Full wwPDB NMR Structure Validation Report (i)

Sep 29, 2024 – 05:50 PM EDT

PDB ID	:	2L1C
Title	:	Shc-PTB:biphosphorylated integrin beta3 cytoplasmic tail complex (1:1)
Authors	:	Deshmukh, L.; Gorbatyuk, V.; Vinogradova, O.
Deposited on	:	2010-07-27

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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

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

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

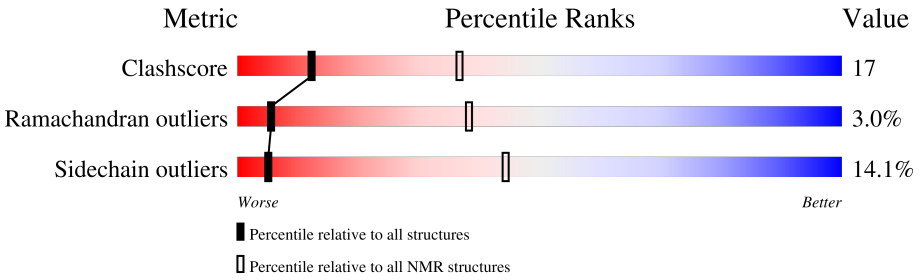
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	211	42% 25% · 20% 9%
2	B	27	22% 41% · 33%

2 Ensemble composition and analysis

This entry contains 15 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:41-A:99, A:105-A:169, A:175-A:198, B:741-B:746, B:748-B:758, B:760-B:760 (166)	0.46	1

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 3 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 8, 12, 14, 15
2	7, 9, 10, 13
3	6, 11

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3384 atoms, of which 1687 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	191	2944	916	1476	269	271	12	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP D3DV78
A	-2	SER	-	expression tag	UNP D3DV78
A	-1	SER	-	expression tag	UNP D3DV78
A	0	HIS	-	expression tag	UNP D3DV78
A	1	HIS	-	expression tag	UNP D3DV78
A	2	HIS	-	expression tag	UNP D3DV78
A	3	HIS	-	expression tag	UNP D3DV78
A	4	HIS	-	expression tag	UNP D3DV78
A	5	HIS	-	expression tag	UNP D3DV78
A	6	SER	-	expression tag	UNP D3DV78
A	7	SER	-	expression tag	UNP D3DV78
A	8	GLY	-	expression tag	UNP D3DV78
A	9	LEU	-	expression tag	UNP D3DV78
A	10	VAL	-	expression tag	UNP D3DV78
A	11	PRO	-	expression tag	UNP D3DV78
A	12	ARG	-	expression tag	UNP D3DV78
A	13	GLY	-	expression tag	UNP D3DV78
A	14	SER	-	expression tag	UNP D3DV78
A	15	HIS	-	expression tag	UNP D3DV78
A	16	MET	-	expression tag	UNP D3DV78

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	27	440	138	211	39	50	2	0

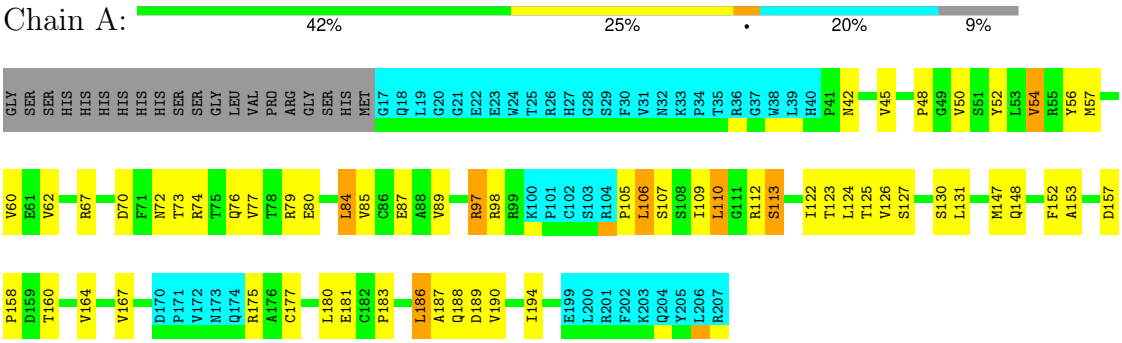
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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.

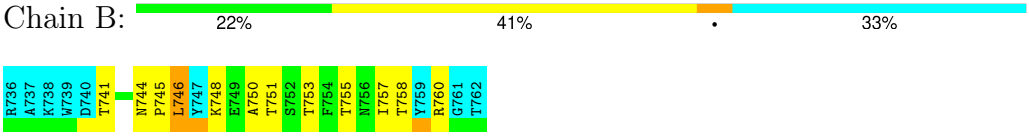
• Molecule 1: SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d

Chain A:



• Molecule 2: Integrin beta-3

Chain B:



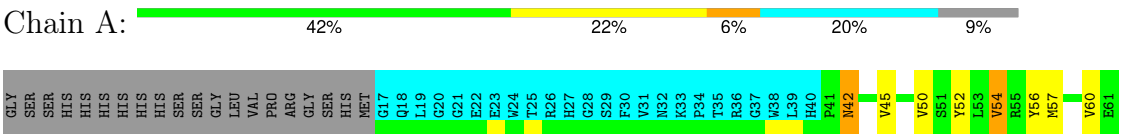
4.2 Scores per residue for each member of the ensemble

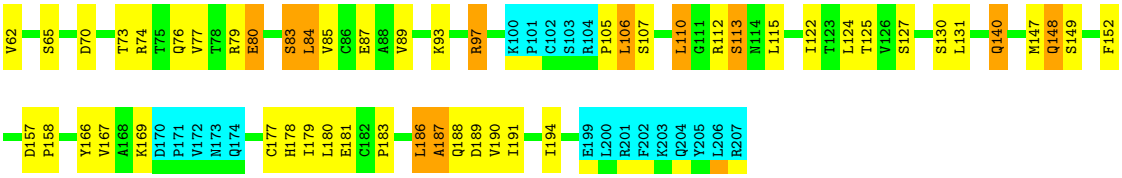
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d

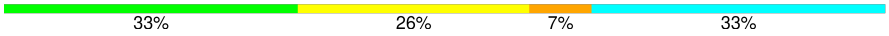
Chain A:





• Molecule 2: Integrin beta-3

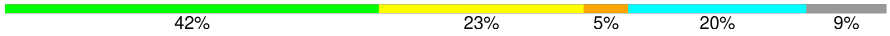
Chain B:

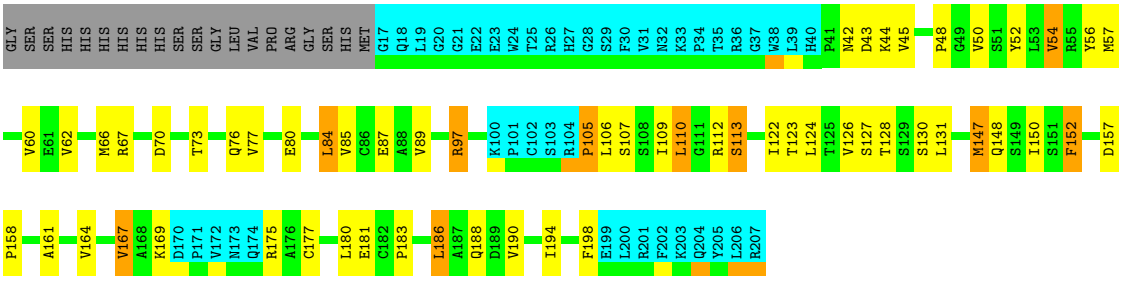


4.2.2 Score per residue for model 2

• Molecule 1: SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d

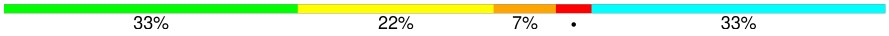
Chain A:





• Molecule 2: Integrin beta-3

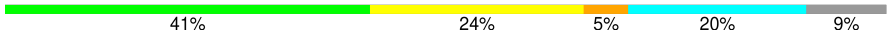
Chain B:

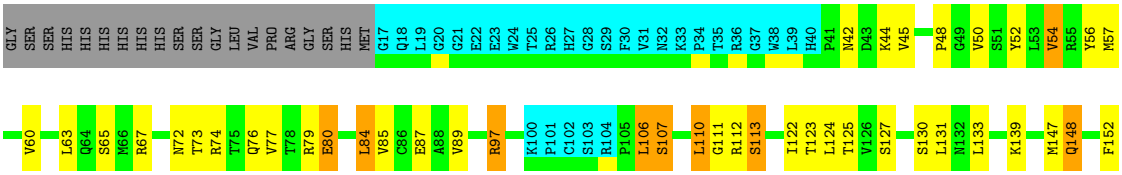


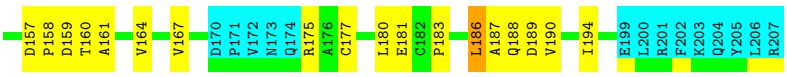
4.2.3 Score per residue for model 3

• Molecule 1: SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d

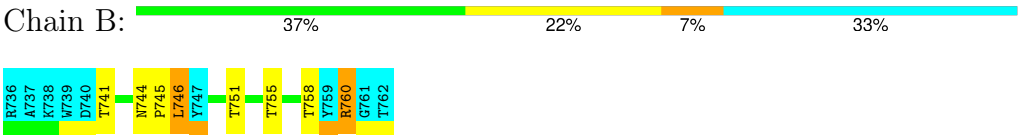
Chain A:





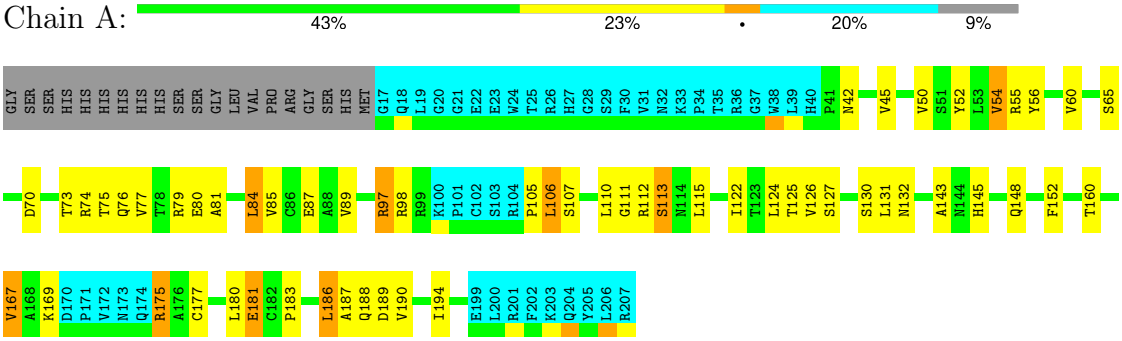


• Molecule 2: Integrin beta-3

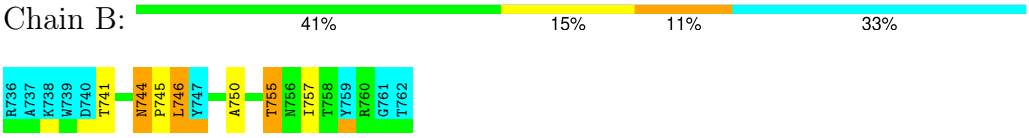


4.2.4 Score per residue for model 4

• Molecule 1: SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d

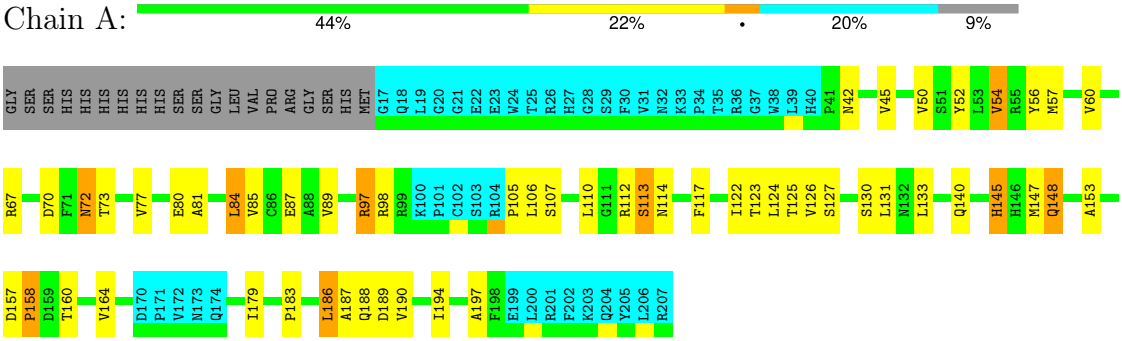


• Molecule 2: Integrin beta-3



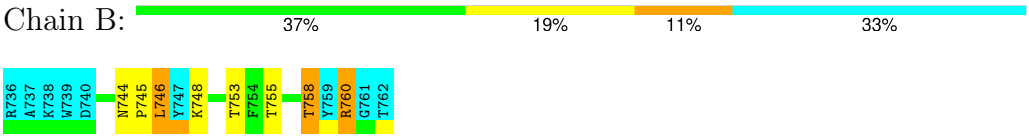
4.2.5 Score per residue for model 5

• Molecule 1: SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d



• Molecule 2: Integrin beta-3

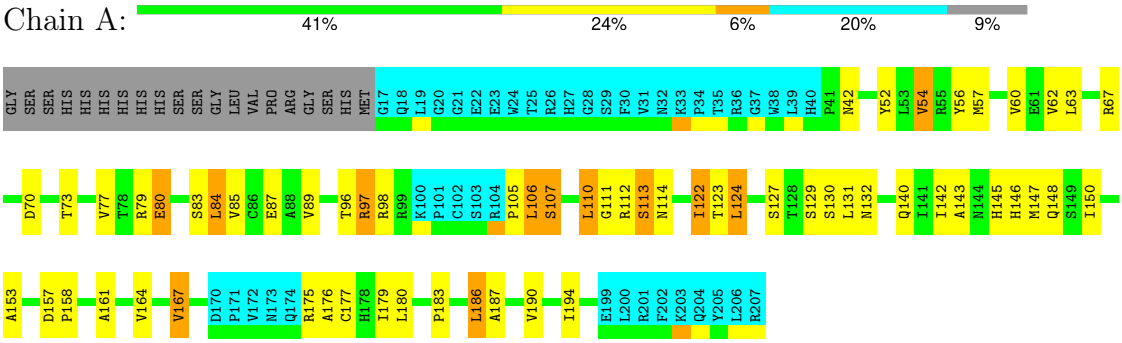
Chain B:



4.2.6 Score per residue for model 6

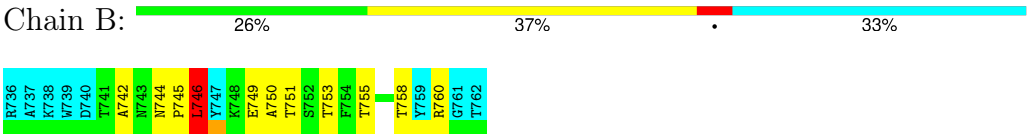
• Molecule 1: SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d

Chain A:



• Molecule 2: Integrin beta-3

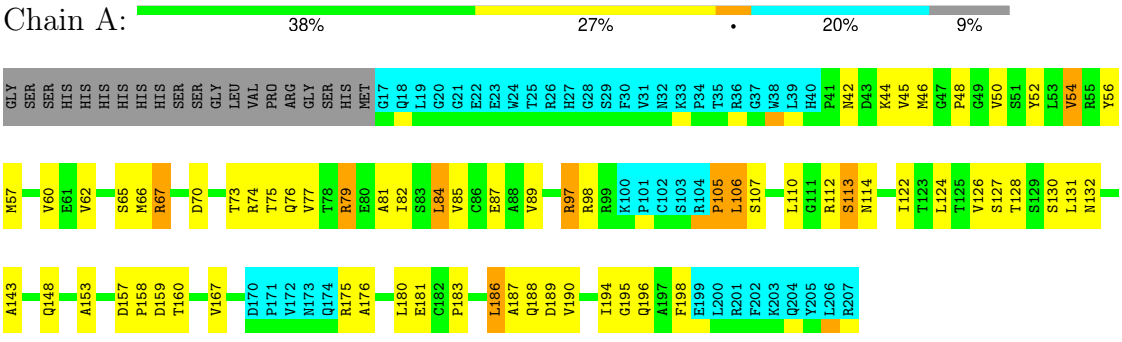
Chain B:



4.2.7 Score per residue for model 7

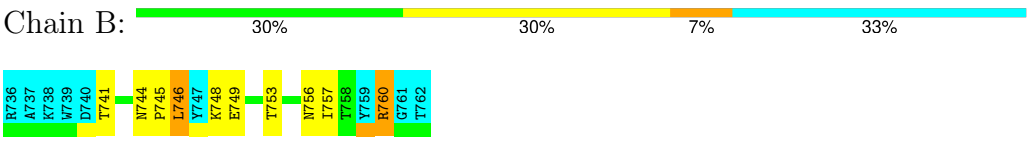
• Molecule 1: SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d

Chain A:



• Molecule 2: Integrin beta-3

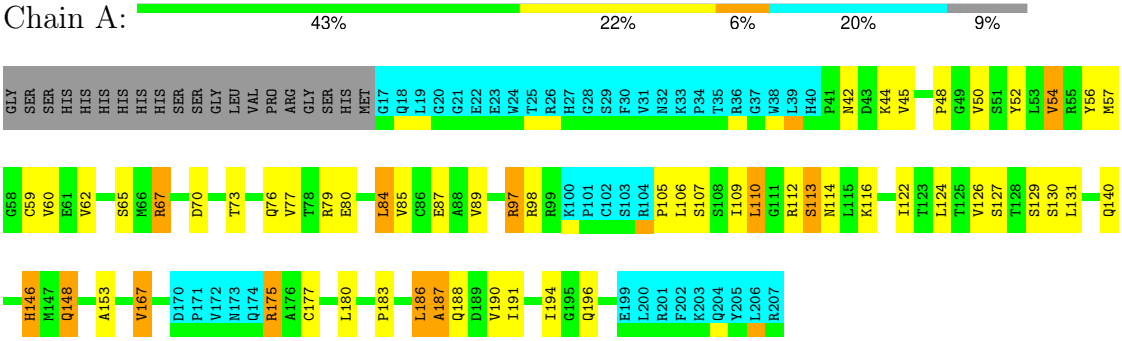
Chain B:



4.2.8 Score per residue for model 8

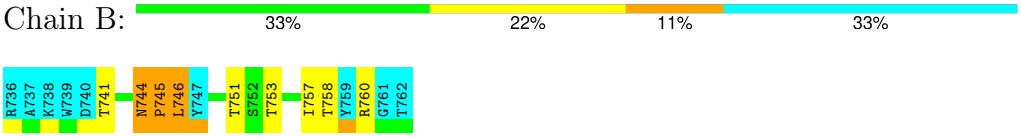
• Molecule 1: SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d

Chain A:



• Molecule 2: Integrin beta-3

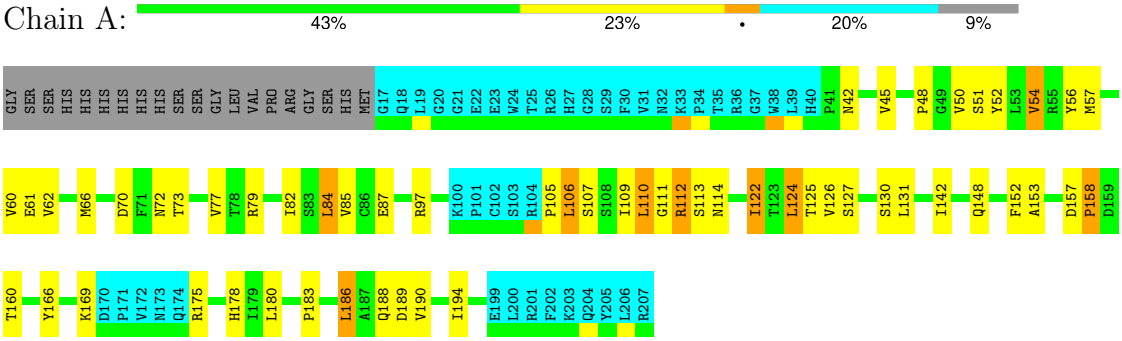
Chain B:



4.2.9 Score per residue for model 9

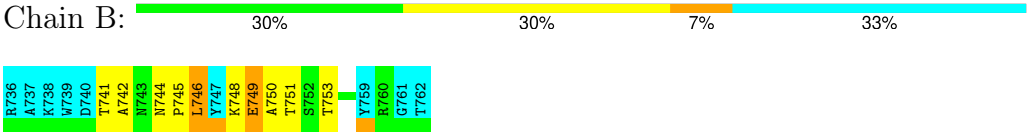
• Molecule 1: SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d

Chain A:



• Molecule 2: Integrin beta-3

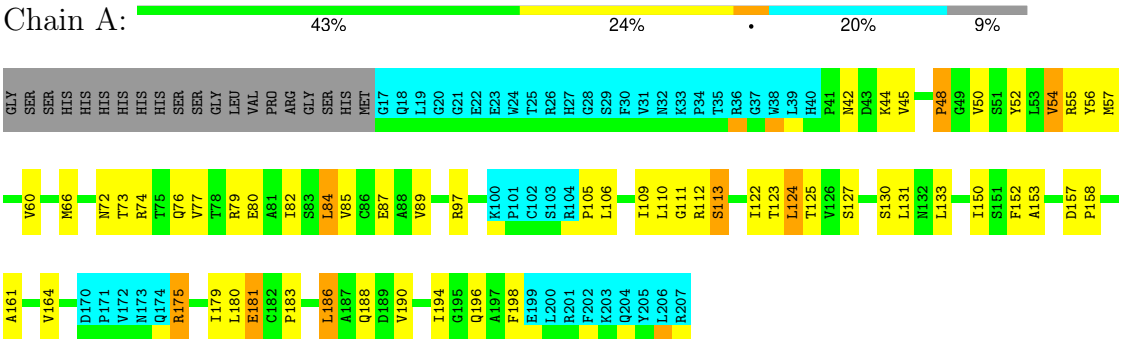
Chain B:



4.2.10 Score per residue for model 10

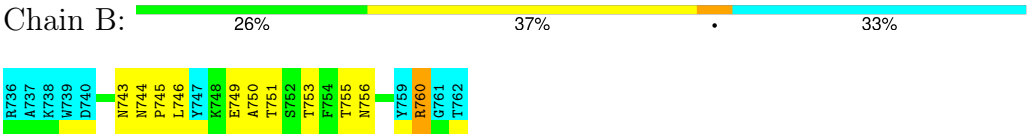
• Molecule 1: SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d

Chain A:



• Molecule 2: Integrin beta-3

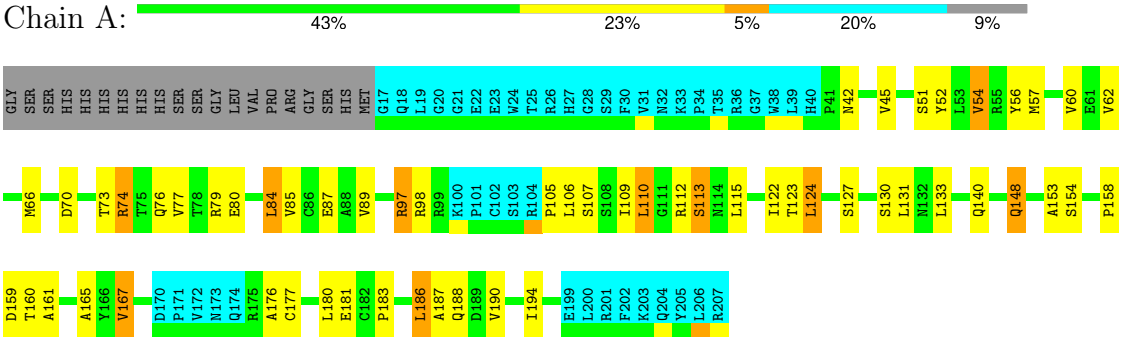
Chain B:



4.2.11 Score per residue for model 11

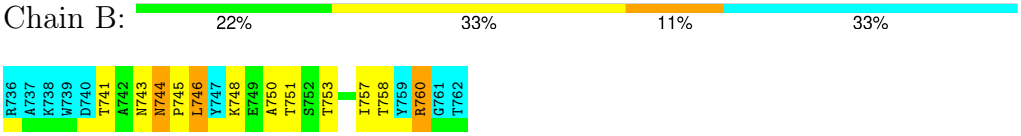
• Molecule 1: SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d

Chain A:



• Molecule 2: Integrin beta-3

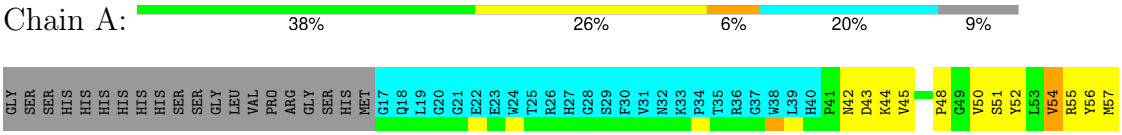
Chain B:

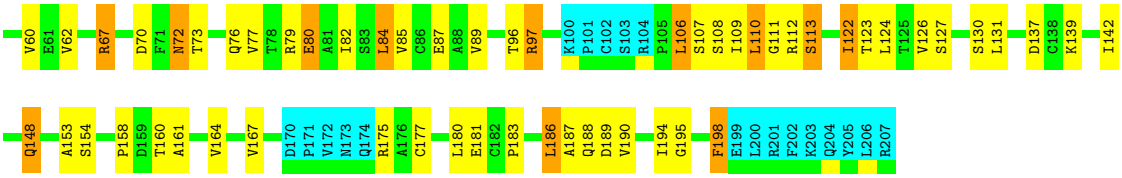


4.2.12 Score per residue for model 12

• Molecule 1: SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d

Chain A:





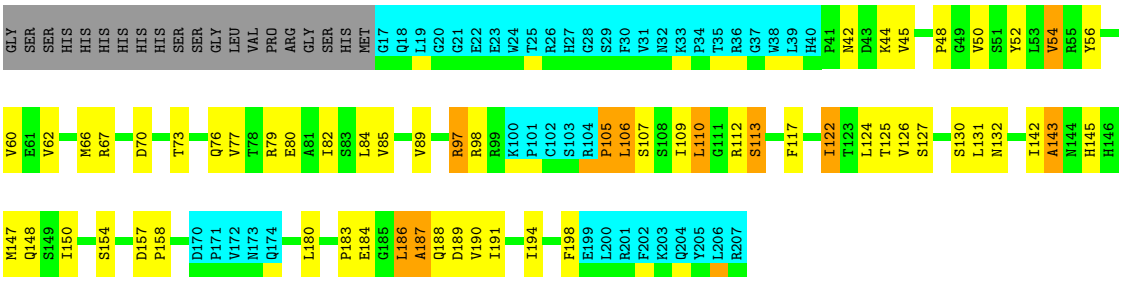
• Molecule 2: Integrin beta-3

Chain B:

4.2.13 Score per residue for model 13

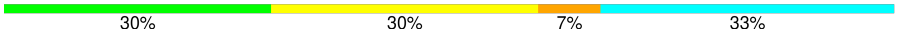
• Molecule 1: SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d

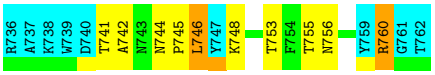
Chain A:



• Molecule 2: Integrin beta-3

Chain B:

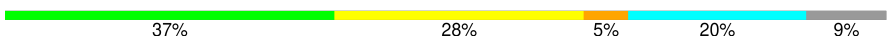


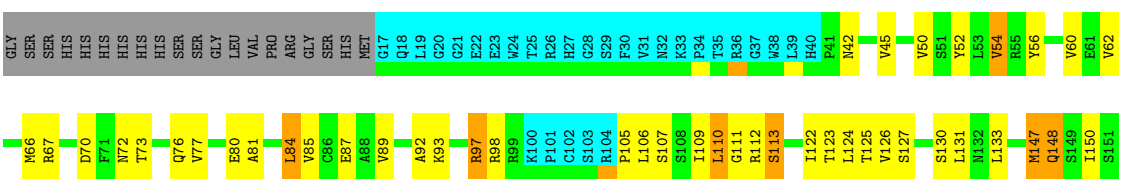


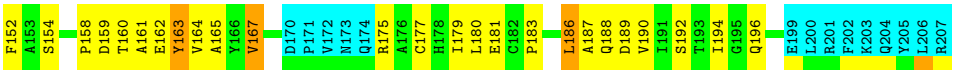
4.2.14 Score per residue for model 14

• Molecule 1: SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d

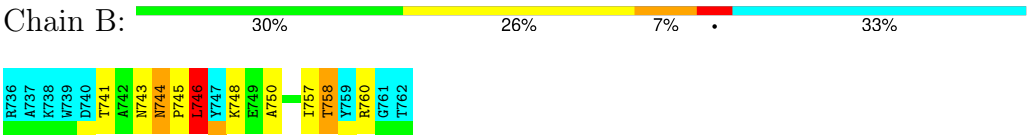
Chain A:





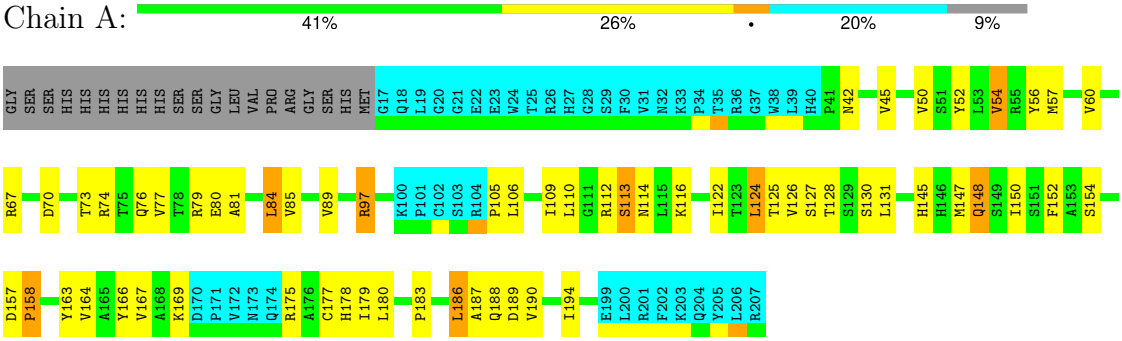


• Molecule 2: Integrin beta-3

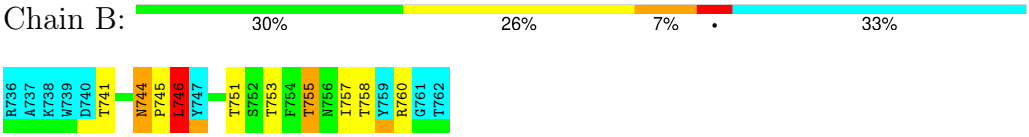


4.2.15 Score per residue for model 15

• Molecule 1: SHC (Src homology 2 domain containing) transforming protein 1, isoform CRA_d



• Molecule 2: Integrin beta-3



5 Refinement protocol and experimental data overview

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

Of the 80 calculated structures, 15 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
CYANA	structure solution	2.1
CNS	refinement	1.21

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

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

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	1106	1124	1121	40±4
2	B	138	138	138	8±2
All	All	18660	18930	18885	632

