	25±4
2	B	788	824	824	63±7
All	All	24600	24520	24520	1429

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 29.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
2:B:54:LYS:HB2	2:B:66:GLN:HB3	0.97	1.34	2	17
1:A:386:GLU:HB3	2:B:60:LYS:HD2	0.96	1.34	11	8
2:B:55:ILE:HG22	2:B:65:LEU:HD12	0.94	1.37	19	19
1:A:388:GLU:HG2	2:B:57:PRO:HG3	0.93	1.39	2	18
1:A:383:GLU:HB3	2:B:76:ASN:HD22	0.88	1.25	14	1
2:B:34:ALA:HB2	2:B:41:PHE:HA	0.88	1.45	19	17
2:B:56:SER:HB2	2:B:60:LYS:HD3	0.87	1.43	11	1
2:B:7:GLU:HB2	2:B:28:ALA:HB2	0.85	1.48	19	2
1:A:386:GLU:HB2	2:B:60:LYS:HD2	0.85	1.46	4	5
2:B:15:VAL:HG11	2:B:24:LEU:HB2	0.83	1.50	13	20
1:A:388:GLU:HG3	2:B:57:PRO:HG3	0.82	1.51	1	1
2:B:7:GLU:HG2	2:B:28:ALA:HB2	0.80	1.52	12	3
2:B:18:LYS:HE3	2:B:18:LYS:HA	0.80	1.50	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:387:PHE:HB3	2:B:54:LYS:HB3	0.80	1.51	16	19
1:A:390:VAL:HB	2:B:53:GLN:HB2	0.79	1.54	5	20
2:B:55:ILE:HG21	2:B:93:LYS:HD3	0.79	1.52	8	6
2:B:16:ARG:HG2	2:B:21:ASP:HB3	0.78	1.56	11	7
2:B:26:LEU:HD11	2:B:92:VAL:HA	0.77	1.54	3	20
1:A:387:PHE:CZ	2:B:64:GLN:HB2	0.77	2.14	12	8
2:B:55:ILE:HD13	2:B:93:LYS:HD2	0.77	1.56	13	14
2:B:56:SER:HB3	2:B:60:LYS:HG2	0.76	1.57	12	2
2:B:9:LEU:HD13	2:B:99:LEU:HD13	0.75	1.57	13	11
1:A:411:ARG:HB2	1:A:414:LEU:HG	0.75	1.59	13	4
2:B:7:GLU:H	2:B:28:ALA:HB2	0.75	1.42	15	9
2:B:56:SER:HB2	2:B:60:LYS:HG2	0.74	1.58	1	4
1:A:387:PHE:HZ	2:B:64:GLN:HB2	0.74	1.42	12	5
2:B:68:VAL:HA	2:B:74:THR:HG22	0.74	1.60	17	20
2:B:31:ILE:HD13	2:B:67:LEU:HD11	0.74	1.60	13	20
1:A:386:GLU:HB3	2:B:60:LYS:HD3	0.73	1.60	1	5
2:B:84:THR:HB	2:B:88:GLU:OE1	0.73	1.84	9	1
2:B:9:LEU:HD21	2:B:28:ALA:HA	0.72	1.60	2	3
2:B:22:GLY:HA3	2:B:35:PRO:HA	0.72	1.59	8	20
1:A:386:GLU:CB	2:B:60:LYS:HD2	0.71	2.15	20	6
1:A:387:PHE:CE2	2:B:64:GLN:HB2	0.71	2.21	10	3
1:A:388:GLU:HG2	2:B:57:PRO:CG	0.71	2.16	15	17
1:A:392:ASP:HB2	2:B:101:PRO:HD3	0.70	1.62	4	8
1:A:387:PHE:HA	2:B:55:ILE:O	0.70	1.86	15	20
1:A:383:GLU:HG2	1:A:384:ASP:H	0.70	1.46	18	2
2:B:56:SER:HB3	2:B:60:LYS:HD3	0.69	1.64	20	3
2:B:17:GLN:O	2:B:20:GLN:HG2	0.69	1.87	17	3
2:B:26:LEU:HD21	2:B:92:VAL:HG13	0.69	1.63	13	20
1:A:395:ILE:HG12	2:B:98:GLN:HG2	0.69	1.62	8	10
2:B:48:ALA:HA	2:B:104:LYS:HA	0.69	1.63	16	3
2:B:22:GLY:HA2	2:B:36:GLU:N	0.69	2.02	12	13
2:B:22:GLY:CA	2:B:35:PRO:HA	0.69	2.18	20	14
2:B:13:LYS:N	2:B:13:LYS:HE3	0.68	2.03	3	1
2:B:65:LEU:HB2	2:B:89:ARG:HG3	0.68	1.64	13	6
1:A:387:PHE:HB3	2:B:54:LYS:HD2	0.68	1.62	15	1
2:B:55:ILE:HG21	2:B:93:LYS:CD	0.67	2.19	20	14
1:A:388:GLU:CG	2:B:57:PRO:HG3	0.66	2.20	1	16
2:B:55:ILE:CG2	2:B:65:LEU:HD12	0.66	2.21	10	10
2:B:81:ASN:HB3	2:B:88:GLU:OE2	0.66	1.90	6	1
