



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 12:17 PM EST

PDB ID : 5LTW  
Title : Complex of human 14-3-3 sigma CLU1 mutant with phosphorylated heat shock protein B6  
Authors : Sluchanko, N.N.; Beelen, S.; Kulikova, A.A.; Weeks, S.D.; Antson, A.A.; Gusev, N.B.; Strelkov, S.V.  
Deposited on : 2016-09-07  
Resolution : 4.50 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

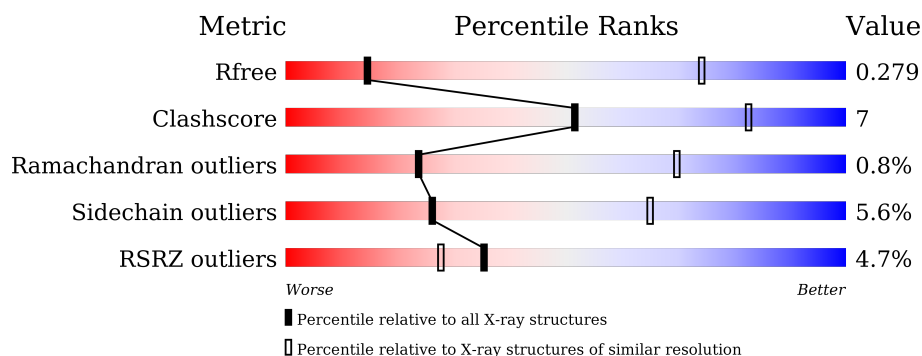
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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.

Mol	Chain	Length	Quality of chain
1	A	234	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div></div> </div> <div>.</div> </div>
1	B	234	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div></div> </div> <div>.</div> </div>
1	E	234	<div> <div>6%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div></div> </div> <div>.</div> </div>
1	F	234	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div></div> </div> <div>..</div> </div>
1	I	234	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div></div> </div> <div>..</div> </div>
1	J	234	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div></div> </div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	C	149	
2	D	149	
2	G	149	
2	H	149	
2	K	149	
2	L	149	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15884 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 14-3-3 protein sigma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1791	1119	305	357	10			
1	B	226	Total	C	N	O	S	0	0	0
			1777	1109	301	358	9			
1	E	227	Total	C	N	O	S	0	0	0
			1790	1118	303	359	10			
1	F	229	Total	C	N	O	S	0	0	0
			1809	1129	307	363	10			
1	I	232	Total	C	N	O	S	0	0	0
			1828	1139	310	369	10			
1	J	229	Total	C	N	O	S	0	0	0
			1809	1129	307	363	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P31947
A	-1	PRO	-	expression tag	UNP P31947
A	0	HIS	-	expression tag	UNP P31947
A	159	ALA	LYS	engineered mutation	UNP P31947
A	160	ALA	LYS	engineered mutation	UNP P31947
A	161	ALA	GLU	engineered mutation	UNP P31947
B	-2	GLY	-	expression tag	UNP P31947
B	-1	PRO	-	expression tag	UNP P31947
B	0	HIS	-	expression tag	UNP P31947
B	159	ALA	LYS	engineered mutation	UNP P31947
B	160	ALA	LYS	engineered mutation	UNP P31947
B	161	ALA	GLU	engineered mutation	UNP P31947
E	-2	GLY	-	expression tag	UNP P31947
E	-1	PRO	-	expression tag	UNP P31947
E	0	HIS	-	expression tag	UNP P31947
E	159	ALA	LYS	engineered mutation	UNP P31947
E	160	ALA	LYS	engineered mutation	UNP P31947

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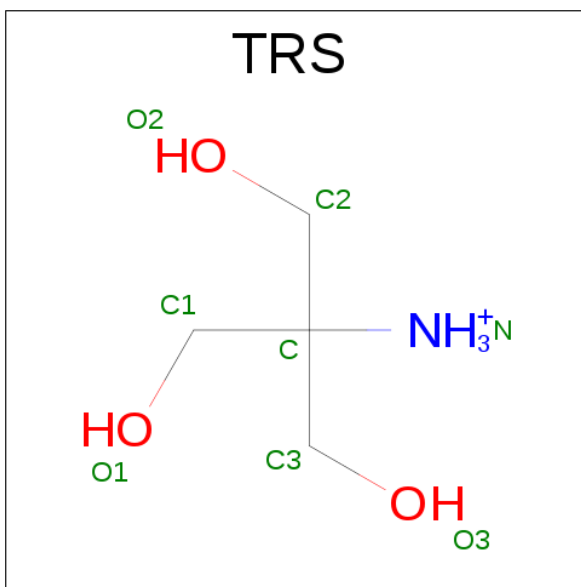
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Chain	Residue	Modelled	Actual	Comment	Reference
E	161	ALA	GLU	engineered mutation	UNP P31947
F	-2	GLY	-	expression tag	UNP P31947
F	-1	PRO	-	expression tag	UNP P31947
F	0	HIS	-	expression tag	UNP P31947
F	159	ALA	LYS	engineered mutation	UNP P31947
F	160	ALA	LYS	engineered mutation	UNP P31947
F	161	ALA	GLU	engineered mutation	UNP P31947
I	-2	GLY	-	expression tag	UNP P31947
I	-1	PRO	-	expression tag	UNP P31947
I	0	HIS	-	expression tag	UNP P31947
I	159	ALA	LYS	engineered mutation	UNP P31947
I	160	ALA	LYS	engineered mutation	UNP P31947
I	161	ALA	GLU	engineered mutation	UNP P31947
J	-2	GLY	-	expression tag	UNP P31947
J	-1	PRO	-	expression tag	UNP P31947
J	0	HIS	-	expression tag	UNP P31947
J	159	ALA	LYS	engineered mutation	UNP P31947
J	160	ALA	LYS	engineered mutation	UNP P31947
J	161	ALA	GLU	engineered mutation	UNP P31947

