



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 07:52 PM UTC

PDB ID : 1G29 / pdb_00001g29
Title : MALK
Authors : Diederichs, K.; Diez, J.; Grellner, G.; Mueller, C.; Breed, J.; Schnell, C.; Vonrhein, C.; Boos, W.; Welte, W.
Deposited on : 2000-10-18
Resolution : 1.90 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

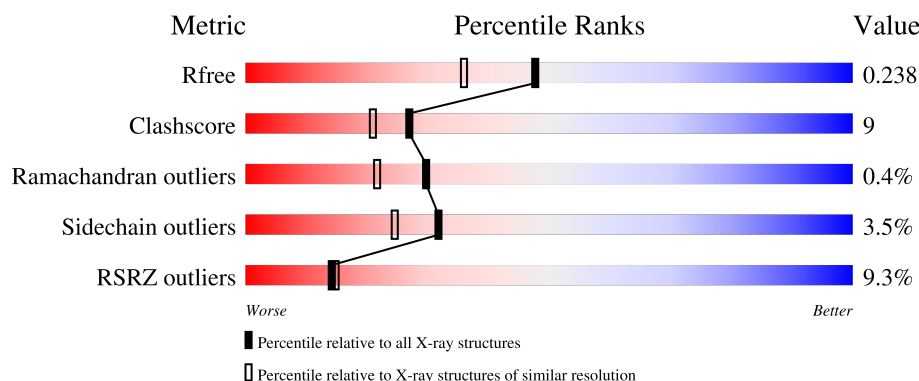
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	1	372	10% 78% 19% .
1	2	372	8% 81% 16% .

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	CL	1	374	-	-	X	-
3	CL	1	375	-	-	X	-
3	CL	2	376	-	-	X	-
3	CL	2	381	-	-	X	-
3	CL	2	396	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6362 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.

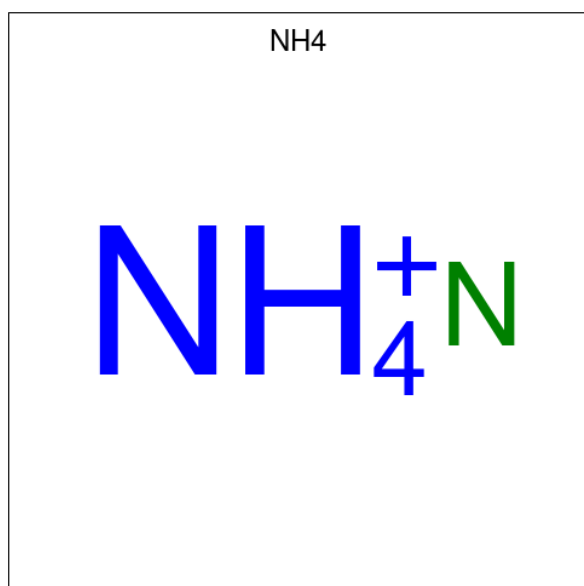
- Molecule 1 is a protein called MALTOSE TRANSPORT PROTEIN MALK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	372	Total	C	N	O	S	0	0	0
			2939	1874	516	534	15			
1	2	372	Total	C	N	O	S	0	0	0
			2939	1874	516	534	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	327	ARG	HIS	SEE REMARK 999	UNP Q9YGA6
2	327	ARG	HIS	SEE REMARK 999	UNP Q9YGA6

- Molecule 2 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1	1	Total	N	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	2	1	Total N 1 1	0	0
2	2	1	Total N 1 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1	4	Total Cl 4 4	0	0
3	2	6	Total Cl 6 6	0	0