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:PRO:HA	1:A:186:LEU:HD23	0.99	1.33	3	15
1:A:127:SER:HB2	1:A:130:SER:HB2	0.82	1.49	1	4
1:A:127:SER:HB3	1:A:130:SER:HB3	0.78	1.55	15	5
2:B:743:ASN:HB2	2:B:748:LYS:HG2	0.74	1.57	14	1
1:A:70:ASP:HB3	1:A:73:THR:HB	0.73	1.59	15	13
1:A:198:PHE:HB3	2:B:756:ASN:HD22	0.71	1.46	10	2
1:A:67:ARG:HA	2:B:760:ARG:HH11	0.70	1.46	8	2
1:A:76:GLN:HE22	2:B:741:THR:HG22	0.70	1.45	11	4
1:A:73:THR:HG23	1:A:109:ILE:HD13	0.68	1.66	9	7
1:A:77:VAL:HB	1:A:110:LEU:HD13	0.67	1.64	7	1
1:A:152:PHE:HB2	1:A:167:VAL:HB	0.67	1.66	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:167:VAL:HB	1:A:177:CYS:HA	0.66	1.68	6	6
1:A:148:GLN:HA	2:B:758:THR:HG22	0.65	1.67	15	3
1:A:96:THR:HG23	1:A:98:ARG:HD3	0.65	1.68	6	1
1:A:87:GLU:O	1:A:97:ARG:HA	0.65	1.92	4	13
1:A:54:VAL:HG12	1:A:186:LEU:HD22	0.64	1.69	8	15
1:A:74:ARG:HB2	1:A:152:PHE:HE2	0.64	1.51	1	3
1:A:67:ARG:HA	2:B:760:ARG:HD2	0.64	1.68	14	2
1:A:127:SER:HB3	1:A:130:SER:HB2	0.63	1.71	9	5
1:A:66:MET:HG2	2:B:760:ARG:HG2	0.63	1.69	7	1
1:A:66:MET:HG2	2:B:760:ARG:HD3	0.62	1.69	13	1
1:A:148:GLN:HA	2:B:758:THR:CG2	0.61	2.25	15	6
1:A:127:SER:HB2	1:A:130:SER:HB3	0.60	1.72	13	1
1:A:106:LEU:HD22	1:A:107:SER:N	0.60	2.12	12	5
1:A:157:ASP:N	1:A:158:PRO:HD3	0.59	2.12	7	10
1:A:62:VAL:HG13	1:A:175:ARG:HG3	0.59	1.74	12	2
2:B:743:ASN:HB2	2:B:748:LYS:HD3	0.59	1.75	12	1
1:A:67:ARG:HG2	2:B:760:ARG:HB2	0.58	1.75	15	1
1:A:62:VAL:HA	1:A:110:LEU:HB2	0.58	1.75	13	9
2:B:744:ASN:HB3	2:B:745:PRO:HD2	0.58	1.75	6	7
1:A:67:ARG:CA	2:B:760:ARG:HD2	0.57	2.29	7	1
1:A:70:ASP:HB3	1:A:73:THR:CB	0.57	2.30	9	11
1:A:60:VAL:HG22	1:A:113:SER:HA	0.56	1.77	8	15
1:A:77:VAL:HB	1:A:110:LEU:HD23	0.56	1.76	13	5
1:A:76:GLN:NE2	2:B:741:THR:HG22	0.56	2.15	11	4
1:A:77:VAL:HG12	1:A:106:LEU:HD11	0.56	1.77	8	7
1:A:148:GLN:HA	2:B:758:THR:HG23	0.56	1.77	1	3
1:A:54:VAL:HB	1:A:180:LEU:HB3	0.56	1.78	9	14
1:A:183:PRO:HA	1:A:186:LEU:CD2	0.55	2.26	12	10
1:A:50:VAL:O	1:A:125:THR:HA	0.55	2.01	10	9
1:A:44:LYS:HA	1:A:48:PRO:HD2	0.55	1.78	10	7
1:A:67:ARG:HA	2:B:760:ARG:HD3	0.55	1.77	8	1
1:A:42:ASN:HA	1:A:45:VAL:HG12	0.55	1.76	9	10
1:A:77:VAL:HG12	1:A:106:LEU:HD21	0.54	1.80	5	6
1:A:67:ARG:HA	2:B:760:ARG:HE	0.54	1.61	12	1
1:A:147:MET:HG2	1:A:198:PHE:CE1	0.54	2.38	13	1
2:B:743:ASN:ND2	2:B:748:LYS:HB2	0.54	2.16	11	1
1:A:62:VAL:O	1:A:175:ARG:HB2	0.54	2.02	2	4
1:A:147:MET:O	1:A:150:ILE:HG12	0.54	2.01	2	4
1:A:76:GLN:OE1	2:B:741:THR:HG22	0.54	2.02	7	3
1:A:87:GLU:HB3	1:A:98:ARG:H	0.54	1.63	5	2
1:A:77:VAL:HG12	1:A:110:LEU:HD22	0.54	1.78	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:ARG:HB2	1:A:152:PHE:CE2	0.54	2.38	3	3
2:B:744:ASN:CB	2:B:745:PRO:HD2	0.54	2.33	1	4
1:A:55:ARG:HB3	1:A:181:GLU:HB3	0.54	1.78	12	1
1:A:152:PHE:HB2	1:A:167:VAL:CG2	0.53	2.34	3	3
1:A:52:TYR:CD1	1:A:190:VAL:HG12	0.52	2.39	15	11
1:A:169:LYS:HA	1:A:175:ARG:HG3	0.52	1.82	4	1
1:A:55:ARG:HD2	1:A:181:GLU:HB3	0.52	1.81	4	1
2:B:744:ASN:OD1	2:B:745:PRO:HD2	0.52	2.04	8	4
1:A:66:MET:HG2	1:A:152:PHE:HD1	0.52	1.64	9	1
1:A:192:SER:O	1:A:196:GLN:HG2	0.52	2.05	14	1
1:A:79:ARG:O	1:A:79:ARG:HD3	0.52	2.05	4	1
1:A:75:THR:HA	2:B:753:THR:CG2	0.52	2.35	7	1
2:B:748:LYS:HB2	2:B:748:LYS:HZ3	0.52	1.65	2	1
1:A:66:MET:SD	1:A:74:ARG:HD2	0.52	2.44	10	1
1:A:84:LEU:HB3	2:B:746:LEU:HG	0.51	1.81	7	12
1:A:97:ARG:HD3	1:A:97:ARG:O	0.51	2.05	15	1
1:A:67:ARG:HA	2:B:760:ARG:NE	0.51	2.20	12	1
1:A:66:MET:HG2	1:A:74:ARG:HG3	0.51	1.81	11	1
1:A:195:GLY:HA2	1:A:198:PHE:CZ	0.50	2.41	12	1
1:A:127:SER:CB	1:A:130:SER:HB2	0.50	2.32	1	1
1:A:106:LEU:HD12	1:A:107:SER:N	0.50	2.21	4	1
1:A:52:TYR:CE2	1:A:190:VAL:HG12	0.50	2.40	8	1
2:B:760:ARG:N	2:B:760:ARG:HD3	0.50	2.21	10	1
1:A:150:ILE:HD12	2:B:755:THR:HG21	0.50	1.83	10	3
1:A:198:PHE:HB3	2:B:756:ASN:HD21	0.50	1.67	2	1
1:A:80:GLU:OE1	1:A:106:LEU:HD12	0.49	2.07	6	5
1:A:52:TYR:CE1	1:A:190:VAL:HG12	0.49	2.42	6	2
1:A:46:MET:HA	1:A:128:THR:HG23	0.49	1.83	7	1
1:A:131:LEU:HB2	1:A:147:MET:HE1	0.49	1.83	13	1
1:A:50:VAL:CG2	1:A:126:VAL:HB	0.49	2.38	8	7
2:B:748:LYS:HB2	2:B:748:LYS:NZ	0.49	2.21	2	1
1:A:131:LEU:HD11	1:A:194:ILE:HD13	0.49	1.84	2	15
1:A:152:PHE:HB2	1:A:167:VAL:CB	0.48	2.37	15	3
1:A:52:TYR:CD2	1:A:190:VAL:HG12	0.48	2.42	8	4
1:A:130:SER:OG	1:A:145:HIS:HA	0.48	2.08	5	5
1:A:167:VAL:HB	1:A:177:CYS:CA	0.48	2.36	6	3
1:A:160:THR:HG22	1:A:160:THR:O	0.48	2.08	12	3
1:A:106:LEU:HD12	1:A:107:SER:H	0.48	1.68	4	1
1:A:153:ALA:O	2:B:753:THR:HA	0.48	2.08	12	8
1:A:98:ARG:HB3	2:B:745:PRO:HB2	0.48	1.85	4	3
1:A:59:CYS:SG	1:A:116:LYS:HE2	0.48	2.48	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:750:ALA:O	2:B:751:THR:HB	0.48	2.09	1	2
1:A:67:ARG:CA	2:B:760:ARG:HD3	0.48	2.39	8	1
1:A:72:ASN:OD1	2:B:749:GLU:HG3	0.48	2.09	9	1
1:A:66:MET:HG2	2:B:760:ARG:CD	0.48	2.38	13	1
1:A:79:ARG:CZ	1:A:160:THR:HG21	0.47	2.39	4	1
1:A:57:MET:O	1:A:85:VAL:HG11	0.47	2.08	5	12
1:A:154:SER:OG	2:B:753:THR:HB	0.47	2.09	13	2
1:A:62:VAL:HG23	1:A:110:LEU:HB3	0.47	1.87	2	7