- Molecule 2 is a protein called Heat shock protein beta-6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	113	Total	C	N	O	P	S	0	0	0
			890	565	163	160	1	1			
2	D	98	Total	C	N	O	P	S	0	0	0
			769	488	141	138	1	1			
2	G	118	Total	C	N	O	P	S	0	0	0
			920	584	168	166	1	1			
2	H	98	Total	C	N	O	P	S	0	0	0
			769	488	141	138	1	1			
2	K	114	Total	C	N	O	P	S	0	0	0
			897	569	164	162	1	1			
2	L	100	Total	C	N	O	P	S	0	0	0
			784	497	143	142	1	1			

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		
3	E	1	Total	C	N	O	0	0
			8	4	1	3		
3	F	1	Total	C	N	O	0	0
			8	4	1	3		
3	I	1	Total	C	N	O	0	0
			8	4	1	3		
3	J	1	Total	C	N	O	0	0
			8	4	1	3		

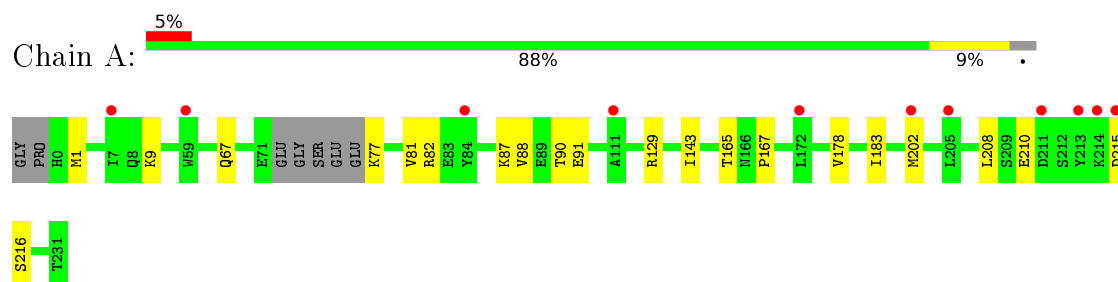
- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Ni	0	0
			1	1		
4	L	1	Total	Ni	0	0
			1	1		
4	D	1	Total	Ni	0	0
			1	1		

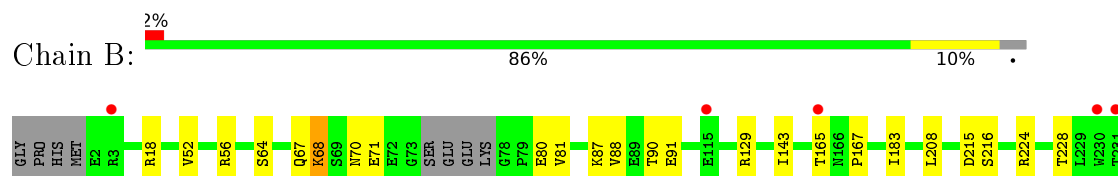
### 3 Residue-property plots [i](#)

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

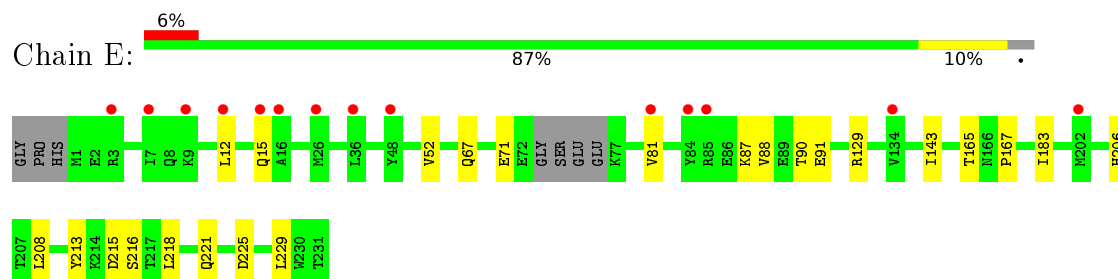
- Molecule 1: 14-3-3 protein sigma



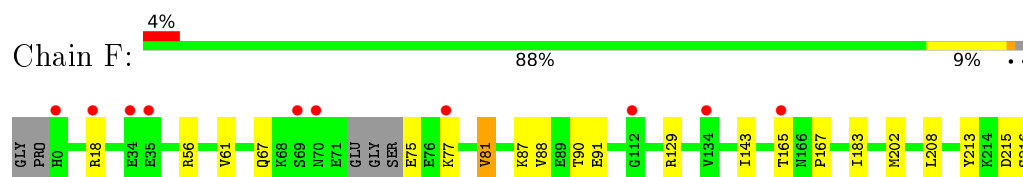
- Molecule 1: 14-3-3 protein sigma



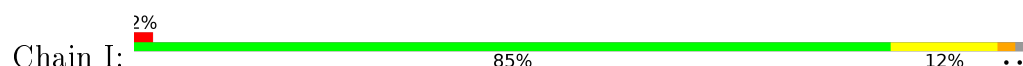
- Molecule 1: 14-3-3 protein sigma

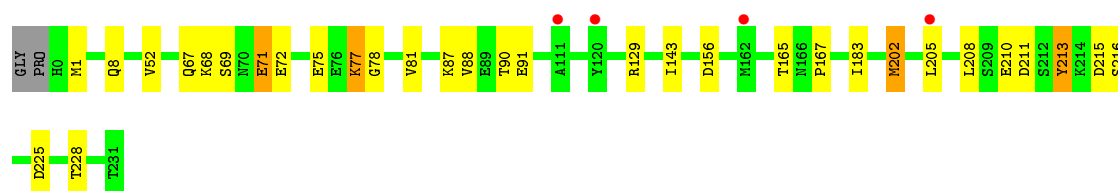


- Molecule 1: 14-3-3 protein sigma

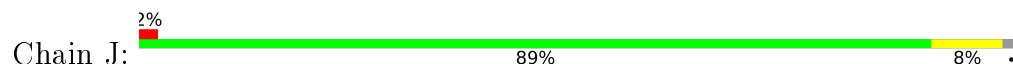


- Molecule 1: 14-3-3 protein sigma





- Molecule 1: 14-3-3 protein sigma



- Molecule 2: Heat shock protein beta-6



- Molecule 2: Heat shock protein beta-6



- Molecule 2: Heat shock protein beta-6



- Molecule 2: Heat shock protein beta-6







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.06Å 341.29Å 144.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.17 – 4.50 47.62 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.17-4.50) 99.7 (47.62-4.50)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 4.45Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.236 , 0.256 0.263 , 0.279	Depositor DCC
$R_{free}$ test set	933 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	227.4	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 68.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	15884	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, TRS, SEP