1:A:384:ASP:HA	1:A:387:PHE:CE1	0.65	2.27	17	8
2:B:7:GLU:N	2:B:28:ALA:HB2	0.65	2.07	18	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:432:ARG:HD2	2:B:101:PRO:O	0.64	1.92	6	3
2:B:55:ILE:HG21	2:B:93:LYS:HD2	0.64	1.67	15	6
2:B:8:VAL:HG22	2:B:27:MET:HG3	0.64	1.68	4	6
2:B:56:SER:HB3	2:B:64:GLN:HG2	0.63	1.70	9	1
2:B:38:LYS:HE2	2:B:38:LYS:HA	0.63	1.69	10	1
1:A:388:GLU:O	2:B:54:LYS:HA	0.63	1.93	6	18
2:B:55:ILE:HD13	2:B:93:LYS:CD	0.63	2.24	10	13
1:A:384:ASP:HA	1:A:387:PHE:CZ	0.63	2.29	14	2
2:B:16:ARG:HA	2:B:20:GLN:O	0.62	1.94	6	19
2:B:55:ILE:HG22	2:B:65:LEU:CD1	0.62	2.24	7	5
2:B:55:ILE:HD13	2:B:93:LYS:HD3	0.61	1.69	8	1
2:B:63:ILE:HG21	2:B:85:ALA:O	0.61	1.95	6	20
1:A:432:ARG:O	1:A:436:ASP:HB2	0.61	1.94	19	1
1:A:386:GLU:HB2	2:B:60:LYS:HZ3	0.61	1.55	12	1
2:B:94:ASP:O	2:B:98:GLN:HG2	0.61	1.96	12	2
1:A:387:PHE:CB	2:B:54:LYS:HD2	0.61	2.26	7	6
1:A:387:PHE:CB	2:B:54:LYS:HB3	0.61	2.26	19	5
2:B:55:ILE:HB	2:B:89:ARG:HE	0.60	1.55	20	2
1:A:386:GLU:HB3	2:B:60:LYS:CD	0.60	2.25	5	6
1:A:383:GLU:HB2	2:B:76:ASN:CB	0.60	2.26	12	1
2:B:56:SER:HB2	2:B:60:LYS:CG	0.60	2.27	9	2
2:B:69:LEU:HD12	2:B:73:ASP:HB3	0.60	1.73	16	18
2:B:55:ILE:HG21	2:B:93:LYS:HG3	0.60	1.72	2	3
2:B:56:SER:HB3	2:B:64:GLN:HG3	0.59	1.74	7	2
1:A:418:MET:SD	1:A:423:LYS:HA	0.59	2.37	10	20
1:A:411:ARG:CB	1:A:414:LEU:HG	0.59	2.26	13	2
1:A:386:GLU:O	2:B:56:SER:HA	0.59	1.97	2	5
2:B:63:ILE:HG21	2:B:85:ALA:C	0.59	2.17	12	14
2:B:35:PRO:HG2	2:B:38:LYS:HG3	0.59	1.73	19	1
1:A:386:GLU:HB3	2:B:60:LYS:HE3	0.59	1.72	2	1
2:B:29:GLU:HB3	2:B:103:PHE:CE1	0.59	2.33	14	3
2:B:7:GLU:HG3	2:B:28:ALA:CB	0.59	2.28	6	6
1:A:396:VAL:HG21	1:A:426:TYR:HB2	0.59	1.75	14	6
2:B:10:LEU:HB3	2:B:26:LEU:HD12	0.59	1.75	1	7
1:A:393:ASP:O	2:B:98:GLN:HA	0.59	1.96	12	9
1:A:383:GLU:CD	1:A:383:GLU:H	0.58	2.01	20	1
1:A:382:GLU:HG2	2:B:78:HIS:HB2	0.58	1.73	20	1
1:A:383:GLU:HG2	1:A:384:ASP:N	0.58	2.13	18	1
2:B:67:LEU:O	2:B:74:THR:HA	0.58	1.99	6	20
2:B:55:ILE:HG12	2:B:93:LYS:HD2	0.58	1.75	1	1
1:A:387:PHE:HE2	2:B:64:GLN:HB2	0.58	1.55	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:387:PHE:HB2	2:B:54:LYS:HE2	0.58	1.76	17	2
2:B:57:PRO:HD2	2:B:60:LYS:HE2	0.58	1.74	2	1
2:B:8:VAL:HG22	2:B:27:MET:SD	0.57	2.39	19	2
2:B:12:VAL:HG13	2:B:88:GLU:HG3	0.57	1.75	4	1
2:B:63:ILE:HG12	2:B:86:VAL:N	0.57	2.14	7	17
2:B:7:GLU:HG3	2:B:28:ALA:HB2	0.57	1.76	6	6
2:B:24:LEU:HD12	2:B:79:PHE:CZ	0.57	2.35	8	11
2:B:25:TYR:HB3	2:B:27:MET:SD	0.57	2.39	19	4
2:B:12:VAL:HG11	2:B:79:PHE:CD2	0.57	2.35	10	4
1:A:382:GLU:HA	2:B:76:ASN:HB2	0.57	1.76	10	1
2:B:7:GLU:CB	2:B:28:ALA:HB2	0.57	2.27	19	1
2:B:55:ILE:O	2:B:57:PRO:HD3	0.57	2.00	2	16