1:A:85:VAL:O	1:A:89:VAL:HG22	0.47	2.09	12	14
1:A:137:ASP:OD2	1:A:139:LYS:HE3	0.47	2.10	12	1
1:A:76:GLN:OE1	1:A:106:LEU:HD12	0.47	2.10	2	3
1:A:77:VAL:CG1	1:A:106:LEU:HD11	0.47	2.39	8	4
1:A:126:VAL:HG13	1:A:194:ILE:HG12	0.47	1.87	5	7
1:A:73:THR:O	1:A:77:VAL:HG13	0.47	2.10	3	3
1:A:62:VAL:O	1:A:175:ARG:HG2	0.47	2.09	8	3
1:A:149:SER:HB2	1:A:169:LYS:HD2	0.47	1.87	1	1
1:A:79:ARG:HB2	2:B:751:THR:HG22	0.47	1.86	10	5
1:A:92:ALA:HA	1:A:181:GLU:OE2	0.47	2.09	14	1
1:A:109:ILE:HD11	2:B:741:THR:HG21	0.46	1.88	2	3
1:A:158:PRO:C	1:A:160:THR:H	0.46	2.14	7	3
1:A:66:MET:HG3	1:A:152:PHE:CD1	0.46	2.45	10	3
1:A:158:PRO:HD2	1:A:161:ALA:HB2	0.46	1.87	14	7
1:A:74:ARG:O	1:A:77:VAL:HG22	0.46	2.09	4	1
1:A:132:ASN:HA	1:A:143:ALA:HB3	0.46	1.87	6	2
1:A:152:PHE:HA	2:B:755:THR:OG1	0.46	2.11	4	1
1:A:79:ARG:O	1:A:83:SER:HB2	0.46	2.09	1	2
1:A:97:ARG:HD3	1:A:97:ARG:C	0.46	2.31	12	1
1:A:57:MET:O	1:A:179:ILE:HB	0.46	2.10	5	2
1:A:79:ARG:HA	1:A:82:ILE:HD12	0.46	1.88	7	5
1:A:107:SER:HB3	1:A:109:ILE:HG13	0.46	1.87	8	1
1:A:106:LEU:HG	1:A:107:SER:N	0.46	2.26	2	4
1:A:97:ARG:HD2	1:A:97:ARG:C	0.46	2.31	3	1
1:A:67:ARG:HB3	2:B:760:ARG:HB3	0.46	1.88	13	1
1:A:147:MET:O	2:B:758:THR:HG21	0.45	2.11	3	2
1:A:107:SER:HB3	1:A:109:ILE:CG1	0.45	2.40	8	1
1:A:77:VAL:CG2	1:A:106:LEU:HD21	0.45	2.41	14	1
1:A:42:ASN:HA	1:A:45:VAL:HG22	0.45	1.88	4	4
1:A:154:SER:HA	2:B:752:SER:O	0.45	2.11	12	1
1:A:66:MET:HG2	1:A:152:PHE:CD1	0.45	2.46	9	1
2:B:745:PRO:O	2:B:746:LEU:HB2	0.45	2.12	12	1
1:A:123:THR:O	1:A:133:LEU:HA	0.44	2.12	3	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:GLU:OE1	1:A:96:THR:HG22	0.44	2.12	12	1
1:A:66:MET:C	2:B:760:ARG:HD2	0.44	2.32	13	1
1:A:84:LEU:HB2	2:B:746:LEU:HD11	0.44	1.89	9	2
1:A:122:ILE:HG21	1:A:142:ILE:HD11	0.44	1.88	6	4
1:A:167:VAL:HA	1:A:176:ALA:O	0.44	2.12	11	3
1:A:85:VAL:HG22	1:A:115:LEU:HD22	0.44	1.89	11	3
1:A:186:LEU:O	1:A:190:VAL:HG22	0.44	2.13	1	13
1:A:164:VAL:HG23	1:A:183:PRO:HB3	0.44	1.88	5	3
1:A:129:SER:O	1:A:146:HIS:HA	0.44	2.11	6	2
1:A:106:LEU:HD21	1:A:109:ILE:HD12	0.44	1.89	13	2
1:A:97:ARG:O	1:A:98:ARG:HD3	0.44	2.12	13	1
1:A:63:LEU:HD23	1:A:111:GLY:CA	0.44	2.42	3	1
1:A:72:ASN:OD1	2:B:749:GLU:HG2	0.44	2.13	10	1
1:A:63:LEU:HD23	1:A:111:GLY:HA3	0.43	1.90	3	1
1:A:51:SER:HA	1:A:124:LEU:O	0.43	2.14	9	2
1:A:107:SER:OG	2:B:741:THR:HG23	0.43	2.13	12	3
1:A:67:ARG:HB3	2:B:760:ARG:HB2	0.43	1.89	6	1
1:A:67:ARG:HA	2:B:760:ARG:CD	0.43	2.41	14	1
1:A:167:VAL:HG22	1:A:177:CYS:HA	0.43	1.88	3	1
1:A:63:LEU:HD13	1:A:111:GLY:CA	0.43	2.43	6	1
1:A:149:SER:CB	1:A:169:LYS:HD2	0.43	2.43	1	1
1:A:60:VAL:HG21	1:A:81:ALA:CB	0.43	2.43	4	5
1:A:50:VAL:HG22	1:A:126:VAL:HB	0.43	1.89	5	2
1:A:74:ARG:HG3	1:A:75:THR:N	0.43	2.28	4	1
1:A:183:PRO:O	1:A:186:LEU:HB3	0.43	2.13	8	1
1:A:66:MET:HB2	2:B:760:ARG:HG3	0.43	1.91	11	1
1:A:187:ALA:O	1:A:191:ILE:HG12	0.42	2.14	1	3
1:A:154:SER:OG	1:A:165:ALA:HB3	0.42	2.14	14	2
1:A:93:LYS:HD3	1:A:163:TYR:CE1	0.42	2.48	14	1
1:A:127:SER:CB	1:A:130:SER:HB3	0.42	2.39	15	1
1:A:79:ARG:HB3	2:B:748:LYS:O	0.42	2.13	7	1
1:A:57:MET:HG2	1:A:85:VAL:CG1	0.42	2.44	2	1
1:A:73:THR:CG2	1:A:109:ILE:HG21	0.42	2.45	9	1
1:A:84:LEU:HB2	2:B:746:LEU:CD1	0.42	2.44	1	1
1:A:179:ILE:N	1:A:179:ILE:HD12	0.42	2.29	6	4
1:A:44:LYS:HB2	1:A:50:VAL:HG13	0.42	1.89	3	3
1:A:77:VAL:HG22	1:A:106:LEU:HD21	0.42	1.91	14	1
1:A:166:TYR:CE1	1:A:178:HIS:HB2	0.42	2.48	9	3
1:A:164:VAL:CG2	1:A:183:PRO:HB3	0.42	2.45	5	7
1:A:105:PRO:HB3	1:A:112:ARG:HA	0.42	1.90	9	1
1:A:77:VAL:HG23	1:A:106:LEU:HD11	0.42	1.91	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:760:ARG:O	2:B:760:ARG:HD2	0.42	2.15	5	1
1:A:51:SER:HB3	1:A:123:THR:CG2	0.42	2.45	12	1
1:A:75:THR:HA	2:B:753:THR:HG22	0.42	1.90	7	1
1:A:114:ASN:CG	1:A:116:LYS:HE3	0.41	2.35	15	1
1:A:198:PHE:HB3	2:B:756:ASN:ND2	0.41	2.30	2	1
1:A:54:VAL:HG11	1:A:124:LEU:HB2	0.41	1.92	6	3
1:A:167:VAL:HG22	1:A:177:CYS:CB	0.41	2.45	1	4
2:B:749:GLU:H	2:B:749:GLU:CD	0.41	2.19	9	1
1:A:55:ARG:HE	1:A:181:GLU:HB3	0.41	1.75	10	1
1:A:75:THR:CG2	2:B:749:GLU:HG2	0.41	2.45	7	1
1:A:160:THR:CB	2:B:751:THR:HB	0.41	2.45	9	1
1:A:52:TYR:O	1:A:123:THR:HA	0.41	2.16	2	2
1:A:154:SER:HA	2:B:753:THR:HA	0.41	1.92	15	1
1:A:77:VAL:HG12	1:A:106:LEU:CD2	0.41	2.46	10	2
1:A:77:VAL:HG12	1:A:106:LEU:CD1	0.41	2.46	8	1
1:A:184:GLU:HG2	1:A:184:GLU:O	0.41	2.16	13	1
1:A:114:ASN:ND2	1:A:116:LYS:HE3	0.41	2.30	15	1
1:A:72:ASN:HD22	1:A:72:ASN:C	0.40	2.20	5	1
1:A:157:ASP:N	1:A:158:PRO:CD	0.40	2.83	7	1
1:A:169:LYS:HB3	1:A:175:ARG:CD	0.40	2.46	2	1
1:A:62:VAL:HG23	1:A:110:LEU:HB2	0.40	1.92	7	1
1:A:183:PRO:CA	1:A:186:LEU:HD23	0.40	2.32	8	1
1:A:72:ASN:C	1:A:72:ASN:HD22	0.40	2.20	12	1
1:A:142:ILE:O	1:A:143:ALA:HB3	0.40	2.17	13	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	148/211 (70%)	126±2 (85±1%)	19±2 (13±1%)	3±1 (2±1%)	8	50
2	B	18/27 (67%)	9±2 (50±11%)	7±2 (39±11%)	2±1 (11±5%)	1	8
All	All	2490/3570 (70%)	2019 (81%)	396 (16%)	75 (3%)	5	38