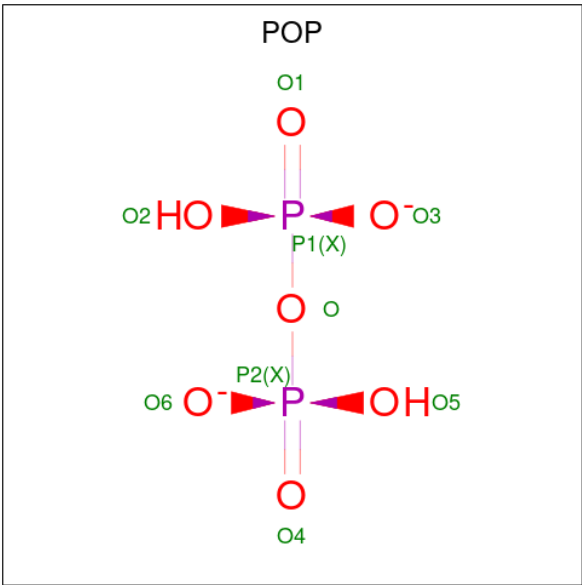
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1	15	Total Na 15 15	0	0
4	2	13	Total Na 13 13	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

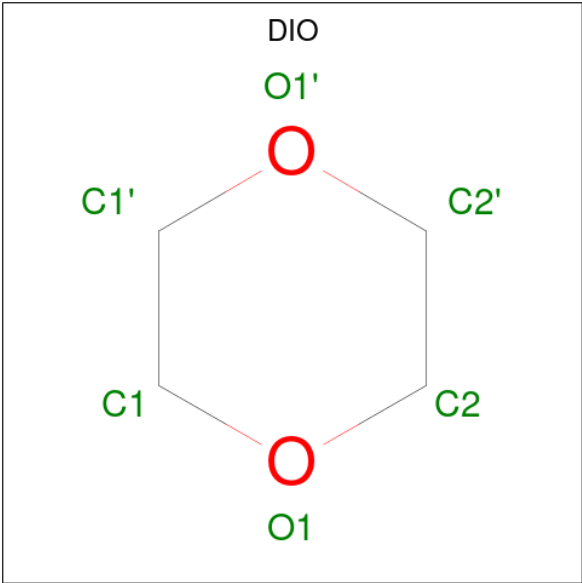
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1	4	Total Mg 4 4	0	0
5	2	7	Total Mg 7 7	0	0

- Molecule 6 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	1	1	Total	O	P	0	0
			9	7	2		
6	2	1	Total	O	P	0	0
			9	7	2		

- Molecule 7 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: C₄H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	1	1	Total	C	O	0	0
			6	4	2		
7	1	1	Total	C	O	0	0
			6	4	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	1	1	Total	C	O	0	0
			6	4	2		

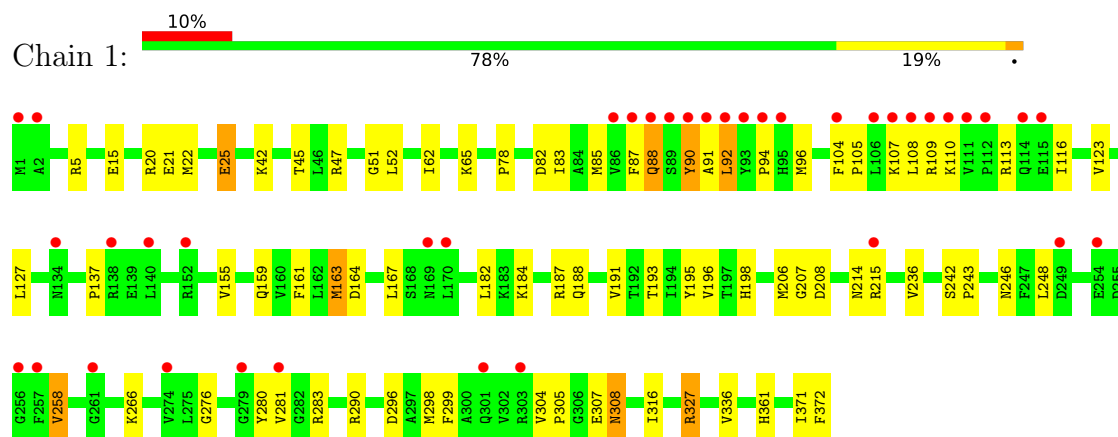
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	1	198	Total	O	0	0
			198	198		
8	2	198	Total	O	0	0
			198	198		

