Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 07:17 AM BST

PDB ID	:	5NJK
Title	:	PTB domain of human Numb isoform-1
Authors	:	Mapelli, M.; Di Fiore, P.P.
Deposited on	:	2017-03-29
Resolution	:	3.13 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

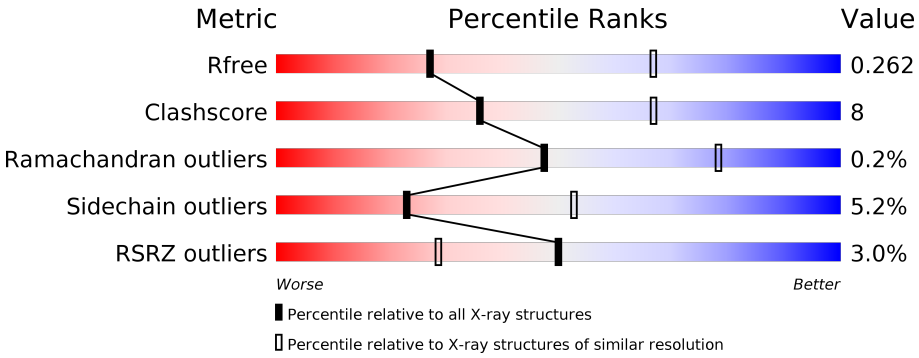
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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}	130704	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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% 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	156	68% 24% • 6%
1	B	156	2% 74% 18% •• 7%
1	C	156	10% 77% 8% • 15%
1	D	156	72% 14% • 13%
1	E	156	% 71% 13% • 15%
1	F	156	% 65% 22% • • 9%

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Mol	Chain	Length	Quality of chain
2	G	7	43% 43% 14%
2	H	7	43% 43% 14%
2	I	7	14% 86% 14%
2	J	7	57% 43%
2	K	7	29% 57% 43%
2	M	7	14% 43% 43% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	E	201	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6984 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.

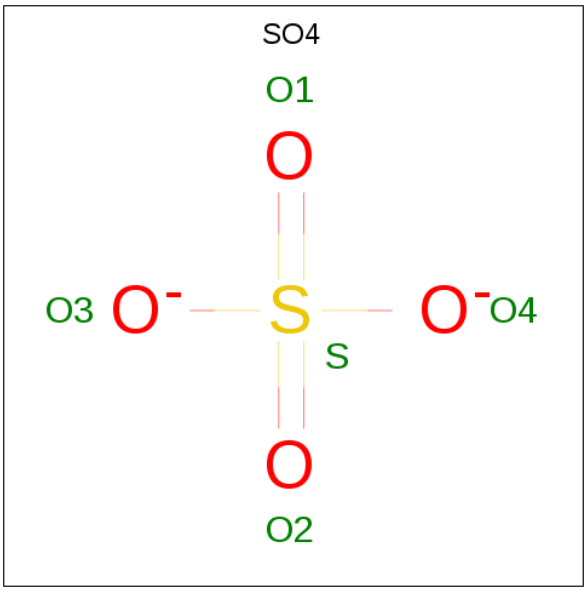
- Molecule 1 is a protein called Protein numb homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1156	727	211	208	10			
1	B	145	Total	C	N	O	S	0	0	0
			1142	719	208	205	10			
1	C	133	Total	C	N	O	S	0	0	0
			1049	654	192	193	10			
1	D	135	Total	C	N	O	S	0	0	0
			1069	672	193	194	10			
1	E	133	Total	C	N	O	S	0	0	0
			1057	663	193	191	10			
1	F	142	Total	C	N	O	S	0	0	0
			1139	717	209	203	10			