2:B:12:VAL:HG11	2:B:79:PHE:CE2	0.56	2.34	3	2
2:B:14:LYS:HD2	2:B:81:ASN:HA	0.56	1.76	1	1
2:B:46:MET:O	2:B:50:ILE:HG13	0.56	2.00	15	15
2:B:30:ARG:HB3	2:B:46:MET:HG2	0.56	1.75	20	2
1:A:387:PHE:CE2	2:B:64:GLN:HG3	0.56	2.36	9	1
2:B:8:VAL:HG23	2:B:27:MET:HG3	0.56	1.78	2	1
2:B:51:LYS:O	2:B:104:LYS:HE3	0.56	2.01	4	1
2:B:63:ILE:HG23	2:B:89:ARG:HD3	0.56	1.78	10	4
2:B:14:LYS:NZ	2:B:81:ASN:HA	0.56	2.16	20	1
2:B:54:LYS:HD3	2:B:66:GLN:OE1	0.55	2.01	17	3
1:A:393:ASP:H	2:B:97:GLN:HG3	0.55	1.62	10	12
1:A:387:PHE:HB2	2:B:54:LYS:HD2	0.55	1.79	9	5
2:B:14:LYS:HA	2:B:21:ASP:HB2	0.55	1.76	4	2
1:A:386:GLU:HB2	2:B:60:LYS:NZ	0.55	2.15	12	1
2:B:102:LYS:HD2	2:B:103:PHE:CZ	0.55	2.37	9	2
2:B:16:ARG:HD2	2:B:80:SER:OG	0.55	2.02	1	1
1:A:396:VAL:HG13	1:A:408:VAL:HG21	0.55	1.79	16	18
1:A:388:GLU:HG2	2:B:57:PRO:HG2	0.55	1.79	16	6
2:B:67:LEU:HD21	2:B:96:LEU:HD13	0.54	1.79	20	4
1:A:390:VAL:CB	2:B:53:GLN:HB2	0.54	2.29	1	11
1:A:383:GLU:HB2	2:B:76:ASN:HB3	0.54	1.79	12	1
2:B:84:THR:HA	2:B:87:LYS:HE3	0.54	1.79	5	2
2:B:9:LEU:HD13	2:B:99:LEU:CD1	0.54	2.32	9	13
2:B:63:ILE:CG1	2:B:86:VAL:HG23	0.54	2.33	8	18
1:A:415:VAL:HA	1:A:418:MET:SD	0.54	2.43	14	10
2:B:50:ILE:HB	2:B:100:LEU:HD21	0.54	1.79	19	3
2:B:56:SER:CB	2:B:60:LYS:HG3	0.54	2.33	18	1
1:A:394:PRO:HG2	1:A:405:TYR:HB2	0.54	1.80	15	2
2:B:17:GLN:O	2:B:20:GLN:HG3	0.54	2.02	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:386:GLU:CB	2:B:60:LYS:HD3	0.54	2.33	3	4
2:B:8:VAL:CG2	2:B:27:MET:HG3	0.54	2.32	2	2
2:B:56:SER:CB	2:B:60:LYS:HD3	0.53	2.27	11	2
2:B:30:ARG:HB3	2:B:46:MET:SD	0.53	2.43	12	1
1:A:385:ASP:OD1	2:B:60:LYS:HE2	0.53	2.04	1	2
1:A:387:PHE:CE1	2:B:64:GLN:HG3	0.53	2.38	8	1
2:B:12:VAL:HG13	2:B:88:GLU:HB3	0.53	1.79	3	2
2:B:54:LYS:CB	2:B:66:GLN:HB3	0.53	2.31	20	5
2:B:48:ALA:HA	2:B:103:PHE:O	0.53	2.04	19	5
1:A:423:LYS:HB2	1:A:423:LYS:HZ3	0.53	1.64	5	3
2:B:84:THR:HB	2:B:88:GLU:HG3	0.53	1.80	18	2
2:B:87:LYS:H	2:B:87:LYS:HD2	0.53	1.63	18	1
1:A:391:ALA:O	2:B:97:GLN:HG3	0.53	2.03	8	16
2:B:51:LYS:HD3	2:B:52:CYS:SG	0.53	2.43	14	1
2:B:71:ALA:HB3	2:B:73:ASP:OD1	0.53	2.04	5	2
1:A:407:GLU:O	1:A:411:ARG:HD2	0.53	2.04	8	1
2:B:47:TYR:HB2	2:B:103:PHE:HB2	0.52	1.81	8	3
1:A:388:GLU:OE1	2:B:55:ILE:HD11	0.52	2.04	1	1
1:A:384:ASP:HA	1:A:387:PHE:CE2	0.52	2.39	20	2
1:A:401:ARG:HB2	1:A:403:PHE:CE2	0.52	2.38	9	4
1:A:396:VAL:HB	1:A:429:MET:HE2	0.52	1.82	9	3
1:A:383:GLU:HB2	2:B:76:ASN:HB2	0.52	1.81	7	1
2:B:31:ILE:HG23	2:B:45:HIS:HB2	0.52	1.82	15	2
2:B:12:VAL:HG11	2:B:79:PHE:HD2	0.52	1.65	10	1
2:B:18:LYS:HA	2:B:18:LYS:CE	0.52	2.35	2	1
2:B:64:GLN:HA	2:B:77:PHE:O	0.51	2.06	3	13
1:A:436:ASP:OD1	2:B:104:LYS:HD2	0.51	2.05	16	1