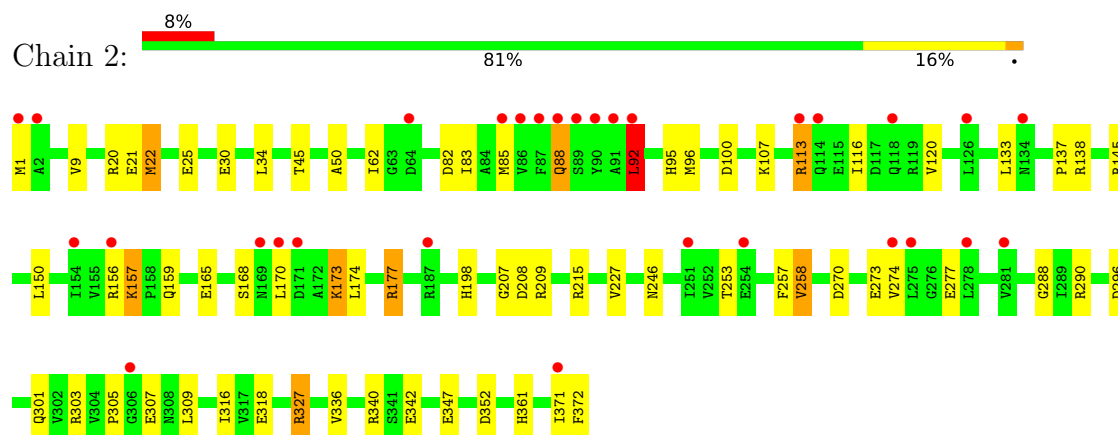
3 Residue-property plots

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: MALTOSE TRANSPORT PROTEIN MALK



• Molecule 1: MALTOSE TRANSPORT PROTEIN MALK



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	190.72Å 65.70Å 77.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.26 – 1.90 34.26 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.26-1.90) 99.2 (34.26-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 1.85Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.211 , 0.247 0.203 , 0.238	Depositor DCC
R_{free} test set	1552 reflections (1.88%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6362	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: POP, NA, MG, CL, DIO, NH4

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	1	0.91	6/2989 (0.2%)	1.09	10/4030 (0.2%)
1	2	0.83	1/2989 (0.0%)	1.10	14/4030 (0.3%)
All	All	0.87	7/5978 (0.1%)	1.10	24/8060 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	206	MET	SD-CE	-7.91	1.59	1.79
1	1	85	MET	SD-CE	-6.96	1.62	1.79
1	2	22	MET	SD-CE	-6.68	1.62	1.79
1	1	298	MET	SD-CE	-6.08	1.64	1.79
1	1	25	GLU	CB-CG	5.35	1.68	1.52
1	1	163	MET	SD-CE	5.29	1.92	1.79
1	1	25	GLU	CG-CD	5.07	1.64	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	371	ILE	N-CA-C	-10.68	101.52	111.45
1	1	371	ILE	N-CA-C	-8.68	101.54	111.00
1	2	307	GLU	N-CA-C	8.35	121.58	111.40
1	1	208	ASP	N-CA-C	-8.28	101.50	111.69
1	2	88	GLN	N-CA-C	7.67	120.31	111.11
1	2	92	LEU	N-CA-C	7.52	122.09	109.76
1	1	90	TYR	N-CA-C	7.32	120.46	110.35
1	1	258	VAL	N-CA-C	-6.88	98.54	108.17
1	1	296	ASP	N-CA-C	-6.46	100.28	109.96
1	2	208	ASP	N-CA-C	-6.42	103.79	111.69
1	2	34	LEU	N-CA-C	-6.10	98.58	108.52
1	2	258	VAL	N-CA-C	-6.00	99.22	107.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	85	MET	N-CA-C	-5.86	98.97	108.41
1	2	62	ILE	N-CA-C	-5.80	98.05	107.28
1	1	25	GLU	CB-CG-CD	5.70	122.29	112.60
1	1	62	ILE	N-CA-C	-5.66	98.29	107.28
1	2	207	GLY	N-CA-C	5.65	120.28	112.37
1	2	296	ASP	N-CA-C	-5.62	101.53	109.96
1	2	133	LEU	N-CA-C	5.41	117.88	111.33
1	1	198	HIS	N-CA-C	-5.31	106.84	113.38
1	1	207	GLY	N-CA-C	5.23	119.85	111.64
1	2	92	LEU	CA-CB-CG	5.06	134.01	116.30
1	1	52	LEU	N-CA-C	-5.03	106.66	112.89
1	2	9	VAL	N-CA-C	5.01	115.51	108.89

