



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:32 PM GMT

PDB ID : 1G40  
Title : CRYSTAL STRUCTURE OF A COMPLEMENT PROTEIN THAT REGULATES BOTH PATHWAYS OF COMPLEMENT ACTIVATION AND BINDS HEPARAN SULFATE PROTEOGLYCANS  
Authors : Murthy, K.H.M.; Smith, S.A.; Ganesh, V.K.; Judge, K.W.; Mullin, N.; Barlow, P.N.; Ogata, C.M.; Kotwal, G.K.  
Deposited on : 2000-10-25  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

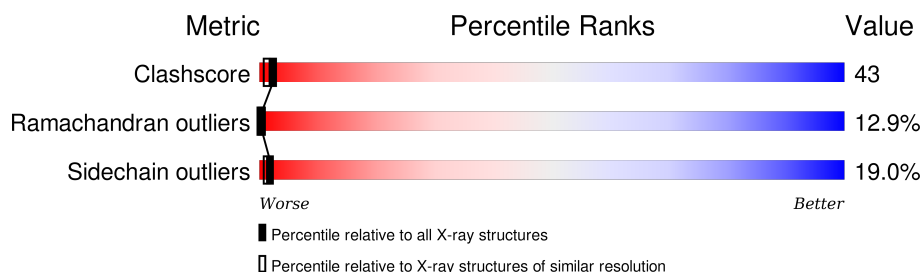
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

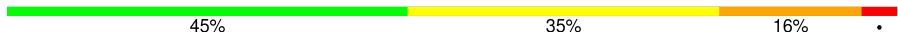
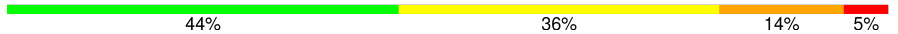
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	244	 45% 35% 16% 5%
1	B	244	 44% 36% 14% 5%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3698 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called COMPLEMENT CONTROL PROTEIN.

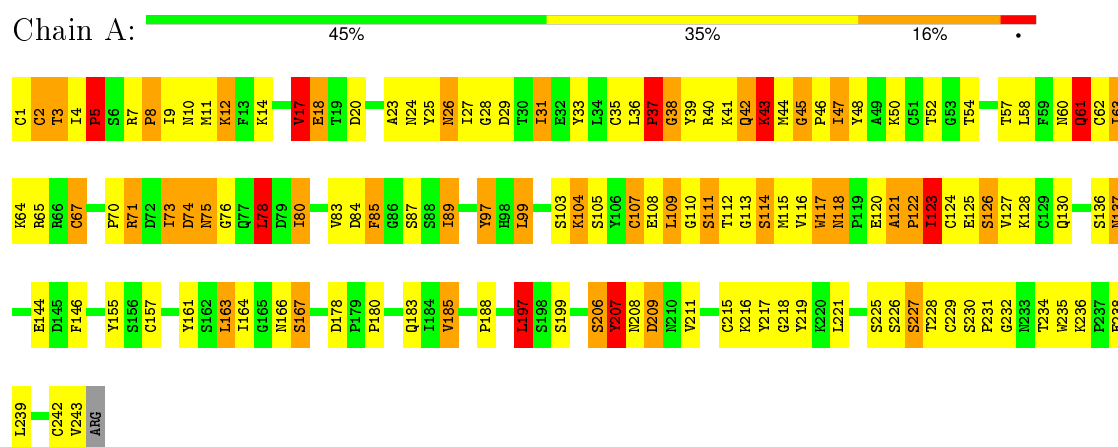
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1849	1150	311	368	20			
1	B	243	Total	C	N	O	S	0	0	0
			1849	1150	311	368	20			

### 3 Residue-property plots [i](#)

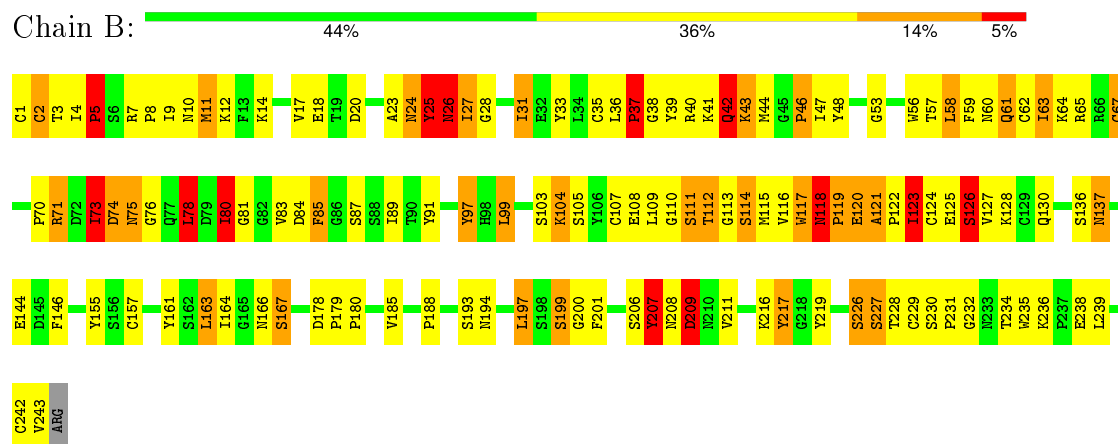
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: COMPLEMENT CONTROL PROTEIN