2:B:29:GLU:O	2:B:46:MET:HG3	0.51	2.06	18	1
2:B:22:GLY:HA2	2:B:36:GLU:H	0.51	1.66	17	4
2:B:13:LYS:O	2:B:14:LYS:HB2	0.51	2.06	12	4
2:B:65:LEU:O	2:B:76:ASN:HA	0.51	2.06	9	6
2:B:84:THR:HB	2:B:88:GLU:CD	0.51	2.25	9	1
1:A:383:GLU:HA	2:B:64:GLN:NE2	0.51	2.21	12	1
2:B:25:TYR:HB3	2:B:27:MET:CE	0.51	2.36	20	1
2:B:31:ILE:HB	2:B:47:TYR:HE1	0.51	1.65	19	3
2:B:99:LEU:HB3	2:B:103:PHE:CE2	0.51	2.41	16	1
2:B:29:GLU:HA	2:B:103:PHE:CE1	0.51	2.41	6	1
1:A:423:LYS:HZ3	1:A:423:LYS:HB2	0.50	1.64	17	3
2:B:16:ARG:HG2	2:B:21:ASP:CB	0.50	2.35	6	2
2:B:86:VAL:HG13	2:B:89:ARG:NH2	0.50	2.21	2	1
2:B:46:MET:C	2:B:48:ALA:H	0.50	2.08	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:32:ALA:HA	2:B:43:ILE:O	0.50	2.05	18	12
2:B:86:VAL:HG22	2:B:89:ARG:NH2	0.50	2.21	1	1
2:B:34:ALA:HB3	2:B:38:LYS:HG3	0.50	1.83	11	1
1:A:386:GLU:HB2	2:B:60:LYS:CE	0.50	2.36	10	2
2:B:15:VAL:HG21	2:B:24:LEU:H	0.50	1.67	10	1
2:B:63:ILE:CG1	2:B:85:ALA:HB1	0.50	2.37	16	1
2:B:62:LYS:HD3	2:B:64:GLN:OE1	0.50	2.06	11	1
1:A:392:ASP:HB3	2:B:100:LEU:HD13	0.50	1.84	7	6
2:B:79:PHE:CD2	2:B:88:GLU:HB3	0.50	2.42	6	1
1:A:423:LYS:HB2	1:A:423:LYS:HZ2	0.50	1.65	14	1
2:B:65:LEU:CD1	2:B:93:LYS:HB2	0.49	2.37	17	12
2:B:18:LYS:O	2:B:19:LYS:HG2	0.49	2.08	9	2
2:B:63:ILE:HD13	2:B:85:ALA:HB3	0.49	1.85	12	1
2:B:62:LYS:HB2	2:B:78:HIS:NE2	0.49	2.22	7	1
1:A:383:GLU:O	1:A:384:ASP:HB2	0.49	2.08	4	1
1:A:386:GLU:HB2	2:B:60:LYS:CD	0.49	2.37	16	2
2:B:29:GLU:OE1	2:B:30:ARG:HD3	0.49	2.08	9	2
2:B:16:ARG:HG2	2:B:21:ASP:HA	0.49	1.84	17	1
2:B:62:LYS:HE3	2:B:64:GLN:NE2	0.49	2.23	9	2
1:A:411:ARG:HH11	1:A:411:ARG:HG3	0.49	1.68	8	1
2:B:62:LYS:HG2	2:B:78:HIS:NE2	0.49	2.23	3	1
2:B:53:GLN:NE2	2:B:97:GLN:HB2	0.49	2.23	20	4
1:A:432:ARG:HD3	2:B:101:PRO:O	0.49	2.07	19	2
2:B:14:LYS:HE2	2:B:81:ASN:HA	0.49	1.85	3	1
2:B:46:MET:H	2:B:46:MET:HE2	0.49	1.68	18	1
2:B:12:VAL:HG21	2:B:92:VAL:CG2	0.48	2.38	1	8
1:A:396:VAL:HB	1:A:429:MET:CE	0.48	2.38	7	5
1:A:387:PHE:CE1	2:B:56:SER:HB3	0.48	2.43	14	1
1:A:395:ILE:HG12	2:B:98:GLN:CG	0.48	2.37	5	3
2:B:38:LYS:HG3	2:B:39:ASP:H	0.48	1.67	10	1
1:A:389:GLU:HA	2:B:54:LYS:HG2	0.48	1.84	16	1
2:B:18:LYS:O	2:B:19:LYS:HB2	0.48	2.08	7	4
2:B:63:ILE:HG23	2:B:89:ARG:HE	0.48	1.68	8	1
1:A:407:GLU:OE1	1:A:407:GLU:HA	0.48	2.08	2	3
1:A:382:GLU:OE2	2:B:64:GLN:HG3	0.48	2.08	15	1
2:B:64:GLN:O	2:B:89:ARG:HD2	0.48	2.08	20	2
2:B:34:ALA:CB	2:B:38:LYS:HG3	0.48	2.38	11	1
1:A:415:VAL:HG13	1:A:418:MET:SD	0.48	2.49	10	7
1:A:386:GLU:CB	2:B:60:LYS:HE3	0.48	2.38	2	1
2:B:14:LYS:HB2	2:B:14:LYS:NZ	0.48	2.24	5	1
2:B:10:LEU:CB	2:B:26:LEU:HD12	0.48	2.39	15	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
2:B:58:GLU:HA	2:B:58:GLU:OE1	0.48	2.09	4	1