- Molecule 2 is a protein called ALA-TYR-ILE-GLY-PRO-PTR-LEU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	7	Total	C	N	O	P	0	0	0
			60	40	7	12	1			
2	G	7	Total	C	N	O	P	0	0	0
			60	40	7	12	1			
2	I	7	Total	C	N	O	P	0	0	0
			60	40	7	12	1			
2	J	7	Total	C	N	O	P	0	0	0
			60	40	7	12	1			
2	K	7	Total	C	N	O	P	0	0	0
			60	40	7	12	1			
2	M	7	Total	C	N	O	P	0	0	0
			60	40	7	12	1			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

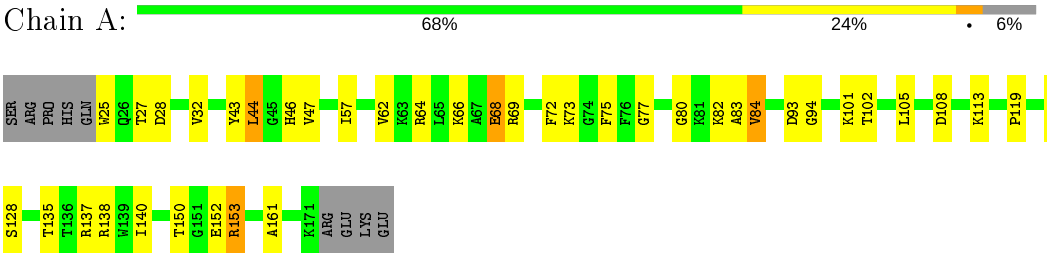
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

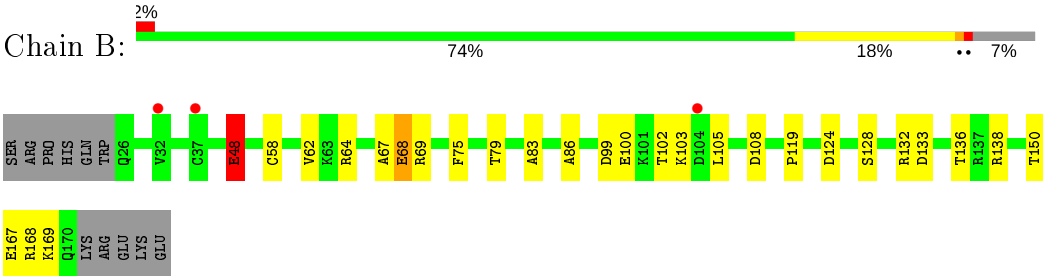
- Molecule 1: Protein numb homolog

Chain A:



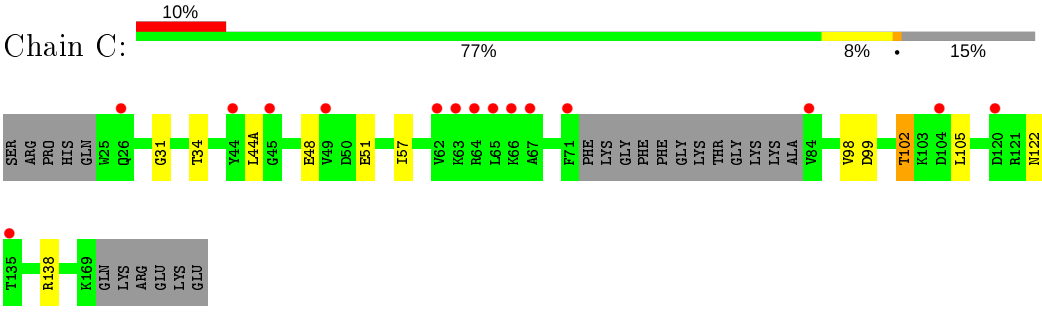
- Molecule 1: Protein numb homolog

Chain B:



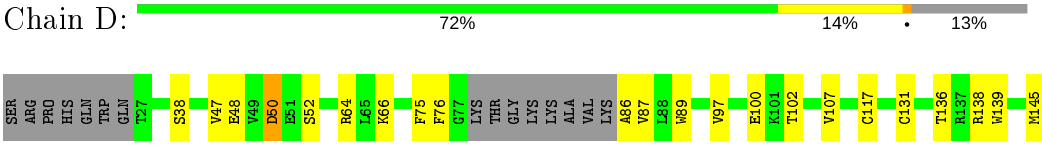
- Molecule 1: Protein numb homolog

Chain C:



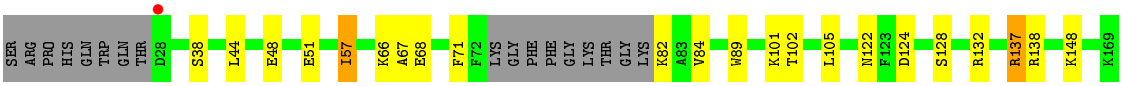
- Molecule 1: Protein numb homolog

Chain D:



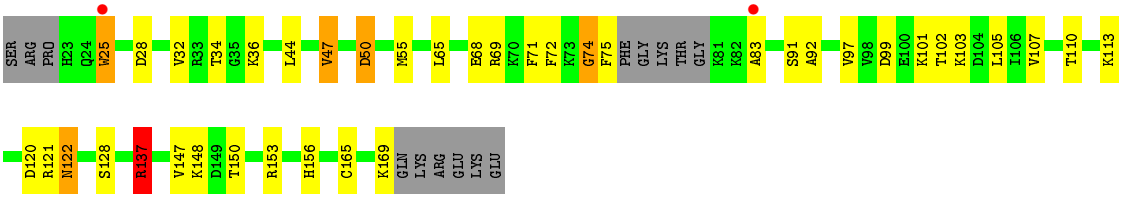
• Molecule 1: Protein numb homolog

Chain E:



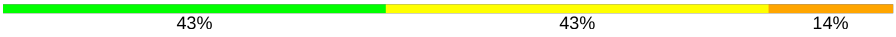
• Molecule 1: Protein numb homolog

Chain F:



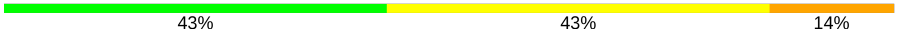
• Molecule 2: ALA-TYR-ILE-GLY-PRO-PTR-LEU

Chain H:



• Molecule 2: ALA-TYR-ILE-GLY-PRO-PTR-LEU

Chain G:



• Molecule 2: ALA-TYR-ILE-GLY-PRO-PTR-LEU

Chain I:

• Molecule 2: ALA-TYR-ILE-GLY-PRO-PTR-LEU

Chain J:

• Molecule 2: ALA-TYR-ILE-GLY-PRO-PTR-LEU

Chain K:

• Molecule 2: ALA-TYR-ILE-GLY-PRO-PTR-LEU

Chain M:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.27Å 81.87Å 235.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.67 – 3.13 55.41 – 3.13	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.67-3.13) 99.4 (55.41-3.13)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.230 , 0.260 0.233 , 0.262	Depositor DCC
R_{free} test set	1336 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	70.3	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6984	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, PTR