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	1	2939	0	3019	54	0
1	2	2939	0	3019	60	0
2	1	1	0	0	0	0
2	2	2	0	0	1	0
3	1	4	0	0	4	0
3	2	6	0	0	7	0
4	1	15	0	0	0	0
4	2	13	0	0	0	0
5	1	4	0	0	0	0
5	2	7	0	0	0	0
6	1	9	0	0	0	0
6	2	9	0	0	0	0
7	1	18	0	24	0	0
8	1	198	0	0	3	0
8	2	198	0	0	2	0
All	All	6362	0	6062	111	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 9.

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)
1:2:327:ARG:HH11	1:2:327:ARG:HG2	1.17	1.07
1:1:327:ARG:CG	1:1:327:ARG:HH11	1.74	0.99
1:2:88:GLN:HG3	1:2:145:ARG:HB3	1.44	0.97
1:1:123:VAL:HG21	1:1:155:VAL:HG12	1.56	0.88
1:2:95:HIS:HD2	1:2:138:ARG:HH11	1.22	0.88
1:1:316:ILE:HB	1:1:327:ARG:HG3	1.59	0.84
1:2:327:ARG:HH11	1:2:327:ARG:CG	1.86	0.84
1:1:327:ARG:NH1	1:1:327:ARG:HG2	1.93	0.83
1:2:309:LEU:HD11	1:2:352:ASP:HB3	1.59	0.83
1:1:327:ARG:HH11	1:1:327:ARG:HG3	1.46	0.78
1:2:327:ARG:HG2	1:2:327:ARG:NH1	1.98	0.78
1:1:327:ARG:CG	1:1:327:ARG:NH1	2.38	0.78
1:2:177:ARG:HH11	1:2:177:ARG:HG3	1.50	0.75
1:1:246:ASN:HD21	1:1:336:VAL:H	1.35	0.74
1:2:30:GLU:OE1	1:2:209:ARG:HD3	1.90	0.71
1:1:246:ASN:ND2	1:1:336:VAL:H	1.90	0.70
1:2:95:HIS:CD2	1:2:138:ARG:HH11	2.07	0.70
1:2:20:ARG:HG2	1:2:21:GLU:HG2	1.74	0.70
1:1:304:VAL:H	1:1:308:ASN:HD21	1.39	0.69
1:1:327:ARG:HH11	1:1:327:ARG:HG2	1.51	0.69
1:2:327:ARG:HD3	1:2:336:VAL:HG22	1.75	0.69
1:2:88:GLN:HE21	1:2:92:LEU:HD22	1.56	0.68
1:1:92:LEU:HD12	1:1:137:PRO:HG3	1.77	0.67
1:2:290:ARG:NH2	3:2:376:CL:CL	2.66	0.66
1:2:327:ARG:CG	1:2:327:ARG:NH1	2.49	0.66
1:2:165:GLU:HG3	1:2:168:SER:HB3	1.77	0.65
1:1:361:HIS:HE1	8:1:975:HOH:O	1.81	0.63
1:2:156:ARG:O	1:2:157:LYS:HB2	2.00	0.61
1:1:94:PRO:HG3	1:2:198:HIS:CE1	2.36	0.60
1:2:361:HIS:HD2	1:2:372:PHE:OXT	1.84	0.60
1:1:164:ASP:OD1	1:2:95:HIS:HE1	1.85	0.60
1:1:87:PHE:HB2	1:1:90:TYR:OH	2.02	0.59
1:2:20:ARG:NH1	3:2:381:CL:CL	2.72	0.59