1:A:396:VAL:HB	1:A:429:MET:SD	0.48	2.49	12	2
2:B:104:LYS:O	2:B:104:LYS:HG3	0.48	2.07	16	1
2:B:40:ARG:HD2	2:B:41:PHE:O	0.48	2.08	10	1
2:B:56:SER:HB2	2:B:60:LYS:HG3	0.48	1.85	18	1
2:B:48:ALA:HA	2:B:104:LYS:CA	0.48	2.37	16	1
1:A:386:GLU:HB3	2:B:60:LYS:CE	0.48	2.39	2	1
2:B:16:ARG:NH1	2:B:21:ASP:HB3	0.48	2.24	3	2
2:B:25:TYR:HB2	2:B:32:ALA:O	0.47	2.08	5	2
2:B:29:GLU:HB3	2:B:103:PHE:CZ	0.47	2.44	7	1
2:B:60:LYS:O	2:B:60:LYS:HG3	0.47	2.09	13	1
2:B:54:LYS:HG3	2:B:66:GLN:OE1	0.47	2.08	4	1
1:A:432:ARG:HG2	2:B:104:LYS:O	0.47	2.09	6	1
1:A:387:PHE:CZ	2:B:64:GLN:HG3	0.47	2.43	9	1
2:B:46:MET:N	2:B:46:MET:HE2	0.47	2.23	18	1
1:A:384:ASP:HA	1:A:387:PHE:CD1	0.47	2.44	13	2
2:B:16:ARG:CG	2:B:21:ASP:HB3	0.47	2.40	8	1
1:A:423:LYS:HZ2	1:A:423:LYS:HB2	0.47	1.70	10	1
1:A:383:GLU:OE2	1:A:385:ASP:HB2	0.47	2.10	10	1
2:B:12:VAL:O	2:B:23:ALA:HA	0.47	2.10	6	2
2:B:63:ILE:CG2	2:B:89:ARG:HB2	0.47	2.40	3	1
2:B:34:ALA:HB2	2:B:41:PHE:CA	0.47	2.37	14	2
2:B:56:SER:CB	2:B:64:GLN:HG3	0.47	2.40	7	1
2:B:24:LEU:HD21	2:B:31:ILE:HD11	0.47	1.87	5	1
1:A:392:ASP:HB3	2:B:100:LEU:CD1	0.46	2.40	7	2
2:B:47:TYR:CE2	2:B:96:LEU:HD23	0.46	2.45	6	3
2:B:24:LEU:HD12	2:B:79:PHE:HZ	0.46	1.70	20	2
1:A:431:GLN:O	1:A:435:GLU:HG2	0.46	2.10	20	2
2:B:63:ILE:HG12	2:B:86:VAL:HG23	0.46	1.88	12	2
2:B:50:ILE:HG23	2:B:69:LEU:HD23	0.46	1.87	12	12
2:B:86:VAL:HG22	2:B:89:ARG:HH12	0.46	1.71	2	1
1:A:383:GLU:HG2	2:B:76:ASN:HB2	0.46	1.88	14	1
2:B:12:VAL:HG13	2:B:88:GLU:CD	0.46	2.31	1	1
2:B:30:ARG:HD3	2:B:46:MET:SD	0.46	2.50	16	1
1:A:389:GLU:OE1	2:B:54:LYS:HE3	0.46	2.10	5	1
2:B:12:VAL:O	2:B:23:ALA:HB1	0.46	2.11	15	2
2:B:65:LEU:HD11	2:B:93:LYS:HB2	0.46	1.85	1	2
1:A:390:VAL:CG2	2:B:53:GLN:HB2	0.46	2.41	20	3
2:B:82:GLU:HA	2:B:85:ALA:HB3	0.46	1.87	18	1
2:B:93:LYS:HZ3	2:B:93:LYS:HB3	0.46	1.70	19	2
2:B:14:LYS:NZ	2:B:14:LYS:HB2	0.45	2.25	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:65:LEU:HB2	2:B:89:ARG:HG2	0.45	1.87	3	2
2:B:58:GLU:OE1	2:B:86:VAL:HG11	0.45	2.11	12	1
2:B:63:ILE:HD13	2:B:85:ALA:HB1	0.45	1.88	6	1
2:B:63:ILE:HD12	2:B:63:ILE:N	0.45	2.27	9	3
1:A:382:GLU:HG2	2:B:78:HIS:CB	0.45	2.41	11	1
1:A:394:PRO:HB2	1:A:429:MET:SD	0.45	2.51	17	3
2:B:93:LYS:HD2	2:B:94:ASP:N	0.45	2.26	18	1
2:B:46:MET:O	2:B:50:ILE:HG12	0.45	2.12	7	1
1:A:432:ARG:HG3	2:B:104:LYS:O	0.45	2.11	9	1
1:A:404:SER:O	1:A:408:VAL:HG23	0.45	2.11	11	7
1:A:383:GLU:HA	2:B:64:GLN:OE1	0.45	2.11	8	1
2:B:66:GLN:HB2	2:B:76:ASN:OD1	0.45	2.11	18	1
1:A:394:PRO:HB3	2:B:101:PRO:CG	0.45	2.42	7	2
2:B:96:LEU:O	2:B:100:LEU:HG	0.45	2.12	16	3
1:A:383:GLU:HB3	2:B:64:GLN:OE1	0.45	2.12	17	1
2:B:68:VAL:HG13	2:B:74:THR:CG2	0.45	2.42	19	5