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	0.83	1/1177 (0.1%)	0.93	1/1576 (0.1%)
1	B	0.74	1/1163 (0.1%)	0.93	1/1557 (0.1%)
1	C	0.56	0/1066	0.77	0/1431
1	D	0.61	0/1089	0.64	0/1460
1	E	0.71	0/1075	0.95	2/1440 (0.1%)
1	F	0.81	1/1161 (0.1%)	0.99	2/1555 (0.1%)
2	G	1.43	0/44	1.44	0/58
2	H	1.02	0/44	0.96	0/58
2	I	1.01	0/44	0.79	0/58
2	J	0.86	0/44	1.05	0/58
2	K	0.88	0/44	1.13	0/58
2	M	1.23	0/44	1.29	0/58
All	All	0.74	3/6995 (0.0%)	0.89	6/9367 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	1
1	F	0	1
2	H	0	1
2	J	0	1
2	K	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	48	GLU	CB-CG	9.00	1.69	1.52
1	F	25	TRP	CB-CG	5.82	1.60	1.50
1	A	108	ASP	CB-CG	5.03	1.62	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	68	GLU	N-CA-C	-7.09	91.84	111.00
1	A	68	GLU	N-CA-C	-6.72	92.85	111.00
1	E	68	GLU	N-CA-C	-6.08	94.58	111.00
1	B	68	GLU	N-CA-C	-5.92	95.01	111.00
1	F	137	ARG	CG-CD-NE	-5.56	100.12	111.80
1	E	137	ARG	CB-CG-CD	5.11	124.89	111.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	67	ALA	Mainchain
1	E	67	ALA	Mainchain
1	F	74	GLY	Peptide
2	H	1	ALA	Peptide
2	J	1	ALA	Peptide
2	K	1	ALA	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1156	0	1147	33	0
1	B	1142	0	1137	18	1
1	C	1049	0	1031	6	0
1	D	1069	0	1045	16	0
1	E	1057	0	1052	10	0
1	F	1139	0	1130	30	0
2	G	60	0	55	4	0
2	H	60	0	55	2	0
2	I	60	0	55	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	60	0	55	1	0
2	K	60	0	55	1	0
2	M	60	0	55	5	0
3	A	5	0	0	1	0
3	E	5	0	0	2	0
4	B	1	0	0	0	0
4	D	1	0	0	0	1
All	All	6984	0	6872	111	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:HD21	1:B:108:ASP:HB2	1.61	0.83
1:A:28:ASP:OD2	1:A:153:ARG:NH1	2.12	0.83
1:B:100:GLU:N	1:B:100:GLU:OE1	2.09	0.81
1:F:55:MET:HG3	1:F:121:ARG:HH21	1.49	0.76
2:G:1:ALA:HB1	2:G:2:TYR:HA	1.68	0.73
1:B:167:GLU:HG2	1:B:169:LYS:HG3	1.74	0.70
1:F:147:VAL:HG12	1:F:148:LYS:HG3	1.75	0.69
1:A:72:PHE:O	1:A:73:LYS:HB3	1.92	0.69
1:C:51:GLU:HB2	1:C:57:ILE:HD12	1.74	0.67
1:D:86:ALA:HA	1:D:100:GLU:OE1	1.95	0.67
1:A:69:ARG:CZ	1:A:73:LYS:HD2	2.25	0.66
1:B:133:ASP:HB3	1:B:136:THR:HG22	1.80	0.63