1:1:290:ARG:NH2	3:1:374:CL:CL	2.72	0.59
1:1:82:ASP:HB3	1:1:159:GLN:HG3	1.84	0.59
1:2:88:GLN:HG2	1:2:92:LEU:HD13	1.85	0.58
1:2:50:ALA:HA	1:2:83:ILE:HD12	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:316:ILE:HB	1:2:327:ARG:HG3	1.87	0.57
1:1:361:HIS:HD2	1:1:372:PHE:O	1.87	0.57
1:2:303:ARG:NH1	3:2:396:CL:CL	2.75	0.57
1:2:22:MET:HE1	1:2:45:THR:OG1	2.05	0.56
1:2:92:LEU:HD21	1:2:137:PRO:HB2	1.87	0.56
1:1:304:VAL:H	1:1:308:ASN:ND2	2.03	0.55
1:1:161:PHE:CE2	1:1:191:VAL:HG11	2.42	0.55
1:2:92:LEU:HD11	1:2:137:PRO:HB3	1.88	0.55
1:1:47:ARG:NH1	3:1:375:CL:CL	2.69	0.54
1:2:88:GLN:CG	1:2:145:ARG:HB3	2.30	0.54
1:2:95:HIS:HD2	1:2:138:ARG:NH1	1.98	0.54
1:1:123:VAL:HG21	1:1:155:VAL:CG1	2.33	0.54
1:1:299:PHE:HB2	8:1:893:HOH:O	2.07	0.54
1:2:303:ARG:HD3	3:2:396:CL:CL	2.45	0.53
1:1:87:PHE:H	1:1:90:TYR:HE1	1.56	0.53
1:2:82:ASP:OD2	1:2:159:GLN:HG3	2.08	0.53
1:2:361:HIS:HE1	8:2:639:HOH:O	1.91	0.52
1:2:20:ARG:NH2	3:2:381:CL:CL	2.80	0.52
1:1:109:ARG:HG3	1:1:109:ARG:HH11	1.75	0.52
1:1:20:ARG:HG2	1:1:21:GLU:HG2	1.91	0.51
1:2:173:LYS:NZ	1:2:173:LYS:HB2	2.25	0.51
1:2:303:ARG:HH12	1:2:305:PRO:HG3	1.75	0.51
1:2:177:ARG:HG3	1:2:177:ARG:NH1	2.20	0.51
1:2:25:GLU:HG3	8:2:688:HOH:O	2.10	0.51
1:2:156:ARG:HG2	1:2:157:LYS:N	2.25	0.51
1:1:316:ILE:HD12	1:1:327:ARG:HD2	1.94	0.50
1:2:273:GLU:O	1:2:277:GLU:HG3	2.12	0.50
1:2:303:ARG:NH1	1:2:305:PRO:HG3	2.26	0.50
1:1:92:LEU:HD12	1:1:137:PRO:CG	2.42	0.50
1:2:215:ARG:O	3:2:381:CL:CL	2.67	0.50
1:1:108:LEU:C	1:1:110:LYS:H	2.20	0.50
1:1:163:MET:HE3	1:1:193:THR:HG23	1.93	0.49
1:2:30:GLU:OE1	1:2:209:ARG:CD	2.58	0.49
1:1:308:ASN:HD22	1:1:308:ASN:C	2.22	0.47
1:2:318:GLU:OE2	1:2:327:ARG:NH2	2.41	0.47
1:1:308:ASN:ND2	1:1:308:ASN:C	2.71	0.47
1:1:214:ASN:OD1	1:1:215:ARG:HD2	2.16	0.46
1:1:15:GLU:HG3	8:1:987:HOH:O	2.15	0.46