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	0.41	0/1817	0.63	0/2445
1	B	0.42	0/1802	0.66	1/2426 (0.0%)
1	E	0.41	0/1815	0.64	0/2442
1	F	0.42	0/1835	0.66	0/2469
1	I	0.43	0/1855	0.67	0/2497
1	J	0.42	0/1835	0.65	0/2469
2	C	0.42	0/905	0.71	1/1229 (0.1%)
2	D	0.39	0/782	0.70	0/1066
2	G	0.48	0/937	0.74	0/1275
2	H	0.40	0/782	0.65	0/1066
2	K	0.45	0/912	0.72	0/1239
2	L	0.40	0/798	0.69	0/1089
All	All	0.42	0/16075	0.67	2/21712 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	ASN	C-N-CA	5.82	136.24	121.70
2	C	31	GLN	C-N-CA	5.67	135.87	121.70

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	1791	0	1769	24	0
1	B	1777	0	1746	23	0
1	E	1790	0	1768	24	0
1	F	1809	0	1781	23	0
1	I	1828	0	1796	34	0
1	J	1809	0	1781	11	0
2	C	890	0	867	23	0
2	D	769	0	753	23	0
2	G	920	0	899	43	0
2	H	769	0	753	37	0
2	K	897	0	874	16	0
2	L	784	0	764	13	0
3	A	8	0	12	1	0
3	B	8	0	12	1	0
3	E	8	0	12	1	0
3	F	8	0	12	1	0
3	I	8	0	12	1	0
3	J	8	0	12	1	0
4	D	1	0	0	0	0
4	H	1	0	0	0	0
4	L	1	0	0	0	0
All	All	15884	0	15623	214	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (214) 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:F:202:MET:SD	2:G:107:PRO:HD2	1.86	1.14
1:E:165:THR:HB	1:E:208:LEU:HD11	1.31	1.09
1:A:165:THR:HB	1:A:208:LEU:HD11	1.31	1.08
1:J:228:THR:HG21	2:K:85:PRO:HG2	1.38	1.05
1:F:165:THR:HB	1:F:208:LEU:HD11	1.34	1.05
1:I:165:THR:HB	1:I:208:LEU:HD11	1.35	1.04
1:B:165:THR:HB	1:B:208:LEU:HD11	1.34	1.03
2:C:111:GLY:HA3	2:D:120:ARG:O	1.66	0.96
2:H:112:PHE:HZ	1:I:156:ASP:HA	1.30	0.96
1:I:225:ASP:HB3	2:L:12:LEU:HD22	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:73:HIS:HB2	2:G:146:ALA:O	1.79	0.82
2:L:73:HIS:HB2	2:L:146:ALA:O	1.87	0.75
1:A:202:MET:SD	1:I:205:LEU:HD12	2.26	0.74
1:E:165:THR:O	1:E:216:SER:OG	2.06	0.73
2:H:112:PHE:CZ	1:I:156:ASP:HA	2.21	0.73
2:G:11:TRP:HE3	2:G:138:PRO:HB3	1.53	0.73
2:G:111:GLY:HA3	2:H:120:ARG:O	1.88	0.72
2:K:31:GLN:HE22	2:L:115:ARG:HE	1.35	0.72
1:A:165:THR:O	1:A:216:SER:OG	2.08	0.72
2:C:113:VAL:HA	2:D:118:HIS:O	1.90	0.71
2:G:1:MET:O	2:G:93:VAL:HA	1.89	0.71
1:A:167:PRO:HG3	1:A:215:ASP:HB2	1.73	0.70
1:B:165:THR:O	1:B:216:SER:OG	2.09	0.70
1:E:165:THR:OG1	1:E:208:LEU:HD21	1.92	0.70
1:E:167:PRO:HG3	1:E:215:ASP:HB2	1.74	0.69
1:I:165:THR:O	1:I:216:SER:OG	2.09	0.69
1:B:167:PRO:HG3	1:B:215:ASP:HB2	1.75	0.69
2:G:28:LEU:HD21	2:H:119:ARG:NH1	2.08	0.69
1:A:165:THR:OG1	1:A:208:LEU:HD21	1.92	0.69
1:I:167:PRO:HG3	1:I:215:ASP:HB2	1.74	0.68
1:F:165:THR:OG1	1:F:208:LEU:HD21	1.94	0.68
1:A:167:PRO:HB3	1:A:215:ASP:HB3	1.76	0.67
2:D:8:GLN:O	2:H:135:ALA:HA	1.94	0.67
1:B:165:THR:OG1	1:B:208:LEU:HD21	1.94	0.67
1:I:165:THR:OG1	1:I:208:LEU:HD21	1.95	0.67
1:B:167:PRO:HB3	1:B:215:ASP:HB3	1.76	0.67
2:C:120:ARG:O	2:D:111:GLY:HA3	1.94	0.67
1:F:165:THR:O	1:F:216:SER:OG	2.10	0.66
2:G:119:ARG:HG2	2:H:113:VAL:HG23	1.78	0.66
1:I:167:PRO:HB3	1:I:215:ASP:HB3	1.77	0.66
1:E:167:PRO:HB3	1:E:215:ASP:HB3	1.77	0.66
1:I:69:SER:HB2	1:I:75:GLU:HB2	1.78	0.65
1:F:167:PRO:HB3	1:F:215:ASP:HB3	1.78	0.65
1:B:224:ARG:CZ	2:C:86:GLU:OE2	2.44	0.65
2:D:1:MET:N	2:H:91:LYS:HD2	2.12	0.65
2:C:118:HIS:O	2:D:113:VAL:HA	1.98	0.64
2:G:113:VAL:HA	2:H:118:HIS:O	1.98	0.63
1:A:210:GLU:HB2	1:I:210:GLU:OE1	1.98	0.63
1:F:167:PRO:HG3	1:F:215:ASP:HB2	1.79	0.62
1:B:224:ARG:HH22	2:C:86:GLU:HG3	1.64	0.62
1:B:228:THR:HG21	2:C:85:PRO:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:MET:SD	2:G:107:PRO:CD	2.77	0.61
2:K:2:GLU:HA	2:K:92:VAL:O	2.01	0.61
2:G:29:PHE:HD2	2:H:82:HIS:HE2	1.47	0.61
2:G:11:TRP:CZ2	2:G:15:ALA:HB2	2.35	0.61
2:G:31:GLN:HG2	2:G:119:ARG:HD2	1.83	0.61
1:A:165:THR:CB	1:A:208:LEU:HD11	2.21	0.61
2:G:121:TYR:HE1	2:H:110:HIS:HB3	1.64	0.61