1:B:48:GLU:HB3	1:B:138:ARG:NH1	2.13	0.62
1:A:69:ARG:NH2	1:A:73:LYS:HD2	2.15	0.62
1:F:28:ASP:OD2	1:F:153:ARG:NH1	2.33	0.62
1:F:101:LYS:HG3	1:F:102:THR:HG23	1.83	0.61
1:F:150:THR:HG23	1:F:153:ARG:H	1.65	0.61
1:D:50:ASP:N	1:D:50:ASP:OD1	2.34	0.60
3:E:201:SO4:S	1:F:137:ARG:NH2	2.75	0.59
1:E:132:ARG:HH21	1:E:137:ARG:HG2	1.67	0.59
1:B:119:PRO:HG3	1:B:152:GLU:HG2	1.85	0.59
1:B:150:THR:HG23	1:B:153:ARG:H	1.67	0.59
1:A:25:TRP:O	1:A:28:ASP:HB3	2.03	0.58
1:A:47:VAL:HG11	1:A:64:ARG:HD2	1.86	0.57
1:D:47:VAL:HG11	1:D:64:ARG:HH21	1.69	0.57
1:A:69:ARG:CZ	1:A:73:LYS:CD	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:THR:OG1	1:F:36:LYS:HE2	2.05	0.57
1:E:51:GLU:HB2	1:E:57:ILE:HD12	1.87	0.56
2:K:2:TYR:CD2	2:K:2:TYR:N	2.74	0.56
1:A:75:PHE:CZ	1:B:68:GLU:HG2	2.40	0.55
1:B:75:PHE:HB2	1:F:71:PHE:CD2	2.42	0.55
1:E:132:ARG:NH2	1:E:137:ARG:HG2	2.22	0.55
1:A:119:PRO:HG3	1:A:152:GLU:HG2	1.90	0.54
1:A:75:PHE:HZ	1:B:68:GLU:HG2	1.73	0.54
1:B:86:ALA:HA	1:B:100:GLU:OE1	2.08	0.54
1:F:28:ASP:O	1:F:32:VAL:HG23	2.08	0.54
1:A:101:LYS:HG2	1:A:102:THR:HG23	1.89	0.53
1:A:105:LEU:O	1:F:137:ARG:HD3	2.09	0.53
1:D:97:VAL:HB	1:D:107:VAL:HG13	1.89	0.53
1:A:93:ASP:OD1	1:A:94:GLY:N	2.41	0.53
1:E:101:LYS:CG	1:E:102:THR:HG23	2.39	0.52
2:M:1:ALA:HB1	2:M:2:TYR:HA	1.90	0.52
1:A:150:THR:HG23	1:A:153:ARG:H	1.74	0.52
1:A:153:ARG:HH11	1:A:153:ARG:HG3	1.75	0.51
1:C:51:GLU:HB2	1:C:57:ILE:CD1	2.40	0.51
1:A:73:LYS:HB2	1:A:80:GLY:O	2.10	0.51
2:G:2:TYR:CD2	2:G:2:TYR:N	2.79	0.51
2:M:2:TYR:CD2	2:M:2:TYR:N	2.78	0.51
1:E:101:LYS:HG3	1:E:102:THR:HG23	1.93	0.50
1:D:47:VAL:CG1	1:D:64:ARG:HH21	2.24	0.50
2:J:2:TYR:CD2	2:J:2:TYR:N	2.79	0.50
3:E:201:SO4:O4	1:F:137:ARG:NH2	2.41	0.50
1:F:165:CYS:O	1:F:169:LYS:HB3	2.11	0.50
1:D:76:PHE:CE2	1:F:72:PHE:HE1	2.31	0.49
1:F:69:ARG:HD3	1:F:83:ALA:H	1.78	0.49
1:F:50:ASP:OD1	1:F:50:ASP:N	2.46	0.49
1:E:66:LYS:NZ	2:M:6:PTR:O1P	2.45	0.49
1:D:66:LYS:HE2	1:D:145:MET:HE1	1.94	0.48
1:F:47:VAL:HG23	1:F:65:LEU:HD21	1.96	0.48
1:A:138:ARG:HE	1:A:140:ILE:HD11	1.78	0.48
1:C:99:ASP:HB3	1:C:102:THR:HG23	1.96	0.48
1:D:38:SER:HB3	1:D:89:TRP:CE3	2.48	0.48