#### • Molecule 1: COMPLEMENT CONTROL PROTEIN



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.30 Å   104.40 Å   141.90 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	87.0 (8.00-2.20)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.198 , 0.234	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3698	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

## 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  >5	RMSZ	# Z  >5
1	A	0.48	0/1898	1.11	11/2575 (0.4%)
1	B	0.49	0/1898	1.16	20/2575 (0.8%)
All	All	0.48	0/3796	1.13	31/5150 (0.6%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	TYR	CB-CG-CD2	-11.15	114.31	121.00
1	B	207	TYR	CB-CG-CD2	-10.93	114.44	121.00
1	A	207	TYR	CB-CG-CD1	10.43	127.26	121.00
1	B	207	TYR	CB-CG-CD1	10.41	127.25	121.00
1	A	207	TYR	CA-CB-CG	8.84	130.20	113.40
1	B	207	TYR	CA-CB-CG	8.36	129.29	113.40
1	B	78	LEU	CA-CB-CG	7.16	131.77	115.30
1	B	26	ASN	N-CA-C	6.88	129.59	111.00
1	B	207	TYR	N-CA-CB	-6.74	98.46	110.60
1	B	53	GLY	N-CA-C	6.47	129.29	113.10
1	A	78	LEU	CA-CB-CG	6.38	129.98	115.30
1	A	207	TYR	N-CA-CB	-6.21	99.42	110.60
1	B	25	TYR	CA-CB-CG	6.17	125.12	113.40
1	B	42	GLN	N-CA-C	6.05	127.33	111.00
1	B	118	ASN	N-CA-C	6.00	127.19	111.00
1	B	217	TYR	N-CA-C	5.87	126.86	111.00
1	A	163	LEU	CA-CB-CG	5.59	128.17	115.30
1	B	163	LEU	CA-CB-CG	5.57	128.12	115.30
1	B	25	TYR	CB-CA-C	-5.47	99.45	110.40
1	B	209	ASP	N-CA-C	-5.44	96.31	111.00
1	B	73	ILE	CG1-CB-CG2	5.40	123.28	111.40
1	A	43	LYS	N-CA-C	5.34	125.43	111.00
1	B	206	SER	C-N-CA	5.33	135.03	121.70
1	B	56	TRP	N-CA-C	-5.27	96.76	111.00
1	A	206	SER	C-N-CA	5.26	134.85	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ASN	N-CA-C	5.14	124.88	111.00
1	B	80	ILE	N-CA-C	-5.10	97.23	111.00
1	A	197	LEU	CA-CB-CG	5.07	126.97	115.30
1	B	25	TYR	C-N-CA	5.06	134.35	121.70
1	B	226	SER	N-CA-C	-5.05	97.36	111.00
1	A	107	CYS	N-CA-C	-5.04	97.38	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 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	1849	0	1739	164	17
1	B	1849	0	1739	149	17
All	All	3698	0	3478	312	17

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 43.