2:G:30:ASP:HB2	2:G:31:GLN:NE2	2.16	0.61
1:A:167:PRO:CG	1:A:215:ASP:CB	2.80	0.59
2:G:10:SER:HB2	2:G:137:SER:HA	1.82	0.59
1:I:68:LYS:O	1:I:71:GLU:HG3	2.03	0.59
1:I:228:THR:HG22	2:L:9:PRO:HG3	1.85	0.59
1:I:210:GLU:HA	1:I:213:TYR:HD2	1.66	0.59
1:E:229:LEU:HD13	2:H:12:LEU:HB3	1.85	0.59
1:B:56:ARG:HH22	2:C:14:ARG:HH22	1.49	0.58
1:E:91:GLU:CD	1:F:18:ARG:HH22	2.06	0.58
1:B:224:ARG:NH2	2:C:86:GLU:HG3	2.19	0.58
1:E:167:PRO:CG	1:E:215:ASP:CB	2.81	0.58
2:H:112:PHE:HZ	1:I:156:ASP:CA	2.09	0.57
2:C:110:HIS:HB3	2:D:121:TYR:CD1	2.39	0.57
2:G:33:PHE:HB3	2:H:110:HIS:CE1	2.40	0.57
2:L:71:PRO:HD2	2:L:73:HIS:CE1	2.39	0.57
1:B:167:PRO:CG	1:B:215:ASP:CB	2.82	0.57
1:I:91:GLU:CD	1:J:18:ARG:HH22	2.08	0.57
2:G:27:ARG:HG3	2:G:28:LEU:H	1.70	0.56
2:G:33:PHE:HB3	2:H:110:HIS:NE2	2.20	0.56
2:K:33:PHE:HD2	2:K:77:LEU:HB2	1.70	0.56
1:A:167:PRO:HG3	1:A:215:ASP:CB	2.36	0.56
1:E:165:THR:CB	1:E:208:LEU:HD11	2.21	0.56
1:I:143:ILE:HD11	3:I:501:TRS:O3	2.06	0.56
1:B:143:ILE:HD11	3:B:501:TRS:O3	2.06	0.55
1:I:225:ASP:CB	2:L:12:LEU:HD22	2.32	0.55
2:H:112:PHE:CE2	1:I:156:ASP:CG	2.80	0.55
1:I:167:PRO:CG	1:I:215:ASP:HB2	2.37	0.55
1:A:143:ILE:HD11	3:A:501:TRS:O3	2.07	0.55
2:G:121:TYR:HE1	2:H:110:HIS:CB	2.20	0.55
1:E:143:ILE:HD11	3:E:501:TRS:O3	2.07	0.54
1:E:167:PRO:HG3	1:E:215:ASP:CB	2.37	0.54
1:A:167:PRO:CB	1:A:215:ASP:HB3	2.37	0.54
1:A:167:PRO:CG	1:A:215:ASP:HB2	2.37	0.54
1:E:167:PRO:CG	1:E:215:ASP:HB2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:167:PRO:CG	1:I:215:ASP:CB	2.86	0.54
1:B:167:PRO:CG	1:B:215:ASP:HB2	2.38	0.53
1:F:143:ILE:HD11	3:F:501:TRS:O3	2.08	0.53
1:B:167:PRO:HG3	1:B:215:ASP:CB	2.39	0.53
1:B:167:PRO:CB	1:B:215:ASP:HB3	2.38	0.53
1:F:224:ARG:HD2	2:G:86:GLU:OE2	2.09	0.53
2:G:92:VAL:HG11	2:G:129:PRO:HB3	1.92	0.52
2:G:13:ARG:O	2:G:14:ARG:HB3	2.10	0.52
1:E:167:PRO:CB	1:E:215:ASP:HB3	2.38	0.52
1:J:143:ILE:HD11	3:J:501:TRS:O3	2.09	0.51
1:F:167:PRO:CG	1:F:215:ASP:CB	2.88	0.51
1:I:88:VAL:O	1:I:91:GLU:N	2.43	0.51
1:A:91:GLU:CD	1:B:18:ARG:HH22	2.13	0.51
2:G:119:ARG:CG	2:H:113:VAL:HG23	2.40	0.51
2:H:92:VAL:HG11	2:H:129:PRO:HB3	1.92	0.51
1:B:64:SER:O	1:B:68:LYS:HD2	2.10	0.51
2:C:110:HIS:CB	2:D:121:TYR:CE1	2.94	0.51
1:J:165:THR:HB	1:J:208:LEU:HD11	1.93	0.51
2:K:92:VAL:HG11	2:K:129:PRO:HB3	1.91	0.51
1:E:87:LYS:O	1:E:90:THR:HB	2.11	0.51
2:G:120:ARG:O	2:H:111:GLY:HA3	2.11	0.51
1:B:87:LYS:O	1:B:90:THR:HB	2.11	0.51
1:F:87:LYS:O	1:F:90:THR:HB	2.11	0.51
1:A:88:VAL:O	1:A:91:GLU:N	2.44	0.50
1:J:88:VAL:O	1:J:91:GLU:N	2.44	0.50
1:I:167:PRO:CB	1:I:215:ASP:HB3	2.41	0.50
1:B:88:VAL:O	1:B:91:GLU:N	2.44	0.50
2:D:92:VAL:HG11	2:D:129:PRO:HB3	1.93	0.50
1:I:167:PRO:HG3	1:I:215:ASP:CB	2.42	0.50
1:J:87:LYS:O	1:J:90:THR:HB	2.11	0.50
1:E:88:VAL:O	1:E:91:GLU:N	2.44	0.50
2:G:31:GLN:HG2	2:G:119:ARG:HH11	1.76	0.50
2:L:92:VAL:HG11	2:L:129:PRO:HB3	1.93	0.50
1:A:87:LYS:O	1:A:90:THR:HB	2.12	0.49
1:F:165:THR:CB	1:F:208:LEU:HD11	2.25	0.49
2:G:1:MET:HB3	2:G:3:ILE:HD11	1.93	0.49
1:F:88:VAL:O	1:F:91:GLU:N	2.45	0.49
2:G:27:ARG:HG3	2:G:28:LEU:N	2.27	0.49
2:G:120:ARG:HB3	2:H:112:PHE:HB2	1.93	0.49
1:F:167:PRO:CG	1:F:215:ASP:HB2	2.42	0.49
1:A:167:PRO:CG	1:A:215:ASP:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:92:VAL:HG11	2:C:129:PRO:HB3	1.94	0.48
1:J:178:VAL:HG13	2:K:14:ARG:HD2	1.94	0.48
2:G:119:ARG:HG2	2:H:113:VAL:CG2	2.42	0.48
1:F:213:TYR:OH	2:G:108:ASP:HA	2.13	0.48
2:G:1:MET:HB2	2:G:94:GLY:H	1.79	0.48
1:A:77:LYS:HZ1	1:A:82:ARG:HB2	1.79	0.48
2:C:110:HIS:HB3	2:D:121:TYR:CE1	2.48	0.48
2:L:91:LYS:HE2	2:L:100:HIS:CD2	2.49	0.48
1:I:87:LYS:O	1:I:90:THR:HB	2.13	0.48
2:K:91:LYS:HE2	2:K:100:HIS:CD2	2.49	0.48
1:E:229:LEU:HB2	2:H:12:LEU:HD22	1.96	0.47