1:A:32:VAL:HG11	1:A:161:ALA:HA	1.96	0.48
1:C:98:VAL:HG22	1:C:105:LEU:HD12	1.96	0.47
1:D:48:GLU:OE1	1:D:138:ARG:HD2	2.14	0.47
1:B:124:ASP:N	1:B:124:ASP:OD1	2.48	0.47
1:F:71:PHE:CZ	1:F:75:PHE:HE2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ARG:HH21	1:B:83:ALA:HB2	1.80	0.46
1:A:47:VAL:CG1	1:A:64:ARG:HD2	2.45	0.46
1:B:58:CYS:O	1:B:62:VAL:HG23	2.16	0.46
1:F:120:ASP:OD1	1:F:122:ASN:ND2	2.49	0.45
1:F:99:ASP:OD1	1:F:101:LYS:HG2	2.17	0.45
1:B:75:PHE:HB2	1:F:71:PHE:CE2	2.51	0.45
1:F:91:SER:OG	1:F:92:ALA:N	2.50	0.45
1:A:105:LEU:HB3	1:F:137:ARG:NH1	2.32	0.44
2:M:7:LEU:HA	2:M:7:LEU:HD23	1.54	0.44
1:A:135:THR:O	1:F:107:VAL:HA	2.18	0.44
1:A:43:TYR:HB3	1:A:84:VAL:HG13	1.99	0.44
1:A:80:GLY:HA2	1:A:82:LYS:H	1.82	0.44
1:A:137:ARG:HD3	1:F:105:LEU:O	2.17	0.44
1:A:46:HIS:HE1	3:A:201:SO4:O4	2.01	0.44
1:A:73:LYS:HA	1:A:77:GLY:N	2.33	0.44
1:A:153:ARG:NH1	1:A:153:ARG:HG3	2.32	0.44
1:C:31:GLY:HA2	1:C:34:THR:HG22	1.99	0.44
1:B:99:ASP:O	1:B:103:LYS:HA	2.18	0.43
1:B:132:ARG:HD2	1:B:132:ARG:HA	1.74	0.43
2:H:2:TYR:N	2:H:2:TYR:CD2	2.85	0.43
1:A:113:LYS:HA	2:G:6:PTR:HD1	2.01	0.43
1:D:66:LYS:HE2	1:D:145:MET:CE	2.47	0.43
1:E:137:ARG:O	1:E:138:ARG:HG3	2.18	0.43
1:D:76:PHE:CE2	1:F:72:PHE:CE1	3.06	0.43
2:H:6:PTR:O	2:H:7:LEU:HB2	2.19	0.43
1:D:87:VAL:HG23	1:D:100:GLU:HB3	2.00	0.42
1:F:25:TRP:HB3	1:F:156:HIS:CD2	2.54	0.42
1:D:100:GLU:OE1	1:D:100:GLU:N	2.46	0.42
1:B:102:THR:C	1:B:103:LYS:HG2	2.39	0.42
1:D:52:SER:HB3	1:D:139:TRP:CZ2	2.55	0.42
1:A:44:LEU:HD22	1:A:83:ALA:HB2	2.01	0.42
1:A:73:LYS:HA	1:A:77:GLY:H	1.84	0.42
1:A:62:VAL:O	1:A:66:LYS:HB2	2.20	0.42
1:E:51:GLU:HB2	1:E:57:ILE:CD1	2.50	0.41
1:A:68:GLU:HG2	1:D:75:PHE:CZ	2.56	0.41
1:C:48:GLU:OE1	1:C:138:ARG:HD3	2.21	0.41
1:F:99:ASP:O	1:F:103:LYS:HA	2.20	0.41
2:G:7:LEU:HA	2:G:7:LEU:HD23	1.88	0.41
1:E:38:SER:HB3	1:E:89:TRP:CE3	2.56	0.40
1:F:113:LYS:HA	2:M:6:PTR:HD1	2.02	0.40
1:F:55:MET:HG3	1:F:121:ARG:NH2	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLU:HG2	1:D:75:PHE:CE2	2.56	0.40
1:E:48:GLU:OE2	1:E:138:ARG:HD3	2.22	0.40
1:F:97:VAL:HB	1:F:107:VAL:HG12	2.03	0.40