1:2:92:LEU:HG	1:2:137:PRO:HG2	1.97	0.46
1:1:276:GLY:HA2	1:1:281:VAL:HG23	1.98	0.46
1:1:107:LYS:HD2	1:1:116:ILE:HD13	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:47:ARG:HD2	3:1:375:CL:CL	2.53	0.45
1:1:214:ASN:OD1	1:1:215:ARG:NH1	2.46	0.44
1:2:116:ILE:O	1:2:120:VAL:HG23	2.17	0.44
1:1:184:LYS:O	1:1:188:GLN:HG3	2.18	0.44
1:1:242:SER:HA	1:1:243:PRO:C	2.42	0.44
1:1:280:TYR:HA	1:1:283:ARG:HD2	2.00	0.43
1:2:347:GLU:OE1	2:2:374:NH4:N	2.51	0.43
1:2:270:ASP:O	1:2:274:VAL:HG23	2.18	0.43
1:1:266:LYS:HB2	1:1:307:GLU:HG2	2.01	0.43
1:1:94:PRO:HG3	1:2:198:HIS:NE2	2.34	0.43
1:1:51:GLY:C	1:1:78:PRO:HG3	2.43	0.43
1:1:96:MET:O	1:1:137:PRO:HD3	2.19	0.43
1:1:236:VAL:O	3:1:374:CL:CL	2.73	0.43
1:1:113:ARG:HG3	1:1:113:ARG:HH11	1.84	0.42
1:1:104:PHE:N	1:1:105:PRO:HD2	2.34	0.42
1:2:96:MET:HE3	1:2:100:ASP:HB3	2.00	0.42
1:2:227:VAL:O	3:2:376:CL:CL	2.75	0.42
1:2:342:GLU:H	1:2:342:GLU:CD	2.26	0.42
1:1:163:MET:HG3	1:1:195:TYR:CD2	2.55	0.42
1:2:107:LYS:HE2	1:2:113:ARG:NH2	2.34	0.42
1:1:22:MET:HE1	1:1:45:THR:HG21	2.01	0.42
1:1:104:PHE:O	1:1:108:LEU:HD13	2.20	0.42
1:2:253:THR:HG1	1:2:257:PHE:H	1.68	0.42
1:1:42:LYS:HD2	1:1:196:VAL:HG13	2.02	0.41
1:1:5:ARG:HG3	1:1:25:GLU:HG3	2.01	0.41
1:2:113:ARG:NH1	1:2:113:ARG:HA	2.35	0.41
1:2:92:LEU:HD21	1:2:137:PRO:CB	2.49	0.41
1:2:316:ILE:HB	1:2:327:ARG:CG	2.51	0.41
1:2:246:ASN:O	1:2:288:GLY:HA2	2.21	0.41
1:2:340:ARG:HB2	1:2:342:GLU:OE1	2.21	0.41
1:2:113:ARG:CB	1:2:113:ARG:HH11	2.34	0.40
1:1:113:ARG:HG3	1:1:113:ARG:NH1	2.37	0.40
1:2:170:LEU:HD22	1:2:174:LEU:HD23	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	1	370/372 (100%)	362 (98%)	6 (2%)	2 (0%)	24	16
1	2	370/372 (100%)	363 (98%)	6 (2%)	1 (0%)	36	29
All	All	740/744 (100%)	725 (98%)	12 (2%)	3 (0%)	30	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	88	GLN
1	1	91	ALA
1	2	157	LYS