All (312) 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:A:20:ASP:HB2	1:A:23:ALA:HB2	1.24	1.11
1:B:2:CYS:H	1:B:25:TYR:HA	1.10	1.08
1:B:2:CYS:N	1:B:25:TYR:HA	1.80	0.96
1:A:46:PRO:HB3	1:A:111:SER:N	1.81	0.95
1:B:46:PRO:HA	1:B:111:SER:HA	1.47	0.94
1:B:85:PHE:CZ	1:B:109:LEU:HA	2.03	0.93
1:A:12:LYS:HB3	1:A:35:CYS:SG	2.07	0.93
1:A:85:PHE:CZ	1:A:109:LEU:HA	2.03	0.93
1:B:78:LEU:HB2	1:B:89:ILE:CG2	2.00	0.92
1:A:85:PHE:O	1:A:85:PHE:CD1	2.24	0.91
1:A:73:ILE:HG12	1:A:123:ILE:CD1	2.00	0.90
1:B:78:LEU:HB2	1:B:89:ILE:HG21	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PHE:O	1:A:85:PHE:HD1	1.53	0.89
1:B:85:PHE:O	1:B:85:PHE:CD1	2.26	0.89
1:A:11:MET:HG3	1:A:12:LYS:N	1.88	0.87
1:A:209:ASP:O	1:A:227:SER:O	1.92	0.87
1:A:73:ILE:HG23	1:A:123:ILE:HG23	1.56	0.86
1:B:12:LYS:HB3	1:B:35:CYS:SG	2.15	0.86
1:A:123:ILE:N	1:A:123:ILE:HD13	1.92	0.85
1:A:185:VAL:HG11	1:A:232:GLY:H	1.41	0.85
1:B:71:ARG:HE	1:B:120:GLU:HB2	1.40	0.84
1:B:85:PHE:O	1:B:85:PHE:HD1	1.57	0.82
1:A:121:ALA:HB1	1:A:122:PRO:HD2	1.60	0.82
1:A:63:ILE:HG22	1:A:64:LYS:H	1.43	0.81
1:A:14:LYS:HE2	1:A:31:ILE:HD12	1.62	0.81
1:B:67:CYS:HB2	1:B:84:ASP:O	1.81	0.80
1:A:67:CYS:HB2	1:A:84:ASP:O	1.81	0.79
1:A:46:PRO:HA	1:A:111:SER:HA	1.66	0.78
1:B:80:ILE:HB	1:B:89:ILE:HG23	1.66	0.77
1:B:27:ILE:HG13	1:B:28:GLY:H	1.50	0.77
1:B:185:VAL:HG11	1:B:232:GLY:H	1.50	0.77
1:A:2:CYS:CB	1:A:24:ASN:HB3	2.14	0.77
1:B:99:LEU:HA	1:B:124:CYS:HA	1.67	0.76
1:B:108:GLU:H	1:B:117:TRP:HA	1.51	0.76
1:A:99:LEU:HA	1:A:124:CYS:HA	1.68	0.75
1:A:8:PRO:CG	1:A:11:MET:HG2	2.18	0.74
1:A:8:PRO:HG3	1:A:11:MET:HG2	1.68	0.74
1:B:123:ILE:N	1:B:123:ILE:HD13	2.03	0.73
1:B:12:LYS:HB2	1:B:33:TYR:HB3	1.70	0.73
1:B:209:ASP:O	1:B:228:THR:HA	1.89	0.72
1:A:89:ILE:CD1	1:A:105:SER:HB2	2.20	0.72
1:B:8:PRO:HB2	1:B:11:MET:HB2	1.73	0.71
1:B:107:CYS:HA	1:B:117:TRP:HB3	1.71	0.70
1:A:11:MET:SD	1:A:62:CYS:N	2.65	0.70
1:A:89:ILE:HD11	1:A:105:SER:HB2	1.74	0.70
1:B:47:ILE:HB	1:B:58:LEU:HD22	1.74	0.69
1:A:85:PHE:HD2	1:A:114:SER:HA	1.57	0.69
1:B:20:ASP:HB2	1:B:23:ALA:HB2	1.72	0.69
1:B:73:ILE:HG12	1:B:123:ILE:CD1	2.23	0.69
1:A:123:ILE:HG22	1:A:124:CYS:H	1.58	0.69
1:B:85:PHE:HD2	1:B:114:SER:HA	1.57	0.68
1:A:73:ILE:HG12	1:A:123:ILE:HD12	1.74	0.68
1:A:73:ILE:HG12	1:A:123:ILE:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ILE:HG23	1:B:123:ILE:HG23	1.76	0.68
1:A:108:GLU:HB2	1:A:116:VAL:O	1.92	0.68
1:A:123:ILE:H	1:A:123:ILE:HD13	1.59	0.68
1:B:2:CYS:CB	1:B:24:ASN:HB2	2.22	0.68
1:B:2:CYS:HB2	1:B:24:ASN:C	2.14	0.67
1:B:4:ILE:HB	1:B:5:PRO:HD2	1.78	0.66
1:A:2:CYS:SG	1:A:24:ASN:HB3	2.36	0.66
1:B:108:GLU:HB2	1:B:116:VAL:O	1.96	0.66
1:B:1:CYS:HA	1:B:25:TYR:CA	2.26	0.66
1:B:46:PRO:HB3	1:B:111:SER:N	2.11	0.65
1:B:73:ILE:HG21	1:B:123:ILE:HD12	1.78	0.65
1:B:209:ASP:O	1:B:227:SER:O	2.15	0.65
1:B:125:GLU:HG2	1:B:126:SER:N	2.12	0.65
1:B:78:LEU:HB2	1:B:89:ILE:HG22	1.78	0.65
1:B:107:CYS:HA	1:B:117:TRP:CB	2.27	0.65
1:A:206:SER:OG	1:A:207:TYR:N	2.22	0.65
1:A:83:VAL:HG22	1:A:84:ASP:N	2.12	0.65
1:B:1:CYS:HA	1:B:25:TYR:HB3	1.77	0.64
1:A:24:ASN:OD1	1:A:31:ILE:HD11	1.96	0.64
1:A:108:GLU:H	1:A:117:TRP:HA	1.62	0.64
1:B:26:ASN:HB3	1:B:27:ILE:HG12	1.79	0.64
1:B:123:ILE:HG22	1:B:124:CYS:N	2.12	0.64
1:B:8:PRO:HB2	1:B:11:MET:CB	2.28	0.64
1:B:83:VAL:HG22	1:B:84:ASP:N	2.12	0.64
1:B:12:LYS:HG2	1:B:62:CYS:HB2	1.79	0.64
1:A:209:ASP:O	1:A:228:THR:HA	1.97	0.64
1:A:47:ILE:HD11	1:A:58:LEU:HD13	1.79	0.64
1:B:73:ILE:HG12	1:B:123:ILE:HD11	1.80	0.64
1:A:4:ILE:HB	1:A:5:PRO:HD2	1.79	0.63
1:B:85:PHE:CE2	1:B:109:LEU:HA	2.33	0.63
1:A:11:MET:HG3	1:A:12:LYS:H	1.62	0.63
1:A:221:LEU:HG	1:A:225:SER:OG	1.99	0.63
1:A:17:VAL:HA	1:B:201:PHE:HB3	1.82	0.62
1:A:12:LYS:HE3	1:A:62:CYS:HB2	1.82	0.62
1:B:194:ASN:O	1:B:216:LYS:HB2	2.00	0.62
1:B:2:CYS:SG	1:B:24:ASN:HB2	2.40	0.62
1:A:164:ILE:HG21	1:A:231:PRO:HD3	1.82	0.62
1:B:164:ILE:HG21	1:B:231:PRO:HD3	1.82	0.62
1:B:188:PRO:O	1:B:235:TRP:HZ2	1.83	0.62
1:B:80:ILE:HG22	1:B:81:GLY:H	1.65	0.61
1:A:2:CYS:HB2	1:A:24:ASN:C	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:SER:O	1:B:137:ASN:HB2	2.01	0.61
1:A:73:ILE:CG2	1:A:123:ILE:HG23	2.31	0.61
1:A:125:GLU:HG2	1:A:126:SER:N	2.15	0.61
1:A:123:ILE:HG22	1:A:124:CYS:N	2.16	0.60
1:A:20:ASP:CB	1:A:23:ALA:HB2	2.16	0.60
1:B:2:CYS:HB2	1:B:24:ASN:HB2	1.83	0.60
1:A:12:LYS:HB2	1:A:33:TYR:HB3	1.82	0.60
1:A:85:PHE:CE2	1:A:109:LEU:HA	2.36	0.60