All (1) 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:B:168:ARG:NH1	4:D:201:HOH:O[4_455]	2.06	0.14

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	145/156 (93%)	141 (97%)	4 (3%)	0	100	100
1	B	143/156 (92%)	134 (94%)	9 (6%)	0	100	100
1	C	129/156 (83%)	125 (97%)	4 (3%)	0	100	100
1	D	131/156 (84%)	125 (95%)	6 (5%)	0	100	100
1	E	129/156 (83%)	125 (97%)	3 (2%)	1 (1%)	19	53
1	F	138/156 (88%)	133 (96%)	4 (3%)	1 (1%)	22	56
2	G	4/7 (57%)	4 (100%)	0	0	100	100
2	H	4/7 (57%)	4 (100%)	0	0	100	100
2	I	4/7 (57%)	4 (100%)	0	0	100	100
2	J	4/7 (57%)	4 (100%)	0	0	100	100
2	K	4/7 (57%)	4 (100%)	0	0	100	100
2	M	4/7 (57%)	4 (100%)	0	0	100	100
All	All	839/978 (86%)	807 (96%)	30 (4%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	71	PHE
1	F	74	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	121/133 (91%)	113 (93%)	8 (7%)	16	45
1	B	120/133 (90%)	116 (97%)	4 (3%)	38	68
1	C	112/133 (84%)	108 (96%)	4 (4%)	35	66
1	D	113/133 (85%)	107 (95%)	6 (5%)	22	52
1	E	113/133 (85%)	104 (92%)	9 (8%)	12	37
1	F	121/133 (91%)	114 (94%)	7 (6%)	20	49
2	G	4/4 (100%)	4 (100%)	0	100	100
2	H	4/4 (100%)	4 (100%)	0	100	100
2	I	4/4 (100%)	4 (100%)	0	100	100
2	J	4/4 (100%)	4 (100%)	0	100	100
2	K	4/4 (100%)	4 (100%)	0	100	100
2	M	4/4 (100%)	4 (100%)	0	100	100
All	All	724/822 (88%)	686 (95%)	38 (5%)	23	53