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)
1	A	187	ALA	12
2	B	746	LEU	12
1	A	105	PRO	9
2	B	750	ALA	6
1	A	111	GLY	5
1	A	140	GLN	4
1	A	107	SER	4
1	A	158	PRO	3
2	B	760	ARG	3
1	A	159	ASP	2
2	B	755	THR	2
2	B	748	LYS	2
1	A	143	ALA	2
2	B	745	PRO	2
1	A	48	PRO	2
2	B	751	THR	1
1	A	106	LEU	1
2	B	742	ALA	1
1	A	97	ARG	1
2	B	756	ASN	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	121/176 (69%)	103±2 (86±2%)	18±2 (14±2%)	5 43
2	B	16/21 (76%)	14±1 (89±7%)	2±1 (11±7%)	7 51
All	All	2055/2955 (70%)	1765 (86%)	290 (14%)	5 44

All 48 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)
1	A	54	VAL	15
1	A	56	TYR	15
1	A	84	LEU	15

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Mol	Chain	Res	Type	Models (Total)
1	A	112	ARG	15
1	A	122	ILE	15
1	A	124	LEU	15
1	A	186	LEU	15
1	A	110	LEU	14
1	A	113	SER	14
1	A	188	GLN	14
1	A	148	GLN	13
1	A	80	GLU	12
1	A	97	ARG	12
1	A	189	ASP	10
1	A	106	LEU	7
1	A	181	GLU	7
1	A	167	VAL	6
2	B	744	ASN	6
2	B	746	LEU	5
1	A	67	ARG	5
1	A	175	ARG	5
2	B	760	ARG	5
1	A	114	ASN	5
2	B	758	THR	4
1	A	72	ASN	4
1	A	147	MET	3
2	B	755	THR	3
1	A	42	ASN	2
1	A	140	GLN	2
1	A	128	THR	2
2	B	748	LYS	2
1	A	117	PHE	2
2	B	749	GLU	2
1	A	74	ARG	2
1	A	132	ASN	2
1	A	159	ASP	2
1	A	163	TYR	2
1	A	83	SER	1
1	A	93	LYS	1
1	A	152	PHE	1
1	A	139	LYS	1
1	A	145	HIS	1
1	A	79	ARG	1
1	A	98	ARG	1
1	A	146	HIS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	61	GLU	1
1	A	198	PHE	1
1	A	162	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	PTR	B	747	2	15,16,17	0.94±0.04	1±0 (4±2%)
2	PTR	B	759	2	15,16,17	0.91±0.06	1±0 (6±1%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	PTR	B	747	2	17,22,24	0.82±0.05	0±0 (0±1%)
2	PTR	B	759	2	17,22,24	0.76±0.02	1±0 (3±2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTR	B	759	2	-	0±0,10,11,13	0±0,1,1,1
2	PTR	B	747	2	-	0±0,10,11,13	0±0,1,1,1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	759	PTR	P-O1P	2.28	1.57	1.50	10	14
2	B	747	PTR	P-O1P	2.27	1.57	1.50	3	11

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	759	PTR	O3P-P-O2P	2.49	117.14	107.80	9	10
2	B	747	PTR	O3P-P-O2P	2.19	116.00	107.80	12	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no oligosaccharides 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

No chemical shift data were provided