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	1	318/318 (100%)	305 (96%)	13 (4%)	27	19
1	2	318/318 (100%)	309 (97%)	9 (3%)	38	32
All	All	636/636 (100%)	614 (96%)	22 (4%)	32	24

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	65	LYS
1	1	83	ILE
1	1	88	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	92	LEU
1	1	127	LEU
1	1	167	LEU
1	1	182	LEU
1	1	187	ARG
1	1	248	LEU
1	1	258	VAL
1	1	305	PRO
1	1	308	ASN
1	1	327	ARG
1	2	1	MET
1	2	92	LEU
1	2	113	ARG
1	2	150	LEU
1	2	173	LYS
1	2	177	ARG
1	2	258	VAL
1	2	301	GLN
1	2	327	ARG

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

Mol	Chain	Res	Type
1	1	95	HIS
1	1	246	ASN
1	1	308	ASN
1	1	361	HIS
1	2	95	HIS
1	2	144	GLN
1	2	361	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 57 ligands modelled in this entry, 3 are modelled with single atom and 49 are monoatomic - leaving 5 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
7	DIO	1	832	-	6,6,6	0.74	0	6,6,6	0.21	0
7	DIO	1	831	-	6,6,6	0.75	0	6,6,6	0.27	0
6	POP	1	501	-	6,8,8	1.38	1 (16%)	12,13,13	1.10	1 (8%)
7	DIO	1	830	-	6,6,6	0.56	0	6,6,6	1.20	1 (16%)
6	POP	2	500	-	6,8,8	1.08	0	12,13,13	0.67	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
7	DIO	1	832	-	-	-	0/1/1/1
7	DIO	1	831	-	-	-	0/1/1/1
6	POP	1	501	-	-	1/6/6/6	-
7	DIO	1	830	-	-	-	0/1/1/1
6	POP	2	500	-	-	2/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	501	POP	P2-O5	-2.21	1.46	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	1	501	POP	O5-P2-O	2.23	112.12	104.64
7	1	830	DIO	C2-O1-C1	2.08	116.60	109.88

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	2	500	POP	P1-O-P2-O6
6	1	501	POP	P1-O-P2-O4
6	2	500	POP	P1-O-P2-O4

There are no ring outliers.

No monomer is involved in short contacts.

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	1	372/372 (100%)	0.52	39 (10%)	11 12	15, 28, 57, 79	0
1	2	372/372 (100%)	0.36	30 (8%)	18 19	16, 28, 49, 62	0
All	All	744/744 (100%)	0.44	69 (9%)	14 15	15, 28, 52, 79	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	90	TYR	11.3
1	1	87	PHE	9.0
1	1	91	ALA	8.0
1	2	92	LEU	4.8
1	1	169	ASN	4.8
1	1	92	LEU	4.5
1	1	107	LYS	4.2
1	2	87	PHE	4.1
1	1	1	MET	4.0
1	1	254	GLU	3.9
1	1	108	LEU	3.9
1	1	89	SER	3.7
1	1	111	VAL	3.7
1	1	88	GLN	3.6
1	2	156	ARG	3.5
1	2	169	ASN	3.4
1	2	1	MET	3.3
1	1	95	HIS	3.3
1	1	94	PRO	3.3
1	1	112	PRO	3.2
1	2	90	TYR	3.0
1	2	113	ARG	2.9
1	2	154	ILE	2.9
1	2	89	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2	170	LEU	2.8
1	1	170	LEU	2.8
1	1	86	VAL	2.8
1	1	106	LEU	2.7
1	2	114	GLN	2.7
1	1	93	TYR	2.7
1	2	274	VAL	2.7
1	1	109	ARG	2.7
1	2	118	GLN	2.7
1	2	254	GLU	2.7
1	2	306	GLY	2.6
1	2	278	LEU	2.6
1	1	114	GLN	2.6
1	2	171	ASP	2.6
1	1	134	ASN	2.6
1	1	215	ARG	2.5
1	2	2	ALA	2.5
1	1	138	ARG	2.5
1	1	140	LEU	2.4
1	1	279	GLY	2.4
1	2	86	VAL	2.4
1	1	115	GLU	2.4
1	1	249	ASP	2.3
1	2	85	MET	2.3
1	1	110	LYS	2.2
1	2	91	ALA	2.2
1	1	281	VAL	2.2
1	2	126	LEU	2.2
1	1	2	ALA	2.2
1	2	371	ILE	2.2
1	2	275	LEU	2.2
1	1	301	GLN	2.1
1	2	88	GLN	2.1
1	2	251	ILE	2.1
1	2	64	ASP	2.1
1	1	303	ARG	2.1
1	2	281	VAL	2.1
1	1	256	GLY	2.1
1	1	274	VAL	2.1
1	2	187	ARG	2.1
1	1	261	GLY	2.0
1	2	134	ASN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1	152	ARG	2.0
1	1	104	PHE	2.0
1	1	257	PHE	2.0