1:B:123:ILE:HG22	1:B:124:CYS:H	1.64	0.60
1:A:136:SER:O	1:A:137:ASN:HB2	2.00	0.60
1:A:188:PRO:O	1:A:235:TRP:HZ2	1.83	0.60
1:A:8:PRO:HB2	1:A:11:MET:CB	2.32	0.59
1:A:42:GLN:OE1	1:A:43:LYS:HE3	2.02	0.59
1:A:89:ILE:O	1:A:89:ILE:HD13	2.03	0.59
1:A:46:PRO:HB3	1:A:111:SER:H	1.65	0.58
1:B:85:PHE:CZ	1:B:109:LEU:CA	2.83	0.58
1:A:11:MET:CE	1:A:61:GLN:HA	2.33	0.58
1:B:118:ASN:C	1:B:120:GLU:H	2.06	0.58
1:B:73:ILE:CG2	1:B:123:ILE:HG23	2.33	0.58
1:B:163:LEU:HD12	1:B:180:PRO:HB2	1.86	0.58
1:A:62:CYS:O	1:A:63:ILE:HG12	2.03	0.58
1:A:121:ALA:HB1	1:A:122:PRO:CD	2.31	0.58
1:A:163:LEU:HD12	1:A:180:PRO:HB2	1.86	0.57
1:B:24:ASN:OD1	1:B:31:ILE:HD11	2.04	0.57
1:B:73:ILE:HG23	1:B:123:ILE:CG2	2.34	0.57
1:B:123:ILE:HD13	1:B:123:ILE:H	1.70	0.57
1:A:123:ILE:H	1:A:123:ILE:CD1	2.18	0.56
1:A:2:CYS:H	1:A:25:TYR:HA	1.70	0.56
1:B:113:GLY:O	1:B:114:SER:HB3	2.06	0.56
1:A:73:ILE:HG23	1:A:123:ILE:CG2	2.33	0.56
1:A:123:ILE:N	1:A:123:ILE:CD1	2.59	0.56
1:B:125:GLU:O	1:B:126:SER:HB3	2.05	0.56
1:A:83:VAL:HG22	1:A:84:ASP:H	1.71	0.56
1:A:50:LYS:HB2	1:A:58:LEU:CD1	2.35	0.56
1:A:12:LYS:CE	1:A:62:CYS:HB2	2.36	0.56
1:B:83:VAL:HG22	1:B:84:ASP:H	1.71	0.56
1:A:207:TYR:O	1:A:229:CYS:HB3	2.06	0.56
1:B:63:ILE:HG12	1:B:64:LYS:H	1.71	0.56
1:B:1:CYS:HA	1:B:25:TYR:CB	2.35	0.56
1:A:71:ARG:NH2	1:A:117:TRP:HB2	2.21	0.56
1:A:50:LYS:HB2	1:A:58:LEU:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:VAL:HB	1:A:232:GLY:O	2.06	0.56
1:A:17:VAL:HG12	1:A:18:GLU:N	2.21	0.56
1:A:12:LYS:HA	1:A:35:CYS:HA	1.87	0.55
1:B:78:LEU:HD23	1:B:89:ILE:HG21	1.89	0.55
1:A:11:MET:CG	1:A:12:LYS:N	2.63	0.55
1:B:41:LYS:O	1:B:113:GLY:HA3	2.07	0.55
1:B:75:ASN:O	1:B:124:CYS:HB3	2.06	0.55
1:B:208:ASN:HB2	1:B:228:THR:HG23	1.89	0.55
1:A:113:GLY:O	1:A:114:SER:HB3	2.06	0.55
1:A:41:LYS:O	1:A:113:GLY:HA3	2.07	0.55
1:B:118:ASN:O	1:B:120:GLU:N	2.40	0.55
1:B:80:ILE:CB	1:B:89:ILE:HG23	2.36	0.55
1:B:70:PRO:HB3	1:B:117:TRP:CH2	2.41	0.54
1:A:47:ILE:HD11	1:A:58:LEU:CD1	2.37	0.54
1:B:85:PHE:CZ	1:B:111:SER:O	2.61	0.54
1:A:36:LEU:CD1	1:A:37:PRO:HD2	2.38	0.54
1:A:125:GLU:O	1:A:126:SER:HB3	2.08	0.54
1:A:80:ILE:HB	1:A:89:ILE:HG22	1.89	0.54
1:B:36:LEU:CD1	1:B:37:PRO:HD2	2.37	0.53
1:B:185:VAL:HB	1:B:232:GLY:O	2.07	0.53
1:A:42:GLN:NE2	1:A:63:ILE:HB	2.23	0.53
1:A:208:ASN:HB2	1:A:228:THR:HG23	1.90	0.53
1:B:80:ILE:HG22	1:B:81:GLY:N	2.22	0.53
1:B:47:ILE:CB	1:B:58:LEU:HD22	2.39	0.53
1:A:85:PHE:CZ	1:A:111:SER:O	2.61	0.53
1:A:63:ILE:HG22	1:A:64:LYS:N	2.19	0.52
1:A:11:MET:SD	1:A:62:CYS:CB	2.98	0.52
1:A:85:PHE:CZ	1:A:109:LEU:CA	2.85	0.52
1:B:1:CYS:HA	1:B:25:TYR:HA	1.92	0.52
1:B:211:VAL:O	1:B:211:VAL:HG23	2.10	0.52
1:B:239:LEU:HD22	1:B:239:LEU:H	1.75	0.52
1:B:91:TYR:HE1	1:B:105:SER:HB2	1.74	0.52
1:A:46:PRO:CA	1:A:111:SER:HA	2.38	0.52
1:A:12:LYS:CG	1:A:33:TYR:HB3	2.40	0.51
1:B:8:PRO:HB2	1:B:11:MET:CG	2.40	0.51
1:B:108:GLU:N	1:B:117:TRP:HA	2.21	0.51
1:B:123:ILE:CD1	1:B:123:ILE:N	2.69	0.51
1:A:118:ASN:O	1:A:120:GLU:N	2.43	0.51
1:A:75:ASN:O	1:A:124:CYS:HB3	2.11	0.51
1:B:73:ILE:HG12	1:B:123:ILE:HD12	1.93	0.51
1:A:239:LEU:HD22	1:A:239:LEU:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PRO:HB2	1:A:11:MET:HB2	1.92	0.50
1:A:85:PHE:C	1:A:85:PHE:CD1	2.85	0.50
1:B:193:SER:O	1:B:194:ASN:HB2	2.12	0.50
1:A:219:TYR:HB2	1:A:242:CYS:SG	2.52	0.50
1:A:70:PRO:HB3	1:A:117:TRP:CH2	2.47	0.50
1:B:4:ILE:HB	1:B:5:PRO:CD	2.42	0.50
1:B:199:SER:HB3	1:B:211:VAL:HA	1.93	0.49
1:A:199:SER:O	1:A:211:VAL:HG12	2.11	0.49
1:B:27:ILE:HG13	1:B:28:GLY:N	2.24	0.49
1:B:199:SER:O	1:B:211:VAL:HG12	2.12	0.49
1:A:2:CYS:CB	1:A:24:ASN:CB	2.89	0.49
1:B:85:PHE:C	1:B:85:PHE:CD1	2.86	0.49
1:B:157:CYS:SG	1:B:163:LEU:HD13	2.53	0.49
1:A:197:LEU:HD23	1:A:211:VAL:HB	1.95	0.49
1:A:41:LYS:O	1:A:113:GLY:CA	2.60	0.49
1:A:157:CYS:SG	1:A:163:LEU:HD13	2.53	0.49
1:A:4:ILE:HB	1:A:5:PRO:CD	2.43	0.48
1:A:11:MET:SD	1:A:12:LYS:HG2	2.54	0.48
1:A:46:PRO:HB3	1:A:110:GLY:C	2.32	0.48
1:B:219:TYR:HB2	1:B:242:CYS:SG	2.54	0.48
1:B:11:MET:HG3	1:B:62:CYS:HB3	1.96	0.48
1:A:230:SER:OG	1:A:236:LYS:HB2	2.13	0.48
1:B:123:ILE:CG2	1:B:124:CYS:H	2.25	0.48
1:A:221:LEU:HD13	1:A:242:CYS:HB2	1.95	0.48
1:A:215:CYS:SG	1:A:221:LEU:HD22	2.54	0.48
1:A:113:GLY:O	1:A:114:SER:CB	2.62	0.47
1:A:33:TYR:HB2	1:A:41:LYS:HZ3	1.80	0.47
1:B:113:GLY:O	1:B:114:SER:CB	2.62	0.47
1:B:123:ILE:CG2	1:B:124:CYS:N	2.77	0.47
1:A:215:CYS:SG	1:A:221:LEU:CD2	3.02	0.47
1:A:11:MET:O	1:A:36:LEU:HD23	2.14	0.47