2:K:85:PRO:HG3	2:K:136:LEU:HD23	1.96	0.47
2:G:91:LYS:HE2	2:G:100:HIS:CD2	2.49	0.47
2:H:91:LYS:HE2	2:H:100:HIS:CD2	2.49	0.47
2:C:91:LYS:HE2	2:C:100:HIS:CD2	2.49	0.47
2:D:1:MET:H3	2:H:91:LYS:HD2	1.77	0.47
2:G:121:TYR:CE1	2:H:110:HIS:HB3	2.48	0.47
1:E:167:PRO:CG	1:E:215:ASP:HB3	2.44	0.47
2:H:112:PHE:HE2	1:I:156:ASP:CG	2.17	0.47
2:K:33:PHE:HB3	2:L:110:HIS:NE2	2.30	0.47
1:E:15:GLN:O	1:F:61:VAL:HG11	2.14	0.47
2:C:38:LEU:HD22	2:C:38:LEU:H	1.80	0.47
1:A:202:MET:HG2	1:I:202:MET:HB3	1.97	0.47
1:F:167:PRO:HG3	1:F:215:ASP:CB	2.44	0.47
1:A:178:VAL:HG13	2:D:14:ARG:HD2	1.96	0.47
2:D:91:LYS:HE2	2:D:100:HIS:CD2	2.49	0.47
1:B:167:PRO:CG	1:B:215:ASP:HB3	2.46	0.46
1:A:129:ARG:HG3	1:A:183:ILE:HG13	1.98	0.46
2:D:9:PRO:HB2	2:D:11:TRP:HD1	1.81	0.46
2:G:31:GLN:N	2:G:31:GLN:CD	2.69	0.46
2:K:113:VAL:HG23	2:L:119:ARG:HG2	1.98	0.46
1:A:77:LYS:NZ	1:A:82:ARG:HB2	2.31	0.46
1:E:12:LEU:HD22	1:F:81:VAL:HG13	1.97	0.46
2:C:110:HIS:CB	2:D:121:TYR:HE1	2.30	0.45
1:F:167:PRO:CB	1:F:215:ASP:HB3	2.43	0.45
2:G:33:PHE:HB2	2:G:77:LEU:O	2.16	0.45
2:C:119:ARG:HG2	2:D:113:VAL:HG23	1.97	0.45
2:C:112:PHE:CD2	2:D:120:ARG:NH2	2.83	0.45
2:C:121:TYR:HE1	2:D:110:HIS:HB3	1.82	0.45
2:G:31:GLN:HB3	2:G:79:ASP:O	2.17	0.45
2:G:29:PHE:HB3	2:H:81:LYS:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:33:PHE:HB3	2:L:110:HIS:CE1	2.51	0.44
2:H:112:PHE:CE2	1:I:156:ASP:OD1	2.70	0.44
2:H:85:PRO:HG3	2:H:136:LEU:HD23	1.99	0.44
1:E:129:ARG:HG3	1:E:183:ILE:HG13	2.00	0.44
2:G:85:PRO:HG3	2:G:136:LEU:HD23	1.99	0.44
1:B:224:ARG:NH2	2:C:86:GLU:CG	2.81	0.44
1:I:129:ARG:HG3	1:I:183:ILE:HG13	2.00	0.43
2:K:121:TYR:HE1	2:L:110:HIS:HB3	1.83	0.43
1:E:218:LEU:O	1:E:221:GLN:HB2	2.19	0.43
2:L:85:PRO:HG3	2:L:136:LEU:HD23	1.99	0.43
2:C:85:PRO:HG3	2:C:136:LEU:HD23	2.01	0.43
1:I:210:GLU:OE2	1:I:213:TYR:HE2	2.01	0.43
1:B:129:ARG:HG3	1:B:183:ILE:HG13	2.00	0.43
1:F:129:ARG:HG3	1:F:183:ILE:HG13	2.00	0.43
2:G:118:HIS:O	2:H:113:VAL:HA	2.18	0.43
1:E:15:GLN:C	1:F:61:VAL:HG11	2.39	0.43
1:E:225:ASP:HB3	2:H:12:LEU:HD21	2.00	0.43
1:I:77:LYS:HA	1:I:78:GLY:HA3	1.77	0.42
2:D:85:PRO:HG3	2:D:136:LEU:HD23	2.00	0.42
1:F:56:ARG:NH2	2:G:14:ARG:HH22	2.17	0.42
2:D:19:LEU:HG	2:D:19:LEU:H	1.50	0.42
1:I:8:GLN:NE2	1:J:77:LYS:HD2	2.35	0.42
1:J:129:ARG:HG3	1:J:183:ILE:HG13	2.00	0.42
1:A:9:LYS:HG3	1:B:80:GLU:HB3	2.01	0.41
2:G:30:ASP:HB2	2:G:31:GLN:HE22	1.84	0.41
2:G:110:HIS:HB3	2:H:121:TYR:CE1	2.56	0.41
2:D:135:ALA:HA	2:H:8:GLN:O	2.19	0.41
2:C:31:GLN:HB3	2:C:79:ASP:O	2.20	0.41
2:H:112:PHE:CZ	1:I:156:ASP:OD1	2.73	0.41
2:H:123:LEU:HD23	2:H:123:LEU:HA	1.94	0.41
2:K:26:GLY:HA3	2:K:32:ARG:HH22	1.84	0.41
2:K:71:PRO:HA	2:K:72:GLY:HA2	1.73	0.41
1:J:220:MET:HA	1:J:223:LEU:HD12	2.02	0.41
2:K:31:GLN:CB	2:K:79:ASP:O	2.68	0.41
1:E:229:LEU:HD12	2:H:8:GLN:HG2	2.03	0.41
1:J:229:LEU:HD21	2:K:13:ARG:O	2.21	0.41
1:A:210:GLU:OE1	1:I:210:GLU:OE1	2.39	0.40
2:C:110:HIS:HB2	2:D:121:TYR:CE1	2.56	0.40
2:D:9:PRO:HB2	2:D:11:TRP:CD1	2.57	0.40
2:G:112:PHE:HB2	2:H:120:ARG:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	223/234 (95%)	215 (96%)	8 (4%)	0	100	100
1	B	222/234 (95%)	213 (96%)	9 (4%)	0	100	100
1	E	223/234 (95%)	214 (96%)	9 (4%)	0	100	100
1	F	225/234 (96%)	216 (96%)	8 (4%)	1 (0%)	39	80
1	I	230/234 (98%)	218 (95%)	11 (5%)	1 (0%)	39	80
1	J	225/234 (96%)	216 (96%)	8 (4%)	1 (0%)	39	80
2	C	106/149 (71%)	96 (91%)	7 (7%)	3 (3%)	6	46
2	D	93/149 (62%)	86 (92%)	6 (6%)	1 (1%)	17	64
2	G	113/149 (76%)	97 (86%)	10 (9%)	6 (5%)	2	30
2	H	93/149 (62%)	85 (91%)	8 (9%)	0	100	100
2	K	107/149 (72%)	93 (87%)	11 (10%)	3 (3%)	6	46
2	L	95/149 (64%)	87 (92%)	8 (8%)	0	100	100
All	All	1955/2298 (85%)	1836 (94%)	103 (5%)	16 (1%)	24	70

