



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:41 AM GMT

PDB ID : 2DRE
Title : Crystal structure of Water-soluble chlorophyll protein from lepidium virginicum at 2.00 angstrom resolution
Authors : Horigome, D.; Satoh, H.; Itoh, N.; Mitsunaga, K.; Oonishi, I.; Nakagawa, A.; Uchida, A.
Deposited on : 2006-06-08
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

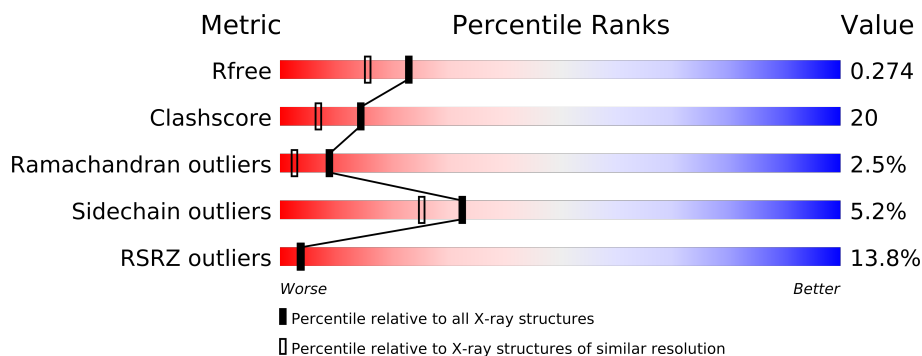
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	180	
1	B	180	
1	C	180	
1	D	180	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CLA	A	1001	-	X
2	CLA	B	1001	-	X
2	CLA	C	1001	-	X

2 Entry composition i

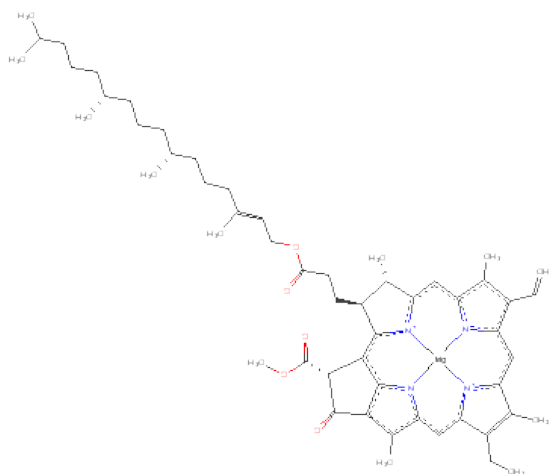
There are 3 unique types of molecules in this entry. The entry contains 6168 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Water-soluble chlorophyll protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1318	831	219	266	2			
1	B	173	Total	C	N	O	S	0	0	0
			1321	830	218	271	2			
1	C	177	Total	C	N	O	S	0	0	0
			1357	851	223	281	2			
1	D	177	Total	C	N	O	S	0	0	0
			1357	851	223	281	2			

- Molecule 2 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
2	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

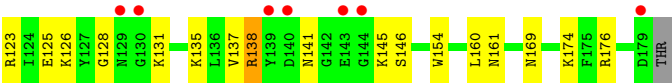
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
2	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	150	Total	O	0	0
			150	150		
3	B	156	Total	O	0	0
			156	156		
3	C	139	Total	O	0	0
			139	139		
3	D	110	Total	O	0	0
			110	110		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.06Å 82.73Å 121.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.99 – 2.00 29.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (28.99-2.00) 99.6 (29.30-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.280 0.240 , 0.274	Depositor DCC
R_{free} test set	2489 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 50391 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6168	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA

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	0.52	1/1349 (0.1%)	0.79	4/1838 (0.2%)
1	B	0.44	0/1351	0.82	3/1840 (0.2%)
1	C	0.33	0/1389	0.67	0/1894
1	D	0.35	0/1389	0.67	0/1894
All	All	0.41	1/5478 (0.0%)	0.74	7/7466 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	PRO	N-CD	-11.64	1.31	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	ARG	N-CA-C	9.46	136.55	111.00
1	A	69	SER	N-CA-C	7.18	130.38	111.00
1	B	28	ASP	C-N-CA	6.42	137.76	121.70
1	A	141	ASN	CA-C-N	-6.39	103.42	116.20
1	B	29	ASN	N-CA-C	5.88	126.86	111.00
1	A	141	ASN	C-N-CA	5.73	134.34	122.30
1	A	141	ASN	O-C-N	5.06	131.81	123.20

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1318	0	1278	51	0
1	B	1321	0	1276	66	0
1	C	1357	0	1300	44	0
1	D	1357	0	1300	55	0
2	A	65	0	72	5	0
2	B	65	0	72	12	0
2	C	65	0	72	5	0
2	D	65	0	72	6	0
3	A	150	0	0	3	0
3	B	156	0	0	9	0
3	C	139	0	0	7	0
3	D	110	0	0	12	0
All	All	6168	0	5442	216	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (216) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:151:LYS:HD2	1:C:151:LYS:H	1.10	1.11
1:B:29:ASN:ND2	1:B:29:ASN:O	1.97	0.97
1:D:29:ASN:N	1:D:29:ASN:HD22	1.61	0.97
1:D:29:ASN:H	1:D:29:ASN:ND2	1.62	0.94
1:D:29:ASN:H	1:D:29:ASN:HD22	0.89	0.85
1:B:123:ARG:HB2	1:B:137:VAL:HG23	1.58	0.85
1:A:2:ASN:HB2	3:A:1151:HOH:O	1.76	0.84
1:C:151:LYS:HD2	1:C:151:LYS:N	1.90	0.82
1:B:131:LYS:HG2	3:B:1155:HOH:O	1.80	0.82
1:B:26:ALA:HB2	1:B:174:LYS:HG3	1.63	0.81
1:C:127:TYR:CE1	1:C:167:ASP:HB3	2.16	0.80
1:D:25:PRO:HG2	1:D:51:ARG:HE	1.47	0.80
1:A:138:ARG:HH11	1:A:138:ARG:HG3	1.46	0.80
1:B:100:VAL:HG21	1:B:138:ARG:HD3	1.63	0.79
1:C:3:ASP:HB2	1:C:78:ASN:HD22	1.48	0.78
1:B:123:ARG:HB2	1:B:137:VAL:CG2	2.14	0.76
1:B:8:LYS:HE2	1:B:132:ASN:ND2	2.00	0.76
1:C:179:ASP:HA	3:C:1095:HOH:O	1.87	0.75
1:C:6:PRO:HA	1:C:76:LEU:HD23	1.71	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:96:LYS:HE3	3:C:1037:HOH:O	1.90	0.72
1:D:65:SER:OG	1:D:82:ALA:HB3	1.89	0.71
1:D:131:LYS:HG2	3:D:1085:HOH:O	1.90	0.71
1:B:131:LYS:H	1:B:131:LYS:HD2	1.55	0.70
1:B:29:ASN:O	1:B:29:ASN:CG	2.32	0.68
1:A:44:LEU:HD12	2:D:1001:CLA:HBB2	1.75	0.68
1:A:66:THR:O	1:A:66:THR:HG23	1.93	0.68
1:B:114:ASP:HB3	1:B:117:SER:HB3	1.75	0.68
1:A:153:LEU:HD12	1:C:41:LEU:HD11	1.75	0.67
1:D:114:ASP:HB3	1:D:117:SER:HB3	1.74	0.67
1:B:101:ASP:HB3	3:B:1017:HOH:O	1.94	0.66
1:B:131:LYS:HD2	1:B:131:LYS:N	2.11	0.66
1:A:17:ILE:HG12	1:A:18:GLU:HG2	1.78	0.65
1:B:78:ASN:HD22	1:B:78:ASN:N	1.94	0.65
1:A:153:LEU:CD1	1:C:41:LEU:HD11	2.27	0.64
1:A:65:SER:OG	1:A:82:ALA:HB3	1.98	0.64
1:B:106:GLU:O	1:B:159:VAL:HB	1.98	0.63
1:D:126:LYS:HD3	3:D:1102:HOH:O	1.98	0.63
1:B:60:LEU:HD12	1:B:61:PRO:HD3	1.79	0.62
1:D:26:ALA:HB1	1:D:174:LYS:HE3	1.81	0.62
1:A:38:ASN:HD21	1:A:153:LEU:HD23	1.64	0.62
1:C:4:GLU:HG3	3:C:1133:HOH:O	2.00	0.62
1:B:104:SER:HB3	3:B:1017:HOH:O	1.98	0.62
1:B:78:ASN:HD22	1:B:78:ASN:H	1.48	0.62
1:A:42:SER:HB3	3:A:1111:HOH:O	1.99	0.61
1:D:114:ASP:HB3	1:D:117:SER:CB	2.31	0.60
1:B:8:LYS:HE2	1:B:132:ASN:HD21	1.66	0.60
1:D:77:THR:HG21	3:D:1060:HOH:O	2.00	0.60
1:D:169:ASN:ND2	3:D:1073:HOH:O	2.35	0.60
1:C:151:LYS:CD	1:C:151:LYS:H	1.97	0.59
1:A:44:LEU:HD13	1:D:44:LEU:HD13	1.84	0.59
1:D:8:LYS:HE3	3:D:1111:HOH:O	2.01	0.59
1:A:178:VAL:O	1:A:179:ASP:HB2	2.02	0.59
1:B:26:ALA:CB	1:B:174:LYS:HG3	2.32	0.59
2:A:1001:CLA:H11	1:B:89:ILE:HD11	1.84	0.59
1:D:6:PRO:HA	1:D:76:LEU:HD13	1.85	0.59
1:B:167:ASP:O	1:B:167:ASP:OD2	2.21	0.59
1:A:89:ILE:HD12	2:B:1001:CLA:H43	1.85	0.59
2:D:1001:CLA:HBB1	2:D:1001:CLA:HHC	1.86	0.58
1:D:25:PRO:HG2	1:D:51:ARG:NE	2.17	0.58
2:A:1001:CLA:HBB2	1:D:44:LEU:HD12	1.85	0.58
1:D:28:ASP:O	1:D:51:ARG:NH2	2.35	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:1001:CLA:HMB3	2:B:1001:CLA:H121	1.84	0.57
1:B:137:VAL:HA	1:B:145:LYS:O	2.04	0.57
1:D:29:ASN:ND2	1:D:29:ASN:N	2.35	0.57
1:D:25:PRO:HG2	1:D:51:ARG:HG3	1.87	0.57
1:A:67:PRO:HB3	1:A:121:PHE:CZ	2.39	0.56
1:A:138:ARG:HH11	1:A:138:ARG:CG	2.17	0.56
1:B:38:ASN:OD1	2:B:1001:CLA:HMB2	2.06	0.56
1:B:44:LEU:HD12	2:C:1001:CLA:HBB2	1.86	0.56
1:B:37:ALA:HB3	1:B:50:VAL:CG2	2.36	0.56
2:B:1001:CLA:HBB2	1:C:44:LEU:HD12	1.87	0.55
1:D:6:PRO:CA	1:D:76:LEU:HD13	2.36	0.55
1:D:78:ASN:OD1	1:D:125:GLU:HG2	2.05	0.55
1:A:123:ARG:HD2	1:A:139:TYR:CE1	2.41	0.55
2:B:1001:CLA:H171	2:D:1001:CLA:H18	1.90	0.54
1:C:3:ASP:N	1:C:78:ASN:HB2	2.22	0.54
1:C:25:PRO:HG2	1:C:51:ARG:HG2	1.89	0.54
1:A:7:VAL:HG22	1:A:77:THR:HG22	1.89	0.54
1:D:125:GLU:OE1	1:D:135:LYS:HE3	2.08	0.54
1:C:17:ILE:HD11	1:C:73:ASN:OD1	2.08	0.54
1:D:66:THR:HG23	3:D:1078:HOH:O	2.07	0.54
1:B:78:ASN:N	1:B:78:ASN:ND2	2.54	0.53
2:B:1001:CLA:H201	1:D:154:TRP:HZ2	1.72	0.53
1:A:138:ARG:HG3	1:A:138:ARG:NH1	2.19	0.53
1:B:118:GLY:HA2	1:B:121:PHE:CD1	2.44	0.53
1:C:71:GLU:HB3	3:C:1091:HOH:O	2.09	0.53
1:A:8:LYS:HD3	1:A:12:GLY:O	2.08	0.53
1:D:27:SER:OG	1:D:28:ASP:N	2.42	0.53
1:B:44:LEU:HG	1:C:91:LEU:HB3	1.91	0.53
1:B:127:TYR:CZ	1:B:172:PRO:HG3	2.44	0.53
1:A:151:LYS:NZ	3:A:1022:HOH:O	2.41	0.53
1:A:67:PRO:HD2	1:A:80:ASN:O	2.09	0.52
1:A:15:LEU:HB3	1:A:75:VAL:HB	1.91	0.52
1:A:16:LYS:HA	1:A:73:ASN:O	2.09	0.52
1:C:154:TRP:HH2	2:C:1001:CLA:H202	1.73	0.52
1:A:107:LYS:HD3	1:A:107:LYS:N	2.24	0.52
1:D:65:SER:HG	1:D:82:ALA:HB3	1.71	0.52
1:D:26:ALA:CB	1:D:174:LYS:HE3	2.39	0.52
1:D:138:ARG:HG2	1:D:160:LEU:HD11	1.91	0.52
1:B:179:ASP:HA	3:B:1002:HOH:O	2.09	0.52
1:B:72:GLY:C	1:B:73:ASN:HD22	2.13	0.52
1:A:38:ASN:ND2	1:A:153:LEU:HD23	2.26	0.51
1:C:129:ASN:HD22	1:C:129:ASN:C	2.13	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:25:PRO:HG2	1:D:51:ARG:CG	2.41	0.51
1:A:66:THR:O	1:A:66:THR:CG2	2.59	0.51
1:A:104:SER:O	1:A:107:LYS:HD3	2.12	0.50
1:D:100:VAL:HG21	1:D:138:ARG:HD2	1.93	0.50
1:B:165:ASP:OD2	1:B:165:ASP:O	2.29	0.50
1:A:119:GLU:HA	1:A:138:ARG:NH2	2.27	0.50
1:A:2:ASN:OD1	1:A:2:ASN:C	2.49	0.50
1:A:67:PRO:HB3	1:A:121:PHE:CE2	2.47	0.49
1:C:4:GLU:O	1:C:76:LEU:HD22	2.11	0.49
1:B:8:LYS:HE3	3:B:1067:HOH:O	2.12	0.49
1:A:106:GLU:CD	1:A:106:GLU:N	2.66	0.49
1:B:25:PRO:HG2	1:B:51:ARG:HD2	1.95	0.49
1:B:162:ASP:O	1:B:164:ASP:N	2.39	0.49
1:A:41:LEU:HA	2:C:1001:CLA:H191	1.95	0.49
1:C:6:PRO:CA	1:C:76:LEU:HD23	2.42	0.49
1:B:37:ALA:HB3	1:B:50:VAL:HG21	1.94	0.49
1:A:16:LYS:NZ	1:A:74:ASP:OD1	2.40	0.48
1:D:8:LYS:CD	3:D:1086:HOH:O	2.61	0.48
1:C:127:TYR:HB3	1:C:133:THR:HG22	1.96	0.48
2:B:1001:CLA:HBB1	2:B:1001:CLA:HHC	1.95	0.48
1:B:8:LYS:HB2	1:B:132:ASN:ND2	2.28	0.48
1:B:60:LEU:HD12	1:B:61:PRO:CD	2.44	0.47
1:B:29:ASN:HA	1:B:51:ARG:HH22	1.79	0.47
1:A:25:PRO:HG2	1:A:51:ARG:HG3	1.96	0.47
1:C:140:ASP:OD1	1:C:140:ASP:C	2.51	0.47
1:A:117:SER:HB3	1:A:119:GLU:HG2	1.96	0.47
1:C:118:GLY:HA2	1:C:121:PHE:CD1	2.50	0.47
1:D:27:SER:HB3	3:D:1105:HOH:O	2.14	0.47
1:C:129:ASN:ND2	1:C:129:ASN:O	2.46	0.47
1:B:93:PRO:HG3	1:C:45:CYS:O	2.14	0.47
1:A:81:ILE:HG13	1:A:122:PHE:O	2.15	0.47
1:B:138:ARG:HG2	1:B:160:LEU:CD2	2.45	0.47
1:C:16:LYS:HA	1:C:73:ASN:O	2.15	0.47
1:B:138:ARG:HG2	1:B:160:LEU:HD21	1.96	0.46
2:D:1001:CLA:HED2	2:D:1001:CLA:H61	1.96	0.46
1:B:127:TYR:CE1	1:B:167:ASP:HB2	2.50	0.46
1:D:3:ASP:HA	1:D:78:ASN:HB2	1.97	0.46
1:A:138:ARG:CG	1:A:138:ARG:NH1	2.74	0.46
1:B:22:PHE:CE2	1:B:58:PRO:HB2	2.49	0.46
1:A:78:ASN:OD1	1:A:125:GLU:HG2	2.15	0.46
1:B:17:ILE:HD12	1:B:17:ILE:O	2.15	0.46
1:B:65:SER:OG	1:B:82:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:26:ALA:HB2	1:A:172:PRO:HB2	1.97	0.46
1:A:77:THR:O	1:A:79:THR:HG23	2.17	0.45
1:A:118:GLY:HA2	1:A:121:PHE:CD1	2.50	0.45