1:A:11:MET:CG	1:A:12:LYS:H	2.24	0.47
1:B:41:LYS:O	1:B:113:GLY:CA	2.63	0.47
1:A:45:GLY:HA2	1:A:46:PRO:HD2	1.68	0.47
1:A:39:TYR:HB3	1:A:62:CYS:SG	2.55	0.47
1:B:120:GLU:HG3	1:B:120:GLU:O	2.15	0.47
1:B:118:ASN:HB3	1:B:119:PRO:HD3	1.96	0.47
1:B:123:ILE:CD1	1:B:123:ILE:H	2.25	0.47
1:B:230:SER:OG	1:B:236:LYS:HB2	2.15	0.47
1:B:166:ASN:O	1:B:167:SER:HB3	2.15	0.47
1:A:157:CYS:HB3	1:A:161:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:SER:O	1:A:104:LYS:HB2	2.15	0.46
1:B:157:CYS:HB3	1:B:161:TYR:HB2	1.96	0.46
1:B:14:LYS:HD3	1:B:31:ILE:HD12	1.96	0.46
1:B:39:TYR:HB3	1:B:62:CYS:SG	2.56	0.46
1:B:197:LEU:HD23	1:B:211:VAL:HB	1.98	0.46
1:A:78:LEU:HG	1:A:89:ILE:HG12	1.98	0.46
1:A:12:LYS:CB	1:A:33:TYR:HB3	2.46	0.46
1:A:42:GLN:HE21	1:A:63:ILE:HG13	1.81	0.46
1:A:2:CYS:HB2	1:A:24:ASN:HB3	1.93	0.46
1:A:211:VAL:O	1:A:211:VAL:HG23	2.16	0.45
1:B:103:SER:O	1:B:104:LYS:HB2	2.16	0.45
1:B:117:TRP:HD1	1:B:117:TRP:H	1.59	0.45
1:B:46:PRO:HA	1:B:111:SER:CA	2.34	0.45
1:B:47:ILE:HB	1:B:58:LEU:CD2	2.45	0.45
1:B:11:MET:O	1:B:36:LEU:HD23	2.17	0.45
1:A:12:LYS:HE2	1:A:41:LYS:HA	1.98	0.45
1:B:85:PHE:C	1:B:85:PHE:HD1	2.17	0.45
1:A:1:CYS:HA	1:A:25:TYR:O	2.17	0.45
1:B:85:PHE:HZ	1:B:110:GLY:N	2.15	0.45
1:A:83:VAL:CG2	1:A:84:ASP:N	2.79	0.45
1:B:155:TYR:CG	1:B:180:PRO:HG3	2.52	0.45
1:A:8:PRO:CB	1:A:11:MET:HG2	2.47	0.45
1:A:85:PHE:C	1:A:85:PHE:HD1	2.15	0.45
1:A:216:LYS:HB3	1:A:219:TYR:CE2	2.52	0.45
1:B:12:LYS:HE3	1:B:41:LYS:NZ	2.32	0.45
1:A:125:GLU:CG	1:A:126:SER:N	2.80	0.45
1:B:41:LYS:HE3	1:B:48:TYR:HE1	1.82	0.44
1:A:166:ASN:O	1:A:167:SER:HB3	2.16	0.44
1:B:107:CYS:CA	1:B:117:TRP:HB3	2.43	0.44
1:A:74:ASP:O	1:A:75:ASN:HB2	2.18	0.44
1:A:78:LEU:H	1:A:78:LEU:HD13	1.82	0.44
1:B:125:GLU:CG	1:B:126:SER:N	2.80	0.44
1:A:215:CYS:SG	1:A:221:LEU:CD1	3.05	0.44
1:B:207:TYR:O	1:B:229:CYS:HB3	2.18	0.44
1:A:155:TYR:CG	1:A:180:PRO:HG3	2.53	0.44
1:A:85:PHE:CD2	1:A:114:SER:HA	2.46	0.44
1:B:12:LYS:HA	1:B:35:CYS:HA	2.00	0.43
1:B:83:VAL:CG2	1:B:84:ASP:N	2.79	0.43
1:A:107:CYS:HA	1:A:117:TRP:CB	2.47	0.43
1:A:41:LYS:HE3	1:A:48:TYR:HE1	1.83	0.43
1:A:7:ARG:N	1:A:8:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ILE:HG13	1:B:89:ILE:HG23	2.01	0.43
1:A:216:LYS:O	1:A:218:GLY:N	2.51	0.43
1:B:85:PHE:CD2	1:B:114:SER:HA	2.47	0.43
1:B:71:ARG:HE	1:B:120:GLU:CB	2.22	0.43
1:A:80:ILE:CB	1:A:89:ILE:HG22	2.47	0.43
1:A:215:CYS:SG	1:A:221:LEU:HD13	2.58	0.43
1:B:130:GLN:HA	1:B:146:PHE:HD1	1.83	0.43
1:A:75:ASN:ND2	1:A:97:TYR:CZ	2.86	0.43
1:A:89:ILE:HD12	1:A:105:SER:O	2.19	0.42
1:B:157:CYS:SG	1:B:163:LEU:HD22	2.58	0.42
1:B:179:PRO:HA	1:B:180:PRO:HD2	1.96	0.42
1:A:157:CYS:SG	1:A:163:LEU:HD22	2.58	0.42
1:A:11:MET:SD	1:A:62:CYS:HB2	2.59	0.42
1:A:110:GLY:O	1:A:111:SER:HB2	2.18	0.42
1:B:9:ILE:O	1:B:10:ASN:HB2	2.19	0.42
1:A:46:PRO:HA	1:A:111:SER:CA	2.44	0.42
1:B:80:ILE:HB	1:B:89:ILE:CG2	2.44	0.42
1:A:26:ASN:ND2	1:A:26:ASN:H	2.16	0.42
1:B:74:ASP:O	1:B:75:ASN:HB2	2.19	0.42
1:B:41:LYS:HB2	1:B:112:THR:H	1.84	0.42
1:B:125:GLU:HG2	1:B:126:SER:H	1.81	0.42
1:A:17:VAL:CG1	1:A:18:GLU:N	2.83	0.42
1:B:12:LYS:HD2	1:B:41:LYS:HZ3	1.85	0.42
1:B:46:PRO:HB3	1:B:110:GLY:C	2.40	0.42
1:B:120:GLU:O	1:B:121:ALA:HB2	2.20	0.42
1:B:25:TYR:HB2	1:B:26:ASN:H	1.38	0.41
1:A:36:LEU:HD13	1:A:37:PRO:HD2	2.02	0.41
1:B:46:PRO:HB3	1:B:110:GLY:HA2	2.02	0.41
1:A:130:GLN:HA	1:A:146:PHE:HD1	1.83	0.41
1:B:7:ARG:N	1:B:8:PRO:CD	2.83	0.41
1:A:9:ILE:O	1:A:10:ASN:HB2	2.19	0.41
1:B:36:LEU:HD13	1:B:37:PRO:HD2	2.03	0.41
1:B:73:ILE:CG2	1:B:123:ILE:HD12	2.46	0.41
1:A:183:GLN:HG3	1:A:231:PRO:HB3	2.03	0.41
1:A:26:ASN:ND2	1:A:26:ASN:N	2.67	0.41
1:A:123:ILE:CG2	1:A:124:CYS:H	2.29	0.41
1:B:83:VAL:HG21	1:B:87:SER:HB3	2.03	0.41
1:A:52:THR:HB	1:A:57:THR:OG1	2.20	0.41
1:A:107:CYS:HA	1:A:117:TRP:HB3	2.02	0.41
1:A:11:MET:SD	1:A:61:GLN:HA	2.61	0.41
1:A:123:ILE:CG2	1:A:124:CYS:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:LYS:HD3	1:B:31:ILE:CD1	2.50	0.41
1:A:43:LYS:O	1:A:110:GLY:O	2.39	0.41
1:B:83:VAL:CG2	1:B:84:ASP:H	2.34	0.41
1:A:108:GLU:N	1:A:117:TRP:HA	2.32	0.41
1:B:42:GLN:CG	1:B:43:LYS:H	2.34	0.41
1:B:12:LYS:CB	1:B:33:TYR:HB3	2.46	0.41
1:A:207:TYR:O	1:A:229:CYS:CB	2.69	0.41
1:B:70:PRO:HB3	1:B:117:TRP:CZ2	2.56	0.40
1:A:3:THR:HG22	1:A:4:ILE:H	1.86	0.40
1:B:75:ASN:ND2	1:B:97:TYR:CZ	2.89	0.40
1:A:85:PHE:HB3	1:A:113:GLY:O	2.22	0.40
1:A:83:VAL:HG21	1:A:87:SER:HB3	2.04	0.40
1:A:70:PRO:HB3	1:A:117:TRP:CZ2	2.57	0.40