2:B:27:MET:HB2	2:B:30:ARG:HG2	0.45	1.88	17	2
1:A:383:GLU:HB2	2:B:76:ASN:HD22	0.45	1.71	17	2
2:B:29:GLU:HG2	2:B:103:PHE:CD1	0.45	2.46	15	1
1:A:410:GLN:HB3	1:A:411:ARG:NH1	0.45	2.27	8	1
1:A:406:SER:O	1:A:410:GLN:HG2	0.45	2.12	12	2
1:A:433:MET:HA	1:A:436:ASP:HB2	0.45	1.89	16	1
1:A:396:VAL:HG13	1:A:408:VAL:CG2	0.44	2.41	5	5
2:B:12:VAL:C	2:B:13:LYS:HD3	0.44	2.33	10	1
2:B:68:VAL:HG13	2:B:74:THR:HG22	0.44	1.89	19	3
2:B:62:LYS:HD3	2:B:64:GLN:CD	0.44	2.32	11	1
2:B:11:ILE:HG23	2:B:25:TYR:CZ	0.44	2.47	13	1
1:A:432:ARG:HA	1:A:432:ARG:NH1	0.44	2.28	7	1
2:B:63:ILE:HD13	2:B:63:ILE:N	0.44	2.28	16	1
2:B:102:LYS:HE2	2:B:103:PHE:CE2	0.44	2.47	1	1
2:B:56:SER:HB2	2:B:64:GLN:H	0.44	1.72	19	1
1:A:427:ILE:O	1:A:431:GLN:HG2	0.44	2.12	16	1
2:B:62:LYS:HD2	2:B:78:HIS:CE1	0.44	2.47	19	1
2:B:63:ILE:CD1	2:B:86:VAL:HG23	0.44	2.43	16	1
2:B:18:LYS:HD3	2:B:18:LYS:O	0.44	2.12	13	1
2:B:10:LEU:HB3	2:B:26:LEU:CD1	0.44	2.42	15	3
1:A:383:GLU:CG	1:A:384:ASP:H	0.44	2.17	18	1
2:B:16:ARG:HA	2:B:21:ASP:HA	0.43	1.88	19	2
2:B:100:LEU:HB2	2:B:101:PRO:HD3	0.43	1.88	11	1
2:B:29:GLU:HB2	2:B:30:ARG:NH2	0.43	2.28	4	1
2:B:12:VAL:HG21	2:B:92:VAL:HG23	0.43	1.90	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:54:LYS:HB2	2:B:66:GLN:CB	0.43	2.39	8	2
2:B:10:LEU:HD23	2:B:92:VAL:HG23	0.43	1.91	10	1
2:B:79:PHE:CD1	2:B:89:ARG:HB2	0.43	2.49	6	2
2:B:66:GLN:HG3	2:B:74:THR:HB	0.43	1.89	20	2
2:B:62:LYS:HG3	2:B:78:HIS:NE2	0.43	2.27	8	1
2:B:56:SER:CB	2:B:64:GLN:HG2	0.43	2.40	9	1
1:A:431:GLN:O	1:A:435:GLU:HB2	0.43	2.13	13	1
2:B:23:ALA:N	2:B:34:ALA:O	0.43	2.48	14	4
2:B:53:GLN:O	2:B:54:LYS:HG3	0.43	2.14	13	1
2:B:100:LEU:N	2:B:101:PRO:HD2	0.43	2.28	18	3
1:A:413:GLU:O	1:A:417:GLN:HG3	0.43	2.14	12	1
2:B:37:GLY:O	2:B:38:LYS:HB3	0.43	2.14	11	1
1:A:394:PRO:HB3	2:B:101:PRO:HG2	0.43	1.91	7	1
2:B:63:ILE:CG2	2:B:89:ARG:HB3	0.43	2.44	14	2
1:A:414:LEU:O	1:A:418:MET:HB3	0.42	2.14	9	3
2:B:16:ARG:O	2:B:78:HIS:HB3	0.42	2.14	17	1
2:B:81:ASN:H	2:B:85:ALA:HB2	0.42	1.73	17	1
2:B:18:LYS:HA	2:B:18:LYS:HE2	0.42	1.89	20	1
2:B:66:GLN:HA	2:B:75:THR:O	0.42	2.14	2	3
2:B:69:LEU:HG	2:B:73:ASP:O	0.42	2.14	7	5
2:B:70:HIS:NE2	2:B:104:LYS:HE2	0.42	2.29	7	1
2:B:63:ILE:HG23	2:B:89:ARG:NE	0.42	2.28	8	1
1:A:398:VAL:HB	1:A:403:PHE:CD2	0.42	2.49	9	1
2:B:50:ILE:HB	2:B:100:LEU:CD2	0.42	2.44	19	1
2:B:66:GLN:CG	2:B:74:THR:HB	0.42	2.45	20	1
2:B:40:ARG:HE	2:B:40:ARG:HA	0.42	1.75	2	1
2:B:58:GLU:H	2:B:58:GLU:CD	0.42	2.18	14	1
2:B:60:LYS:HD3	2:B:64:GLN:OE1	0.42	2.14	4	1
2:B:63:ILE:HB	2:B:79:PHE:O	0.42	2.14	16	1
2:B:47:TYR:HB3	2:B:100:LEU:HD23	0.42	1.90	18	1
2:B:63:ILE:HG13	2:B:85:ALA:HB1	0.42	1.91	16	1
2:B:56:SER:HB2	2:B:60:LYS:CB	0.42	2.44	9	2