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	13	ARG
2	C	32	ARG
2	G	32	ARG
1	I	72	GLU
2	K	13	ARG
2	G	14	ARG
2	G	22	LEU
2	G	35	GLU
1	J	77	LYS
2	G	13	ARG
2	G	71	PRO
2	K	14	ARG

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Mol	Chain	Res	Type
2	C	14	ARG
2	D	14	ARG
1	F	77	LYS
2	K	35	GLU

### 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	190/195 (97%)	187 (98%)	3 (2%)	70	88
1	B	188/195 (96%)	183 (97%)	5 (3%)	52	80
1	E	190/195 (97%)	184 (97%)	6 (3%)	46	77
1	F	192/195 (98%)	188 (98%)	4 (2%)	61	85
1	I	194/195 (100%)	185 (95%)	9 (5%)	33	70
1	J	192/195 (98%)	187 (97%)	5 (3%)	54	81
2	C	93/120 (78%)	81 (87%)	12 (13%)	5	30
2	D	81/120 (68%)	75 (93%)	6 (7%)	17	56
2	G	96/120 (80%)	82 (85%)	14 (15%)	4	26
2	H	81/120 (68%)	74 (91%)	7 (9%)	13	49
2	K	94/120 (78%)	78 (83%)	16 (17%)	2	19
2	L	83/120 (69%)	76 (92%)	7 (8%)	14	51
All	All	1674/1890 (89%)	1580 (94%)	94 (6%)	26	65

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	67	GLN
1	A	81	VAL
1	B	52	VAL
1	B	67	GLN
1	B	68	LYS