All (17) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:TYR:CD2	1:B:37:PRO:CB[2_564]	0.82	1.38
1:A:36:LEU:CB	1:B:37:PRO:O[2_564]	1.38	0.82
1:A:36:LEU:CB	1:B:37:PRO:C[2_564]	1.50	0.70
1:A:37:PRO:O	1:B:35:CYS:O[2_564]	1.78	0.42
1:A:39:TYR:CG	1:B:37:PRO:CB[2_564]	1.89	0.31
1:A:39:TYR:CE2	1:B:37:PRO:CB[2_564]	1.90	0.30
1:A:39:TYR:N	1:B:37:PRO:CG[2_564]	1.91	0.29
1:A:38:GLY:N	1:B:37:PRO:CD[2_564]	1.96	0.24
1:A:36:LEU:C	1:B:37:PRO:CA[2_564]	1.98	0.22
1:A:39:TYR:CD2	1:B:37:PRO:CG[2_564]	2.01	0.19
1:A:36:LEU:O	1:B:37:PRO:CA[2_564]	2.03	0.17
1:A:36:LEU:O	1:B:37:PRO:CG[2_564]	2.07	0.13
1:A:37:PRO:CB	1:B:35:CYS:O[2_564]	2.10	0.10
1:A:38:GLY:C	1:B:37:PRO:CG[2_564]	2.15	0.05
1:A:39:TYR:CD2	1:B:37:PRO:CA[2_564]	2.17	0.03
1:A:10:ASN:OD1	1:B:64:LYS:NZ[2_564]	2.17	0.03
1:A:36:LEU:CG	1:B:37:PRO:O[2_564]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	241/244 (99%)	162 (67%)	50 (21%)	29 (12%)	0	0
1	B	241/244 (99%)	161 (67%)	47 (20%)	33 (14%)	0	0
All	All	482/488 (99%)	323 (67%)	97 (20%)	62 (13%)	0	0