2:B:16:ARG:HG3	2:B:21:ASP:HB3	0.42	1.92	10	1
1:A:394:PRO:HD3	1:A:433:MET:SD	0.42	2.55	6	1
1:A:383:GLU:CG	1:A:384:ASP:N	0.42	2.81	18	1
2:B:57:PRO:O	2:B:58:GLU:HB3	0.42	2.14	18	1
2:B:11:ILE:HG23	2:B:25:TYR:CE1	0.42	2.49	3	2
1:A:394:PRO:HB2	1:A:429:MET:CE	0.42	2.43	12	1
1:A:394:PRO:HB2	1:A:429:MET:HE3	0.42	1.92	12	1
1:A:433:MET:O	1:A:436:ASP:HB3	0.42	2.15	7	1
1:A:394:PRO:HD2	1:A:405:TYR:CB	0.42	2.44	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:12:VAL:CG1	2:B:88:GLU:HB3	0.42	2.44	3	2
2:B:86:VAL:HG22	2:B:89:ARG:NH1	0.42	2.30	10	1
2:B:16:ARG:HG3	2:B:21:ASP:CA	0.42	2.44	10	1
2:B:14:LYS:HB2	2:B:14:LYS:HZ2	0.42	1.74	5	1
2:B:85:ALA:HA	2:B:88:GLU:OE1	0.42	2.14	18	1
2:B:62:LYS:O	2:B:64:GLN:HG2	0.42	2.14	7	1
2:B:38:LYS:NZ	2:B:38:LYS:HA	0.42	2.30	9	1
2:B:15:VAL:HG21	2:B:24:LEU:N	0.42	2.30	10	1
2:B:14:LYS:HZ2	2:B:81:ASN:HA	0.42	1.75	20	1
1:A:382:GLU:HA	2:B:62:LYS:NZ	0.41	2.30	1	1
1:A:431:GLN:HA	1:A:434:PHE:HB2	0.41	1.91	12	2
1:A:412:PRO:HD2	1:A:413:GLU:OE2	0.41	2.15	13	1
2:B:93:LYS:HB3	2:B:93:LYS:HZ3	0.41	1.74	10	1
1:A:392:ASP:CG	2:B:104:LYS:HZ3	0.41	2.18	1	1
2:B:102:LYS:HE2	2:B:103:PHE:CZ	0.41	2.49	13	1
1:A:398:VAL:O	1:A:401:ARG:HD3	0.41	2.16	5	1
1:A:387:PHE:CB	2:B:54:LYS:HE2	0.41	2.43	18	1
2:B:18:LYS:CE	2:B:18:LYS:HA	0.41	2.33	15	1
2:B:99:LEU:O	2:B:102:LYS:HB3	0.41	2.15	20	2
1:A:418:MET:HE1	1:A:426:TYR:HB2	0.41	1.91	9	1
2:B:22:GLY:HA2	2:B:36:GLU:HG2	0.41	1.92	4	1
2:B:56:SER:HB3	2:B:64:GLN:CG	0.41	2.42	9	1
2:B:63:ILE:HG13	2:B:86:VAL:HG23	0.41	1.91	10	1
1:A:394:PRO:CD	2:B:101:PRO:HG2	0.41	2.46	20	1
2:B:87:LYS:HD2	2:B:87:LYS:N	0.41	2.29	11	1
2:B:63:ILE:CG2	2:B:79:PHE:HB2	0.41	2.46	4	1
2:B:84:THR:HG22	2:B:87:LYS:HD2	0.41	1.92	7	1
1:A:401:ARG:HB2	1:A:403:PHE:CZ	0.41	2.51	15	1
1:A:387:PHE:HE1	2:B:64:GLN:HG3	0.41	1.72	8	1
2:B:62:LYS:HE3	2:B:64:GLN:CD	0.41	2.36	17	1
2:B:13:LYS:HE2	2:B:13:LYS:N	0.41	2.31	8	2
2:B:62:LYS:HD3	2:B:64:GLN:NE2	0.41	2.31	18	1
2:B:35:PRO:HB2	2:B:36:GLU:OE2	0.40	2.16	13	1
1:A:383:GLU:HG3	2:B:18:LYS:H	0.40	1.75	19	1
2:B:11:ILE:O	2:B:13:LYS:HE2	0.40	2.16	3	1
1:A:390:VAL:HG21	2:B:93:LYS:HG3	0.40	1.91	8	1
1:A:433:MET:HG3	2:B:101:PRO:HB3	0.40	1.93	20	1
1:A:394:PRO:HD3	2:B:101:PRO:HG2	0.40	1.93	20	1
1:A:398:VAL:HG13	1:A:418:MET:CB	0.40	2.46	4	1
2:B:63:ILE:HG12	2:B:86:VAL:CA	0.40	2.46	11	1
2:B:56:SER:HB3	2:B:60:LYS:HB2	0.40	1.94	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:384:ASP:O	1:A:385:ASP:HB2	0.40	2.16	19	1
2:B:65:LEU:HG	2:B:66:GLN:N	0.40	2.31	16	1
2:B:102:LYS:HD2	2:B:103:PHE:CE1	0.40	2.52	10	1
1:A:383:GLU:N	1:A:383:GLU:CD	0.40	2.73	20	1
2:B:31:ILE:CD1	2:B:67:LEU:HD11	0.40	2.43	14	1