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Mol	Chain	Res	Type
1	B	71	GLU
1	B	81	VAL
2	C	1	MET
2	C	8	GLN
2	C	14	ARG
2	C	27	ARG
2	C	31	GLN
2	C	32	ARG
2	C	33	PHE
2	C	35	GLU
2	C	70	ASP
2	C	104	GLU
2	C	122	ARG
2	C	123	LEU
2	D	12	LEU
2	D	13	ARG
2	D	19	LEU
2	D	104	GLU
2	D	122	ARG
2	D	123	LEU
1	E	52	VAL
1	E	67	GLN
1	E	71	GLU
1	E	81	VAL
1	E	206	HIS
1	E	213	TYR
1	F	67	GLN
1	F	75	GLU
1	F	81	VAL
1	F	224	ARG
2	G	2	GLU
2	G	3	ILE
2	G	8	GLN
2	G	13	ARG
2	G	14	ARG
2	G	25	PRO
2	G	28	LEU
2	G	31	GLN
2	G	33	PHE
2	G	37	LEU
2	G	38	LEU
2	G	104	GLU

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Mol	Chain	Res	Type
2	G	122	ARG
2	G	123	LEU
2	H	3	ILE
2	H	8	GLN
2	H	12	LEU
2	H	14	ARG
2	H	104	GLU
2	H	122	ARG
2	H	123	LEU
1	I	1	MET
1	I	52	VAL
1	I	67	GLN
1	I	71	GLU
1	I	77	LYS
1	I	81	VAL
1	I	202	MET
1	I	211	ASP
1	I	213	TYR
1	J	1	MET
1	J	67	GLN
1	J	68	LYS
1	J	77	LYS
1	J	81	VAL
2	K	1	MET
2	K	2	GLU
2	K	3	ILE
2	K	8	GLN
2	K	10	SER
2	K	11	TRP
2	K	12	LEU
2	K	14	ARG
2	K	28	LEU
2	K	30	ASP
2	K	32	ARG
2	K	33	PHE
2	K	69	THR
2	K	104	GLU
2	K	122	ARG
2	K	123	LEU
2	L	12	LEU
2	L	13	ARG
2	L	14	ARG

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Mol	Chain	Res	Type
2	L	70	ASP
2	L	104	GLU
2	L	122	ARG
2	L	123	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	8	GLN
1	I	8	GLN
1	I	152	GLN
2	K	31	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SEP	C	16	2	7,9,10	0.96	0	8,12,14	2.33	4 (50%)
2	SEP	D	16	2	7,9,10	0.71	0	8,12,14	3.64	3 (37%)
2	SEP	G	16	2	7,9,10	1.17	1 (14%)	8,12,14	1.68	2 (25%)
2	SEP	H	16	2	7,9,10	0.87	0	8,12,14	2.33	4 (50%)
2	SEP	K	16	2	7,9,10	1.11	1 (14%)	8,12,14	2.01	3 (37%)
2	SEP	L	16	2	7,9,10	0.83	0	8,12,14	2.24	5 (62%)

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	SEP	C	16	2	-	0/5/8/10	0/0/0/0
2	SEP	D	16	2	-	0/5/8/10	0/0/0/0
2	SEP	G	16	2	-	0/5/8/10	0/0/0/0
2	SEP	H	16	2	-	0/5/8/10	0/0/0/0
2	SEP	K	16	2	-	0/5/8/10	0/0/0/0
2	SEP	L	16	2	-	0/5/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	16	SEP	P-OG	-2.63	1.52	1.59
2	K	16	SEP	P-OG	-2.58	1.52	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	16	SEP	O-C-CA	-2.75	118.34	125.72
2	C	16	SEP	O-C-CA	-2.69	118.52	125.72
2	H	16	SEP	O2P-P-O1P	-2.63	102.05	110.63
2	L	16	SEP	O-C-CA	-2.52	118.97	125.72
2	C	16	SEP	O2P-P-O1P	-2.47	102.57	110.63
2	H	16	SEP	O-C-CA	-2.44	119.17	125.72
2	G	16	SEP	O-C-CA	-2.32	119.50	125.72
2	K	16	SEP	O-C-CA	-2.31	119.54	125.72
2	L	16	SEP	O2P-P-O1P	-2.08	103.83	110.63
2	L	16	SEP	O2P-P-OG	2.16	113.04	106.72
2	L	16	SEP	O3P-P-OG	2.39	113.69	106.72
2	K	16	SEP	OG-P-O1P	2.48	113.33	107.08
2	H	16	SEP	O3P-P-OG	2.60	114.31	106.72
2	C	16	SEP	OG-P-O1P	2.65	113.74	107.08
2	D	16	SEP	O2P-P-OG	2.85	115.04	106.72
2	G	16	SEP	OG-CB-CA	3.05	110.92	108.26
2	K	16	SEP	OG-CB-CA	3.39	111.21	108.26
2	L	16	SEP	OG-CB-CA	4.00	111.75	108.26
2	H	16	SEP	OG-CB-CA	4.26	111.97	108.26
2	C	16	SEP	OG-CB-CA	4.30	112.01	108.26
2	D	16	SEP	OG-CB-CA	9.34	116.40	108.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	TRS	A	501	-	7,7,7	0.36	0	9,9,9	0.44	0
3	TRS	B	501	-	7,7,7	0.34	0	9,9,9	0.45	0
3	TRS	E	501	-	7,7,7	0.37	0	9,9,9	0.45	0
3	TRS	F	501	-	7,7,7	0.33	0	9,9,9	0.44	0
3	TRS	I	501	-	7,7,7	0.40	0	9,9,9	0.49	0
3	TRS	J	501	-	7,7,7	0.35	0	9,9,9	0.48	0