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

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

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
4	NA	2	439	1/1	0.68	0.24	63,63,63,63	0
6	POP	1	501	9/9	0.76	0.24	31,33,34,36	9
3	CL	1	391	1/1	0.77	0.25	78,78,78,78	0
5	MG	1	392	1/1	0.79	0.21	60,60,60,60	0
4	NA	1	414	1/1	0.81	0.18	52,52,52,52	0
3	CL	2	395	1/1	0.82	0.29	74,74,74,74	0
3	CL	2	396	1/1	0.82	0.20	74,74,74,74	0
7	DIO	1	832	6/6	0.82	0.20	47,49,49,50	0
6	POP	2	500	9/9	0.83	0.20	28,33,37,37	9
4	NA	1	387	1/1	0.84	0.21	59,59,59,59	0
4	NA	2	424	1/1	0.85	0.16	57,57,57,57	0
4	NA	1	389	1/1	0.85	0.15	56,56,56,56	0
4	NA	1	422	1/1	0.86	0.16	56,56,56,56	0
4	NA	2	392	1/1	0.86	0.19	52,52,52,52	0
4	NA	1	394	1/1	0.86	0.13	57,57,57,57	0
3	CL	2	430	1/1	0.86	0.18	82,82,82,82	0
5	MG	2	389	1/1	0.87	0.19	55,55,55,55	0
4	NA	2	384	1/1	0.87	0.22	59,59,59,59	0
4	NA	2	388	1/1	0.87	0.18	50,50,50,50	0
5	MG	1	393	1/1	0.87	0.14	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	1	376	1/1	0.88	0.20	40,40,40,40	0
5	MG	1	384	1/1	0.88	0.14	48,48,48,48	0
4	NA	2	397	1/1	0.88	0.32	61,61,61,61	0
7	DIO	1	831	6/6	0.88	0.13	39,41,41,42	0
4	NA	1	388	1/1	0.88	0.15	50,50,50,50	0
7	DIO	1	830	6/6	0.89	0.10	15,20,23,26	0
5	MG	2	387	1/1	0.89	0.30	45,45,45,45	0
4	NA	2	391	1/1	0.89	0.14	60,60,60,60	0
4	NA	2	394	1/1	0.92	0.15	54,54,54,54	0
3	CL	2	381	1/1	0.93	0.40	55,55,55,55	0
4	NA	2	380	1/1	0.93	0.09	41,41,41,41	0
3	CL	1	381	1/1	0.93	0.31	61,61,61,61	0
4	NA	1	386	1/1	0.93	0.19	43,43,43,43	0
2	NH4	2	374	1/1	0.93	0.10	26,26,26,26	0
5	MG	2	386	1/1	0.94	0.24	54,54,54,54	0
4	NA	1	383	1/1	0.94	0.19	40,40,40,40	0
5	MG	2	393	1/1	0.95	0.12	53,53,53,53	0
4	NA	1	385	1/1	0.95	0.17	42,42,42,42	0
4	NA	1	379	1/1	0.95	0.13	40,40,40,40	0
4	NA	2	390	1/1	0.95	0.24	44,44,44,44	0
2	NH4	1	373	1/1	0.95	0.07	22,22,22,22	0
4	NA	2	383	1/1	0.95	0.09	40,40,40,40	0
4	NA	2	382	1/1	0.96	0.06	46,46,46,46	0
3	CL	2	378	1/1	0.96	0.32	45,45,45,45	0
5	MG	2	385	1/1	0.96	0.10	42,42,42,42	0
4	NA	1	382	1/1	0.96	0.15	44,44,44,44	0
4	NA	2	377	1/1	0.97	0.10	31,31,31,31	0
5	MG	1	378	1/1	0.97	0.06	38,38,38,38	0
2	NH4	2	373	1/1	0.97	0.06	24,24,24,24	0
4	NA	1	390	1/1	0.97	0.06	47,47,47,47	0
4	NA	1	380	1/1	0.97	0.08	39,39,39,39	0
5	MG	2	379	1/1	0.97	0.15	35,35,35,35	0
3	CL	1	375	1/1	0.97	0.24	46,46,46,46	0
4	NA	1	377	1/1	0.97	0.14	33,33,33,33	0
5	MG	2	375	1/1	0.98	0.12	28,28,28,28	0
3	CL	2	376	1/1	0.99	0.23	40,40,40,40	0
3	CL	1	374	1/1	0.99	0.18	39,39,39,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.