2:B:13:LYS:HE2	2:B:13:LYS:HB2	0.40	1.66	15	1
2:B:70:HIS:NE2	2:B:104:LYS:HE3	0.40	2.32	13	1
1:A:432:ARG:HG2	2:B:101:PRO:O	0.40	2.16	10	1
2:B:14:LYS:CE	2:B:81:ASN:HA	0.40	2.46	3	1
1:A:392:ASP:HB3	2:B:100:LEU:HB3	0.40	1.94	5	1
2:B:29:GLU:HB3	2:B:103:PHE:CD1	0.40	2.51	14	1

6.3 Torsion angles (i)

6.3.1 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 NMR 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	55/64 (86%)	49±1 (89±2%)	5±2 (9±3%)	1±1 (2±2%)	11	48
2	B	98/110 (89%)	87±2 (89±2%)	9±2 (9±2%)	2±1 (2±1%)	14	55
All	All	3060/3480 (88%)	2722 (89%)	271 (9%)	67 (2%)	13	52

All 20 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	82	GLU	10
1	A	386	GLU	8
1	A	392	ASP	6
2	B	36	GLU	5
2	B	83	SER	5
2	B	85	ALA	5
1	A	385	ASP	4
1	A	384	ASP	4
1	A	383	GLU	3
2	B	37	GLY	3

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Mol	Chain	Res	Type	Models (Total)
2	B	57	PRO	2
2	B	60	LYS	2
1	A	382	GLU	2
2	B	58	GLU	2
2	B	59	GLY	1
2	B	18	LYS	1
2	B	35	PRO	1
2	B	7	GLU	1
2	B	101	PRO	1
2	B	61	ALA	1

6.3.2 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 NMR 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	48/56 (86%)	40±2 (83±4%)	8±2 (17±4%)	6	42
2	B	85/94 (90%)	70±3 (82±3%)	15±3 (18±3%)	5	39
All	All	2660/3000 (89%)	2188 (82%)	472 (18%)	6	41

All 69 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	24	LEU	20
1	A	424	GLU	20
2	B	95	LEU	20
1	A	396	VAL	20
1	A	413	GLU	17
2	B	53	GLN	17
2	B	21	ASP	15
2	B	29	GLU	14
2	B	9	LEU	13
1	A	404	SER	13
1	A	383	GLU	13
2	B	17	GLN	12
2	B	76	ASN	12
2	B	82	GLU	12

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Mol	Chain	Res	Type	Models (Total)
1	A	432	ARG	11
1	A	392	ASP	11
2	B	64	GLN	10
2	B	36	GLU	9
2	B	7	GLU	9
1	A	389	GLU	9
2	B	19	LYS	8
2	B	30	ARG	8
1	A	382	GLU	8
2	B	93	LYS	8
2	B	13	LYS	7
2	B	18	LYS	7
2	B	38	LYS	7
2	B	49	ASP	7
1	A	423	LYS	7
2	B	97	GLN	6
2	B	40	ARG	6
2	B	75	THR	6
2	B	98	GLN	6
2	B	83	SER	6
1	A	418	MET	6
2	B	58	GLU	6
2	B	60	LYS	6
2	B	89	ARG	6
2	B	39	ASP	6
1	A	436	ASP	5
1	A	411	ARG	5
2	B	84	THR	5
1	A	401	ARG	5
2	B	56	SER	5
2	B	62	LYS	5
2	B	20	GLN	5
1	A	384	ASP	3
2	B	14	LYS	3
1	A	435	GLU	3
2	B	73	ASP	2
2	B	51	LYS	2
2	B	87	LYS	2
2	B	80	SER	2
1	A	388	GLU	1
1	A	433	MET	1
2	B	47	TYR	1

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Mol	Chain	Res	Type	Models (Total)
2	B	104	LYS	1
2	B	50	ILE	1
2	B	46	MET	1
1	A	410	GLN	1
2	B	88	GLU	1
2	B	94	ASP	1
1	A	434	PHE	1
2	B	16	ARG	1
1	A	385	ASP	1
2	B	43	ILE	1
2	B	81	ASN	1
1	A	429	MET	1
1	A	386	GLU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no carbohydrates in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided