



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:05 PM UTC

PDB ID : 5NJJ / pdb_00005njj
Title : PTB domain of human Numb isoform-1
Authors : Mapelli, M.; Di Fiore, P.P.
Deposited on : 2017-03-29
Resolution : 2.70 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

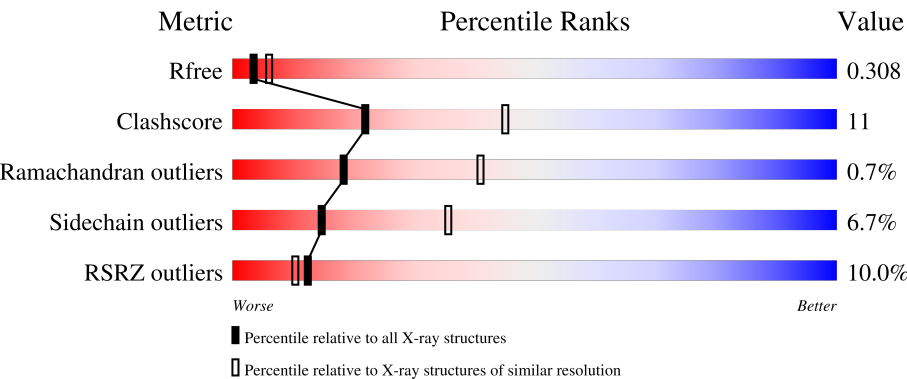
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 of 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 $\leq 5\%$. 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	156	12% 67% 22% • 8%
1	B	156	11% 57% 27% • • 11%
1	C	156	5% 63% 24% • 10%
1	D	156	5% 61% 26% • • 8%
2	E	7	14% 43% 43% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	7	
2	G	7	
2	H	7	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4731 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.

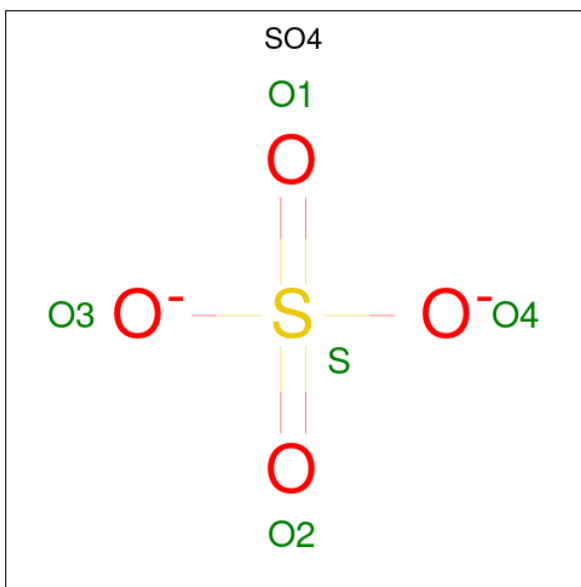
- Molecule 1 is a protein called Protein numb homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	0	0
			1132	713	206	203	10			
1	B	139	Total	C	N	O	S	0	0	0
			1103	695	200	198	10			
1	C	141	Total	C	N	O	S	0	0	0
			1116	703	203	200	10			
1	D	143	Total	C	N	O	S	0	0	0
			1134	714	207	203	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	P	0	0	0
			60	40	7	12	1			
2	F	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	H	7	Total	C	N	O	P	0	0	0
			60	40	7	12	1			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

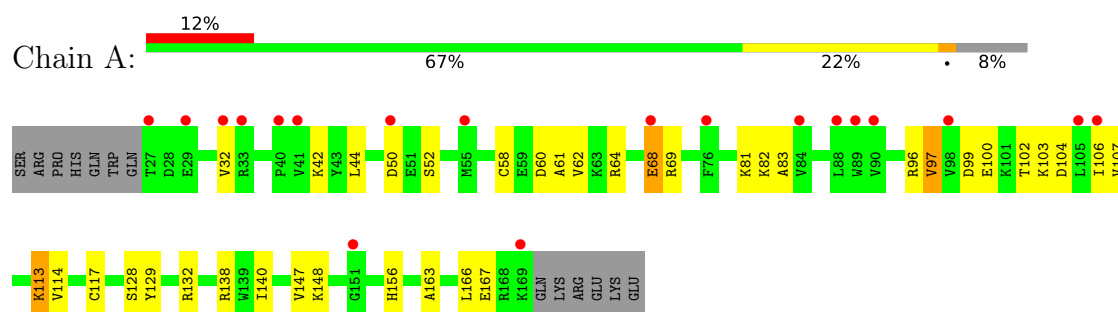
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		

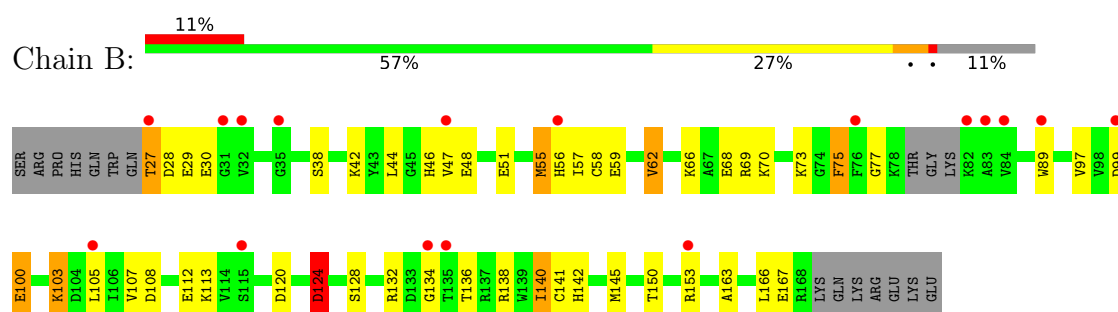
3 Residue-property plots [i](#)

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.

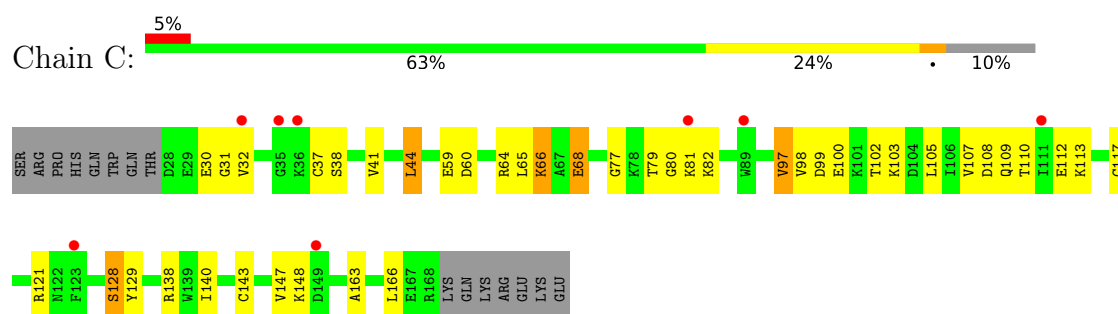
• Molecule 1: Protein numb homolog



• Molecule 1: Protein numb homolog

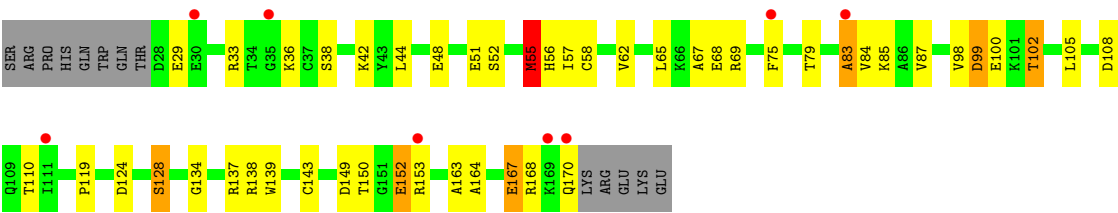


• Molecule 1: Protein numb homolog



• Molecule 1: Protein numb homolog





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



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	113.77Å 120.44Å 237.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.57 – 2.70 39.57 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.57-2.70) 99.5 (39.57-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.269 , 0.303 0.280 , 0.308	Depositor DCC
R_{free} test set	1061 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	72.0	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4731	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PTR, SO4

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	0.67	0/1153	1.26	7/1543 (0.5%)
1	B	0.80	0/1123	1.31	11/1503 (0.7%)
1	C	0.70	0/1137	1.27	7/1522 (0.5%)
1	D	0.81	0/1155	1.37	13/1545 (0.8%)
2	E	0.90	0/44	1.17	0/58
2	F	0.57	0/44	0.81	0/58
2	G	0.54	0/44	0.85	0/58
2	H	0.52	0/44	1.04	0/58
All	All	0.74	0/4744	1.29	38/6345 (0.6%)

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	D	0	1

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	GLU	N-CA-C	-15.01	91.56	112.13
1	A	68	GLU	N-CA-C	-14.84	91.81	112.13
1	D	68	GLU	N-CA-C	-14.64	92.08	112.13
1	B	68	GLU	N-CA-C	-13.72	93.33	112.13
1	A	167	GLU	N-CA-C	11.04	123.39	111.36
1	D	84	VAL	CA-C-N	9.65	134.43	120.82
1	D	84	VAL	C-N-CA	9.65	134.43	120.82
1	B	134	GLY	N-CA-C	8.53	124.48	114.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	124	ASP	N-CA-C	7.02	119.79	111.71
1	B	140	ILE	N-CA-C	6.71	117.70	107.77
1	B	124	ASP	N-CA-C	6.48	119.16	111.71
1	D	38	SER	N-CA-C	6.40	119.15	109.23
1	D	98	VAL	N-CA-C	6.37	117.08	108.17
1	B	62	VAL	N-CA-C	6.36	116.50	110.53
1	D	87	VAL	N-CA-C	6.16	116.74	108.11
1	B	55	MET	N-CA-C	6.13	118.93	111.82
1	D	134	GLY	N-CA-C	5.96	121.37	114.16
1	B	30	GLU	N-CA-C	-5.92	104.95	111.82
1	A	50	ASP	N-CA-C	5.91	120.35	113.20
1	D	83	ALA	CA-C-N	-5.89	115.27	123.10
1	D	83	ALA	C-N-CA	-5.89	115.27	123.10
1	D	85	LYS	N-CA-C	5.85	118.82	110.10
1	D	99	ASP	N-CA-C	-5.83	101.41	110.10
1	D	55	MET	N-CA-C	5.83	118.58	111.82
1	A	32	VAL	N-CA-C	5.54	116.27	110.62
1	A	114	VAL	N-CA-C	5.45	116.56	108.23
1	C	80	GLY	N-CA-C	-5.38	108.75	114.67
1	B	103	LYS	CA-CB-CG	-5.33	103.44	114.10
1	B	167	GLU	N-CA-C	5.21	117.04	111.36
1	C	32	VAL	N-CA-C	5.17	115.89	110.62
1	A	96	ARG	CA-C-N	-5.09	116.33	123.10
1	A	96	ARG	C-N-CA	-5.09	116.33	123.10
1	C	77	GLY	CA-C-N	-5.06	114.61	122.09
1	C	77	GLY	C-N-CA	-5.06	114.61	122.09
1	C	41	VAL	N-CA-C	5.05	115.97	108.65
1	C	66	LYS	CB-CG-CD	5.03	122.86	111.30
1	B	29	GLU	N-CA-C	5.01	116.74	111.28
1	B	73	LYS	N-CA-C	-5.01	107.23	113.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	67	ALA	Mainchain

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	1132	0	1133	21	0
1	B	1103	0	1096	31	0
1	C	1116	0	1113	22	0
1	D	1134	0	1134	25	0
2	E	60	0	55	9	0
2	F	60	0	56	5	0
2	G	60	0	55	2	0
2	H	60	0	55	7	0
3	D	5	0	0	1	0
4	A	1	0	0	0	0
All	All	4731	0	4697	101	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 11.

All (101) 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:100:GLU:HA	1:B:103:LYS:HE2	1.51	0.90
1:D:164:ALA:HB1	1:D:168:ARG:HH12	1.47	0.80
1:B:97:VAL:HG12	1:B:107:VAL:HB	1.68	0.75
1:C:79:THR:H	1:C:82:LYS:HE3	1.51	0.74
1:A:97:VAL:HG12	1:A:107:VAL:HB	1.75	0.69
1:C:147:VAL:HG23	1:C:148:LYS:HG2	1.75	0.69
2:E:6:PTR:CD2	2:E:7:LEU:H	2.06	0.68
1:A:166:LEU:HB2	2:E:1:ALA:HB2	1.77	0.67
1:A:147:VAL:HG23	1:A:148:LYS:HG2	1.76	0.67
1:B:113:LYS:HA	2:F:6:PTR:HD1	1.78	0.66
1:C:163:ALA:HB2	2:H:2:TYR:CE1	2.31	0.65
1:B:42:LYS:HD3	1:B:69:ARG:NH2	2.13	0.63
1:C:97:VAL:CG1	1:C:107:VAL:HB	2.31	0.61
1:A:163:ALA:HA	2:E:1:ALA:CB	2.31	0.60
1:A:97:VAL:CG1	1:A:107:VAL:HB	2.32	0.59
1:D:105:LEU:HD21	1:D:108:ASP:HB2	1.83	0.59
1:B:105:LEU:HD21	1:B:108:ASP:HB2	1.85	0.58
1:D:33:ARG:NH2	1:D:167:GLU:OE1	2.37	0.58
1:C:66:LYS:O	1:C:66:LYS:HG3	2.00	0.57
1:A:97:VAL:O	1:A:106:ILE:HG12	2.04	0.57
2:G:6:PTR:CG	2:G:7:LEU:H	2.18	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:THR:HG23	1:D:153:ARG:H	1.70	0.57
1:B:136:THR:OG1	1:B:138:ARG:NH1	2.39	0.56
1:C:113:LYS:HA	2:E:6:PTR:HD1	1.88	0.56
1:D:137:ARG:HG2	1:D:137:ARG:HH11	1.70	0.56
1:D:137:ARG:HG2	1:D:137:ARG:NH1	2.20	0.55
1:C:68:GLU:OE1	1:C:81:LYS:HD2	2.07	0.55
1:B:51:GLU:HB2	1:B:57:ILE:HD13	1.89	0.54
1:C:166:LEU:HB2	2:H:1:ALA:HB2	1.89	0.54
1:A:102:THR:HG23	1:A:104:ASP:H	1.73	0.54
1:D:51:GLU:HB2	1:D:57:ILE:CD1	2.37	0.53
1:C:31:GLY:C	1:C:37:CYS:HB2	2.34	0.53
1:C:105:LEU:HD21	1:C:108:ASP:HB2	1.90	0.52
1:C:99:ASP:O	1:C:103:LYS:HA	2.10	0.52
1:D:128:SER:HB3	1:D:143:CYS:HA	1.91	0.52
2:E:1:ALA:HB1	2:E:2:TYR:HA	1.91	0.52
1:C:163:ALA:HA	2:H:1:ALA:CB	2.40	0.52
1:A:132:ARG:HG2	2:H:6:PTR:OH	2.10	0.51
1:B:51:GLU:HB2	1:B:57:ILE:CD1	2.40	0.51
1:B:136:THR:HG21	1:B:138:ARG:CZ	2.41	0.51
1:A:132:ARG:HG2	2:H:6:PTR:CZ	2.41	0.50
1:C:60:ASP:O	1:C:64:ARG:HG3	2.12	0.50
2:E:6:PTR:HD2	2:E:7:LEU:H	1.75	0.50
1:B:99:ASP:O	1:B:103:LYS:HA	2.12	0.49
1:B:58:CYS:O	1:B:62:VAL:HG23	2.12	0.49
1:C:117:CYS:HA	1:C:129:TYR:HA	1.94	0.49
1:A:99:ASP:O	1:A:103:LYS:HA	2.12	0.49
1:A:61:ALA:HA	1:A:64:ARG:HD3	1.94	0.49
1:A:52:SER:OG	2:H:7:LEU:HD11	2.14	0.48
1:B:75:PHE:C	1:B:75:PHE:CD1	2.91	0.48
1:B:38:SER:HG	1:B:89:TRP:CD1	2.32	0.48
1:B:48:GLU:HA	1:B:140:ILE:HD13	1.95	0.47
1:B:27:THR:HB	1:B:28:ASP:H	1.55	0.47
1:D:42:LYS:HD2	1:D:69:ARG:NH2	2.30	0.47
1:D:51:GLU:HB2	1:D:57:ILE:HD13	1.96	0.47
1:B:124:ASP:OD2	1:B:124:ASP:N	2.38	0.47
1:B:55:MET:HB3	1:B:55:MET:HE3	1.68	0.47
1:B:55:MET:H	1:D:170:GLN:C	2.23	0.47
1:A:97:VAL:HG13	1:A:106:ILE:CG1	2.44	0.47
1:C:59:GLU:OE2	1:C:121:ARG:HD2	2.15	0.47
1:B:132:ARG:HG2	2:F:6:PTR:OH	2.15	0.46
1:D:119:PRO:HG3	1:D:152:GLU:HG3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:ALA:HB1	1:D:168:ARG:NH1	2.25	0.46
1:B:59:GLU:HA	1:B:120:ASP:OD1	2.16	0.46
1:D:58:CYS:O	1:D:62:VAL:HG23	2.16	0.46
1:B:145:MET:HB3	1:B:145:MET:HE3	1.62	0.46
1:C:112:GLU:O	2:E:6:PTR:HD1	2.16	0.45
1:A:60:ASP:O	1:A:64:ARG:HG3	2.17	0.45
1:D:29:GLU:HG2	1:D:33:ARG:HD2	1.99	0.45
1:D:52:SER:HB3	1:D:139:TRP:CZ2	2.52	0.44
1:B:100:GLU:HA	1:B:103:LYS:CE	2.33	0.44
1:A:117:CYS:HA	1:A:129:TYR:HA	1.99	0.44
1:A:166:LEU:CB	2:E:1:ALA:HB2	2.47	0.44
1:B:42:LYS:HD3	1:B:69:ARG:HH22	1.82	0.44
1:B:112:GLU:O	2:F:6:PTR:HD1	2.17	0.44
1:D:55:MET:HE3	1:D:55:MET:HB3	1.63	0.44
1:C:128:SER:HB3	1:C:143:CYS:SG	2.57	0.44
1:D:65:LEU:HA	1:D:65:LEU:HD23	1.73	0.44
1:D:149:ASP:OD1	1:D:153:ARG:HD3	2.18	0.44
1:C:109:GLN:NE2	1:C:110:THR:O	2.41	0.43
1:B:62:VAL:O	1:B:66:LYS:HB2	2.18	0.43
1:A:156:HIS:HA	2:H:2:TYR:HE2	1.83	0.43
1:C:98:VAL:HG12	1:C:105:LEU:HA	1.99	0.43
1:D:36:LYS:O	1:D:36:LYS:HG2	2.19	0.43
1:B:163:ALA:HA	2:G:1:ALA:O	2.18	0.43
1:C:113:LYS:HA	2:E:6:PTR:CD1	2.48	0.43
1:B:56:HIS:HB3	1:D:170:GLN:HG2	2.01	0.42
1:A:58:CYS:O	1:A:62:VAL:HG23	2.20	0.42
1:A:113:LYS:HE3	1:A:132:ARG:O	2.19	0.42
1:D:99:ASP:HB3	1:D:102:THR:HG23	2.00	0.41
1:A:69:ARG:HH11	1:A:83:ALA:H	1.68	0.41
1:B:46:HIS:HA	1:B:141:CYS:O	2.21	0.41
1:B:46:HIS:HB3	1:B:142:HIS:CE1	2.55	0.41
1:C:138:ARG:HG3	1:C:140:ILE:HD11	2.03	0.41
1:B:113:LYS:HA	2:F:6:PTR:CD1	2.49	0.41
1:D:48:GLU:OE2	1:D:138:ARG:HD2	2.21	0.41
1:D:163:ALA:HA	2:F:1:ALA:O	2.21	0.41
1:A:138:ARG:CZ	1:A:140:ILE:HD11	2.52	0.40
1:C:44:LEU:HB3	1:C:65:LEU:HD13	2.03	0.40
1:B:150:THR:HG23	1:B:153:ARG:H	1.86	0.40
1:D:56:HIS:ND1	3:D:201:SO4:O3	2.52	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	141/156 (90%)	138 (98%)	3 (2%)	0	100	100
1	B	135/156 (86%)	128 (95%)	5 (4%)	2 (2%)	8	22
1	C	139/156 (89%)	135 (97%)	4 (3%)	0	100	100
1	D	141/156 (90%)	134 (95%)	5 (4%)	2 (1%)	9	23
2	E	4/7 (57%)	4 (100%)	0	0	100	100
2	F	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	G	4/7 (57%)	4 (100%)	0	0	100	100
2	H	4/7 (57%)	4 (100%)	0	0	100	100
All	All	572/652 (88%)	550 (96%)	18 (3%)	4 (1%)	18	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	83	ALA
1	B	75	PHE
1	D	75	PHE
1	B	77	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	120/133 (90%)	111 (92%)	9 (8%)	12	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	117/133 (88%)	109 (93%)	8 (7%)	14	35
1	C	118/133 (89%)	111 (94%)	7 (6%)	18	42
1	D	120/133 (90%)	111 (92%)	9 (8%)	12	31
2	E	4/4 (100%)	4 (100%)	0	100	100
2	F	4/4 (100%)	4 (100%)	0	100	100
2	G	4/4 (100%)	4 (100%)	0	100	100
2	H	4/4 (100%)	4 (100%)	0	100	100
All	All	491/548 (90%)	458 (93%)	33 (7%)	15	36

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LYS
1	A	44	LEU
1	A	68	GLU
1	A	81	LYS
1	A	82	LYS
1	A	97	VAL
1	A	100	GLU
1	A	113	LYS
1	A	128	SER
1	B	27	THR
1	B	44	LEU
1	B	47	VAL
1	B	70	LYS
1	B	100	GLU
1	B	124	ASP
1	B	128	SER
1	B	166	LEU
1	C	30	GLU
1	C	38	SER
1	C	44	LEU
1	C	97	VAL
1	C	100	GLU
1	C	102	THR
1	C	128	SER
1	D	44	LEU
1	D	55	MET
1	D	79	THR
1	D	100	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	102	THR
1	D	110	THR
1	D	128	SER
1	D	152	GLU
1	D	167	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	HIS
1	D	122	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	1.22	2 (13%)	17,22,24	1.05	1 (5%)
2	PTR	H	6	2	15,16,17	1.33	1 (6%)	17,22,24	0.54	0
2	PTR	F	6	2	15,16,17	1.28	2 (13%)	17,22,24	0.92	1 (5%)
2	PTR	E	6	2	15,16,17	1.24	1 (6%)	17,22,24	0.47	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	-	1/10/11/13	0/1/1/1
2	PTR	H	6	2	-	0/10/11/13	0/1/1/1
2	PTR	F	6	2	-	2/10/11/13	0/1/1/1
2	PTR	E	6	2	-	1/10/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	6	PTR	OH-CZ	-4.42	1.30	1.40
2	E	6	PTR	OH-CZ	-4.25	1.31	1.40
2	G	6	PTR	OH-CZ	-3.85	1.32	1.40
2	F	6	PTR	OH-CZ	-3.72	1.32	1.40
2	G	6	PTR	P-OH	2.22	1.63	1.59
2	F	6	PTR	P-OH	2.07	1.63	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	6	PTR	O2P-P-OH	3.02	114.24	105.32
2	F	6	PTR	O2P-P-OH	2.65	113.15	105.32

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	6	PTR	CZ-OH-P-O1P
2	E	6	PTR	N-CA-CB-CG
2	G	6	PTR	CZ-OH-P-O1P
2	F	6	PTR	CZ-OH-P-O2P

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	6	PTR	1	0
2	H	6	PTR	2	0
2	F	6	PTR	4	0
2	E	6	PTR	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	D	201	-	4,4,4	0.38	0	6,6,6	0.33	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	201	SO4	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, 95th 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	143/156 (91%)	1.06	19 (13%) 7 6	72, 85, 106, 108	0
1	B	139/156 (89%)	1.03	17 (12%) 8 7	59, 80, 107, 114	0
1	C	141/156 (90%)	0.91	8 (5%) 29 26	65, 79, 100, 108	0
1	D	143/156 (91%)	0.79	8 (5%) 30 26	59, 72, 95, 104	0
2	E	6/7 (85%)	1.70	1 (16%) 4 3	67, 73, 76, 78	0
2	F	6/7 (85%)	1.60	2 (33%) 1 1	60, 63, 77, 93	0
2	G	6/7 (85%)	1.77	2 (33%) 1 1	58, 66, 75, 92	0
2	H	6/7 (85%)	2.53	2 (33%) 1 1	71, 78, 81, 81	0
All	All	590/652 (90%)	0.99	59 (10%) 12 10	58, 80, 105, 114	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1	ALA	7.9
2	E	1	ALA	4.9
2	G	7	LEU	4.5
1	A	98	VAL	3.9
1	C	149	ASP	3.9
2	F	7	LEU	3.7
1	C	35	GLY	3.4
1	C	81	LYS	3.3
1	C	36	LYS	3.2
1	A	29	GLU	3.1
1	A	27	THR	3.1
1	A	50	ASP	3.0
1	B	27	THR	3.0
2	G	1	ALA	2.9
1	B	84	VAL	2.9
1	C	111	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	35	GLY	2.8
1	B	135	THR	2.8
1	A	90	VAL	2.8
1	B	76	PHE	2.8
1	A	106	ILE	2.8
2	H	7	LEU	2.7
1	B	31	GLY	2.6
1	B	35	GLY	2.6
1	A	89	TRP	2.6
1	D	30	GLU	2.5
1	B	99	ASP	2.5
1	B	56	HIS	2.5
1	B	89	TRP	2.5
1	C	123	PHE	2.4
1	A	105	LEU	2.4
1	A	41	VAL	2.4
1	C	89	TRP	2.4
1	D	169	LYS	2.4
1	A	88	LEU	2.4
1	B	115	SER	2.4
1	D	83	ALA	2.3
2	F	1	ALA	2.3
1	D	111	ILE	2.2
1	A	169	LYS	2.2
1	A	84	VAL	2.2
1	D	75	PHE	2.2
1	B	32	VAL	2.2
1	A	32	VAL	2.2
1	A	76	PHE	2.2
1	C	32	VAL	2.1
1	A	55	MET	2.1
1	A	151	GLY	2.1
1	B	83	ALA	2.1
1	D	153	ARG	2.1
1	D	170	GLN	2.1
1	A	68	GLU	2.1
1	B	134	GLY	2.1
1	A	33	ARG	2.0
1	B	82	LYS	2.0
1	A	40	PRO	2.0
1	B	47	VAL	2.0
1	B	105	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	153	ARG	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, 95th 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	F	6	16/17	0.82	0.15	84,88,93,94	0
2	PTR	G	6	16/17	0.85	0.14	79,83,89,89	0
2	PTR	E	6	16/17	0.86	0.12	71,72,73,74	0
2	PTR	H	6	16/17	0.87	0.12	76,78,81,81	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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	D	201	5/5	0.84	0.11	80,81,82,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.