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	37	PRO
1	A	43	LYS
1	A	54	THR
1	A	104	LYS
1	A	111	SER
1	A	121	ALA
1	A	137	ASN
1	A	167	SER
1	A	207	TYR
1	A	217	TYR
1	B	17	VAL
1	B	27	ILE
1	B	37	PRO
1	B	43	LYS
1	B	59	PHE
1	B	104	LYS
1	B	111	SER
1	B	121	ALA
1	B	137	ASN
1	B	167	SER
1	B	217	TYR
1	A	45	GLY
1	A	75	ASN
1	A	80	ILE

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Mol	Chain	Res	Type
1	A	114	SER
1	B	75	ASN
1	B	80	ILE
1	B	114	SER
1	B	123	ILE
1	B	200	GLY
1	B	207	TYR
1	A	5	PRO
1	A	74	ASP
1	A	126	SER
1	A	178	ASP
1	A	226	SER
1	A	238	GLU
1	B	5	PRO
1	B	38	GLY
1	B	126	SER
1	B	178	ASP
1	B	226	SER
1	B	238	GLU
1	B	26	ASN
1	B	61	GLN
1	B	63	ILE
1	B	74	ASP
1	B	199	SER
1	A	38	GLY
1	A	61	GLN
1	A	123	ILE
1	B	25	TYR
1	B	118	ASN
1	A	127	VAL
1	B	127	VAL
1	A	8	PRO
1	A	63	ILE
1	B	46	PRO
1	A	28	GLY
1	A	76	GLY
1	B	76	GLY