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
3	TRS	A	501	-	-	0/9/9/9	0/0/0/0
3	TRS	B	501	-	-	0/9/9/9	0/0/0/0
3	TRS	E	501	-	-	0/9/9/9	0/0/0/0
3	TRS	F	501	-	-	0/9/9/9	0/0/0/0
3	TRS	I	501	-	-	0/9/9/9	0/0/0/0
3	TRS	J	501	-	-	0/9/9/9	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	TRS	1	0
3	B	501	TRS	1	0
3	E	501	TRS	1	0
3	F	501	TRS	1	0
3	I	501	TRS	1	0
3	J	501	TRS	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	227/234 (97%)	0.35	11 (4%) 34 26	71, 93, 120, 135	0
1	B	226/234 (96%)	0.16	5 (2%) 65 56	79, 121, 176, 214	0
1	E	227/234 (97%)	0.38	14 (6%) 24 17	59, 90, 118, 150	0
1	F	229/234 (97%)	0.40	10 (4%) 38 29	62, 91, 119, 161	0
1	I	232/234 (99%)	0.28	4 (1%) 73 64	21, 48, 69, 84	0
1	J	229/234 (97%)	0.29	5 (2%) 65 56	38, 72, 95, 104	0
2	C	112/149 (75%)	0.36	4 (3%) 46 37	79, 112, 220, 262	0
2	D	97/149 (65%)	0.64	15 (15%) 3 4	69, 89, 143, 201	0
2	G	117/149 (78%)	0.28	5 (4%) 39 30	46, 67, 105, 131	0
2	H	97/149 (65%)	0.45	7 (7%) 18 14	49, 78, 133, 160	0
2	K	113/149 (75%)	0.60	9 (7%) 15 12	50, 80, 149, 190	0
2	L	99/149 (66%)	0.43	5 (5%) 32 25	34, 64, 104, 109	0
All	All	2005/2298 (87%)	0.36	94 (4%) 35 28	21, 85, 140, 262	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	69	SER	4.5
2	D	74	PHE	4.4
2	H	72	GLY	4.2
2	D	78	LEU	3.9
1	E	81	VAL	3.8
1	F	165	THR	3.6
2	D	73	HIS	3.6
2	H	119	ARG	3.5
1	E	84	TYR	3.4
1	B	231	THR	3.3
1	E	12	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	205	LEU	3.2
1	E	26	MET	3.2
1	A	213	TYR	3.1
2	K	149	ALA	3.0
1	E	16	ALA	3.0
2	H	148	PRO	3.0
2	D	79	ASP	3.0
2	G	30	ASP	3.0
2	K	74	PHE	2.9
1	F	35	GLU	2.9
2	G	74	PHE	2.9
1	A	84	TYR	2.9
1	F	134	VAL	2.8
1	B	165	THR	2.8
1	E	15	GLN	2.8
2	C	123	LEU	2.8
2	K	115	ARG	2.8
1	I	111	ALA	2.8
2	L	88	ILE	2.8
2	C	97	VAL	2.7
1	A	205	LEU	2.7
2	H	74	PHE	2.7
1	A	215	ASP	2.7
2	D	146	ALA	2.7
1	A	214	LYS	2.6
2	D	115	ARG	2.6
1	J	165	THR	2.6
2	K	107	PRO	2.6
2	D	20	PRO	2.6
1	J	110	GLU	2.6
1	J	0	HIS	2.6
1	E	36	LEU	2.5
2	K	123	LEU	2.5
2	K	83	PHE	2.5
2	K	82	HIS	2.5
1	A	7	ILE	2.5
1	F	77	LYS	2.5
1	I	162	MET	2.4
2	D	144	ILE	2.4
1	A	59	TRP	2.4
2	C	74	PHE	2.4
2	D	148	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	G	147	ALA	2.4
1	F	0	HIS	2.3
2	L	92	VAL	2.3
2	D	99	VAL	2.3
2	D	77	LEU	2.3
2	H	77	LEU	2.3
1	F	112	GLY	2.3
1	A	111	ALA	2.3
1	A	211	ASP	2.3
2	D	94	GLY	2.3
2	D	88	ILE	2.3
2	D	1	MET	2.3
1	E	7	ILE	2.3
2	H	78	LEU	2.2
1	A	202	MET	2.2
2	L	119	ARG	2.2
1	E	3	ARG	2.2
1	E	85	ARG	2.2
1	E	202	MET	2.2
2	D	92	VAL	2.2
2	L	85	PRO	2.2
1	I	120	TYR	2.2
1	F	70	ASN	2.2
2	C	90	VAL	2.1
1	A	172	LEU	2.1
1	E	9	LYS	2.1
2	G	7	VAL	2.1
2	K	31	GLN	2.1
2	G	148	PRO	2.1
1	F	18	ARG	2.1
1	F	34	GLU	2.1
1	B	230	TRP	2.1
2	K	32	ARG	2.1
1	B	115	GLU	2.1
1	J	121	LEU	2.1
2	L	99	VAL	2.0
1	B	3	ARG	2.0
1	E	134	VAL	2.0
1	E	48	TYR	2.0
1	J	108	ILE	2.0
2	H	121	TYR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SEP	H	16	10/11	0.77	0.31	-	65,67,68,69	0
2	SEP	L	16	10/11	0.79	0.26	-	24,28,34,35	0
2	SEP	K	16	10/11	0.75	0.31	-	53,56,58,58	0
2	SEP	D	16	10/11	0.73	0.26	-	71,72,73,74	0
2	SEP	G	16	10/11	0.67	0.32	-	64,65,67,67	0
2	SEP	C	16	10/11	0.82	0.27	-	93,97,99,99	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NI	H	201	1/1	-0.06	0.34	0.23	60,60,60,60	0
4	NI	D	201	1/1	0.54	0.16	-1.35	60,60,60,60	0
4	NI	L	201	1/1	0.89	0.20	-	60,60,60,60	0
3	TRS	F	501	8/8	0.03	1.10	-	99,101,102,106	0
3	TRS	J	501	8/8	0.12	1.05	-	68,71,73,73	0
3	TRS	I	501	8/8	0.74	0.47	-	43,45,45,48	0
3	TRS	E	501	8/8	0.11	0.76	-	99,103,105,109	0
3	TRS	B	501	8/8	0.25	0.79	-	116,119,122,122	0
3	TRS	A	501	8/8	0.29	0.97	-	100,103,104,108	0

## 6.5 Other polymers

There are no such residues in this entry.