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	44	LEU
1	A	57	ILE
1	A	84	VAL
1	A	122	ASN
1	A	124	ASP
1	A	128	SER

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Mol	Chain	Res	Type
1	A	153	ARG
1	B	48	GLU
1	B	64	ARG
1	B	79	THR
1	B	128	SER
1	C	44(A)	LEU
1	C	102	THR
1	C	122	ASN
1	C	128	SER
1	D	50	ASP
1	D	102	THR
1	D	117	CYS
1	D	131	CYS
1	D	136	THR
1	D	149	ASP
1	E	44	LEU
1	E	57	ILE
1	E	82	LYS
1	E	84	VAL
1	E	105	LEU
1	E	122	ASN
1	E	124	ASP
1	E	128	SER
1	E	148	LYS
1	F	44	LEU
1	F	47	VAL
1	F	50	ASP
1	F	110	THR
1	F	122	ASN
1	F	128	SER
1	F	137	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	156	HIS
1	F	122	ASN

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	PTR	G	6	2	15,16,17	1.44	2 (13%)	19,22,24	1.19	1 (5%)
2	PTR	H	6	2	15,16,17	1.25	2 (13%)	19,22,24	0.94	1 (5%)
2	PTR	M	6	2	15,16,17	1.34	2 (13%)	19,22,24	0.56	0
2	PTR	K	6	2	15,16,17	1.40	2 (13%)	19,22,24	0.78	1 (5%)
2	PTR	I	6	2	15,16,17	1.24	1 (6%)	19,22,24	0.86	1 (5%)
2	PTR	J	6	2	15,16,17	1.38	2 (13%)	19,22,24	0.60	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
2	PTR	G	6	2	-	0/10/11/13	0/1/1/1
2	PTR	H	6	2	-	1/10/11/13	0/1/1/1
2	PTR	M	6	2	-	0/10/11/13	0/1/1/1
2	PTR	K	6	2	-	1/10/11/13	0/1/1/1
2	PTR	I	6	2	-	0/10/11/13	0/1/1/1
2	PTR	J	6	2	-	0/10/11/13	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	6	PTR	OH-CZ	-4.14	1.31	1.40
2	M	6	PTR	OH-CZ	-4.14	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	6	PTR	OH-CZ	-4.01	1.31	1.40
2	K	6	PTR	OH-CZ	-3.92	1.31	1.40
2	J	6	PTR	OH-CZ	-3.85	1.31	1.40
2	I	6	PTR	OH-CZ	-3.67	1.32	1.40
2	G	6	PTR	P-OH	3.39	1.64	1.59
2	J	6	PTR	P-OH	2.67	1.63	1.59
2	M	6	PTR	P-OH	2.64	1.63	1.59
2	H	6	PTR	P-OH	2.28	1.62	1.59
2	K	6	PTR	P-OH	2.28	1.62	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	6	PTR	CB-CA-C	-4.55	102.93	111.47
2	H	6	PTR	O2P-P-OH	3.15	115.08	105.24
2	I	6	PTR	CB-CA-C	-2.97	105.90	111.47
2	K	6	PTR	O2P-P-OH	2.19	112.08	105.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	6	PTR	CZ-OH-P-O2P
2	K	6	PTR	CZ-OH-P-O1P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	6	PTR	1	0
2	H	6	PTR	1	0
2	M	6	PTR	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
3	SO4	A	201	-	4,4,4	0.30	0	6,6,6	0.44	0
3	SO4	E	201	-	4,4,4	0.37	0	6,6,6	0.29	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	SO4	1	0
3	E	201	SO4	2	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^{th} 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^2)	Q<0.9
1	A	147/156 (94%)	0.11	0 100 100	38, 50, 76, 104	0
1	B	145/156 (92%)	0.22	3 (2%) 63 44	48, 68, 98, 108	0
1	C	133/156 (85%)	0.77	16 (12%) 4 2	63, 86, 109, 140	0
1	D	135/156 (86%)	0.14	0 100 100	48, 72, 100, 110	0
1	E	133/156 (85%)	0.18	1 (0%) 86 74	45, 59, 88, 103	0
1	F	142/156 (91%)	0.15	2 (1%) 75 59	41, 54, 78, 103	0
2	G	6/7 (85%)	0.42	0 100 100	38, 42, 49, 55	0
2	H	6/7 (85%)	0.78	0 100 100	52, 53, 58, 62	0
2	I	6/7 (85%)	1.12	1 (16%) 1 1	62, 64, 70, 77	0
2	J	6/7 (85%)	0.37	0 100 100	60, 64, 71, 82	0
2	K	6/7 (85%)	0.97	2 (33%) 0 0	60, 63, 67, 82	0
2	M	6/7 (85%)	0.42	1 (16%) 1 1	40, 42, 48, 53	0
All	All	871/978 (89%)	0.27	26 (2%) 50 29	38, 64, 99, 140	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	67	ALA	3.8
1	C	135	THR	3.7
1	E	28	ASP	3.7
2	I	1	ALA	3.4
1	C	45	GLY	3.1
1	C	71	PHE	2.7
1	B	37	CYS	2.6
1	C	84	VAL	2.6
1	C	66	LYS	2.5
1	C	65	LEU	2.5
2	K	7	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	62	VAL	2.4
1	C	44	TYR	2.4
1	F	83	ALA	2.3
1	C	104	ASP	2.3
1	C	64	ARG	2.3
1	C	26	GLN	2.2
1	C	123	PHE	2.2
1	F	25	TRP	2.2
2	M	1	ALA	2.2
2	K	1	ALA	2.1
1	C	63	LYS	2.1
1	C	49	VAL	2.1
1	C	120	ASP	2.1
1	B	104	ASP	2.0
1	B	32	VAL	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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	PTR	I	6	16/17	0.87	0.21	76,78,81,81	0
2	PTR	K	6	16/17	0.88	0.18	76,78,81,81	0
2	PTR	J	6	16/17	0.93	0.16	78,79,81,82	0
2	PTR	H	6	16/17	0.94	0.18	56,56,57,58	0
2	PTR	G	6	16/17	0.94	0.22	52,52,52,52	0
2	PTR	M	6	16/17	0.97	0.22	50,51,51,51	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
3	SO4	A	201	5/5	0.95	0.12	70,70,70,71	0
3	SO4	E	201	5/5	0.97	0.12	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.