### 5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	213/214 (100%)	171 (80%)	42 (20%)	1	1
1	B	213/214 (100%)	174 (82%)	39 (18%)	2	1
All	All	426/428 (100%)	345 (81%)	81 (19%)	2	1

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	CYS
1	A	3	THR
1	A	5	PRO
1	A	12	LYS
1	A	17	VAL
1	A	18	GLU
1	A	26	ASN
1	A	27	ILE
1	A	29	ASP
1	A	31	ILE
1	A	37	PRO
1	A	40	ARG
1	A	42	GLN
1	A	43	LYS
1	A	44	MET
1	A	47	ILE
1	A	60	ASN
1	A	61	GLN
1	A	65	ARG
1	A	67	CYS
1	A	71	ARG
1	A	73	ILE
1	A	78	LEU
1	A	85	PHE
1	A	89	ILE
1	A	97	TYR
1	A	99	LEU
1	A	109	LEU
1	A	112	THR
1	A	115	MET
1	A	117	TRP

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Mol	Chain	Res	Type
1	A	122	PRO
1	A	123	ILE
1	A	128	LYS
1	A	144	GLU
1	A	185	VAL
1	A	197	LEU
1	A	207	TYR
1	A	209	ASP
1	A	227	SER
1	A	234	THR
1	A	243	VAL
1	B	2	CYS
1	B	3	THR
1	B	5	PRO
1	B	11	MET
1	B	18	GLU
1	B	24	ASN
1	B	31	ILE
1	B	37	PRO
1	B	40	ARG
1	B	42	GLN
1	B	44	MET
1	B	57	THR
1	B	58	LEU
1	B	60	ASN
1	B	61	GLN
1	B	65	ARG
1	B	67	CYS
1	B	71	ARG
1	B	73	ILE
1	B	78	LEU
1	B	85	PHE
1	B	97	TYR
1	B	99	LEU
1	B	112	THR
1	B	115	MET
1	B	117	TRP
1	B	119	PRO
1	B	120	GLU
1	B	122	PRO
1	B	123	ILE
1	B	126	SER

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Mol	Chain	Res	Type
1	B	128	LYS
1	B	144	GLU
1	B	197	LEU
1	B	207	TYR
1	B	209	ASP
1	B	227	SER
1	B	234	THR
1	B	243	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	75	ASN
1	A	130	GLN
1	A	233	ASN
1	B	75	ASN
1	B	130	GLN
1	B	233	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.