2:A:1001:CLA:H201	1:C:153:LEU:HD21	1.98	0.45
1:B:145:LYS:HD3	1:B:160:LEU:HD21	1.99	0.45
1:B:131:LYS:O	3:B:1155:HOH:O	2.21	0.45
2:B:1001:CLA:H193	1:D:41:LEU:CD2	2.46	0.45
1:A:45:CYS:O	1:D:93:PRO:HD3	2.16	0.45
1:C:154:TRP:CH2	2:C:1001:CLA:H202	2.52	0.45
1:B:66:THR:HA	1:B:67:PRO:HD3	1.49	0.45
1:D:79:THR:O	1:D:123:ARG:HG2	2.17	0.44
1:A:89:ILE:HD11	2:B:1001:CLA:H11	2.00	0.44
1:A:38:ASN:OD1	2:A:1001:CLA:HMB2	2.18	0.44
1:D:135:LYS:NZ	3:D:1009:HOH:O	2.51	0.44
1:C:17:ILE:HG12	1:C:73:ASN:HA	1.99	0.44
1:B:136:LEU:HB2	1:B:147:VAL:CG2	2.48	0.44
1:D:25:PRO:CG	1:D:51:ARG:HG3	2.47	0.44
1:D:128:GLY:CA	3:D:1107:HOH:O	2.65	0.44
1:A:105:GLU:HG3	1:A:105:GLU:H	1.43	0.44
1:A:121:PHE:O	1:A:138:ARG:NH1	2.51	0.44
1:B:114:ASP:HB3	1:B:117:SER:CB	2.45	0.43
1:D:26:ALA:HB2	1:D:174:LYS:HG3	2.00	0.43
1:B:80:ASN:N	1:B:123:ARG:HH11	2.17	0.43
1:D:115:PRO:HG3	3:D:1050:HOH:O	2.18	0.43
1:C:138:ARG:HG2	1:C:139:TYR:N	2.33	0.43
1:D:79:THR:HG22	1:D:80:ASN:N	2.34	0.43
1:D:137:VAL:HG13	1:D:145:LYS:O	2.18	0.43
1:C:78:ASN:OD1	1:C:125:GLU:HG2	2.18	0.43
1:B:107:LYS:HA	3:B:1017:HOH:O	2.18	0.43
1:C:138:ARG:HG2	1:C:139:TYR:H	1.83	0.43
1:B:97:THR:HG22	1:B:98:TRP:O	2.19	0.43
1:D:13:ASN:HB3	1:D:14:PRO:HD2	2.01	0.43
2:B:1001:CLA:C20	1:D:154:TRP:HZ2	2.31	0.43
1:B:146:SER:HB2	1:B:165:ASP:HA	2.00	0.43
1:C:17:ILE:HG12	1:C:73:ASN:HB3	2.00	0.42
1:D:4:GLU:O	1:D:76:LEU:HD12	2.19	0.42
1:B:170:ALA:O	1:B:172:PRO:HD3	2.19	0.42
1:D:145:LYS:HB3	1:D:161:ASN:O	2.19	0.42
1:C:3:ASP:HB3	3:C:1127:HOH:O	2.19	0.42
1:A:17:ILE:N	1:A:17:ILE:HD13	2.35	0.42
1:C:24:GLN:HA	1:C:25:PRO:HD3	1.80	0.42
1:B:29:ASN:ND2	1:B:29:ASN:C	2.71	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:75:VAL:HA	3:C:1118:HOH:O	2.19	0.42
1:D:66:THR:HA	1:D:67:PRO:HD3	1.93	0.42
1:A:60:LEU:HD12	1:A:61:PRO:HD2	2.02	0.42
1:C:81:ILE:O	1:C:81:ILE:HD12	2.19	0.42
2:C:1001:CLA:H43	1:D:89:ILE:HG21	2.01	0.42
1:B:161:ASN:HB3	3:B:1144:HOH:O	2.20	0.42
1:A:54:LEU:HB2	1:A:57:GLN:HG2	2.01	0.42
1:B:125:GLU:HB3	3:B:1092:HOH:O	2.20	0.41
1:D:8:LYS:HD2	3:D:1086:HOH:O	2.20	0.41
1:B:5:GLU:O	1:B:77:THR:HG23	2.20	0.41
1:A:27:SER:C	1:A:29:ASN:H	2.23	0.41
1:D:146:SER:O	1:D:161:ASN:ND2	2.53	0.41
1:B:95:SER:N	1:B:112:GLY:HA2	2.36	0.41
2:B:1001:CLA:HED1	2:B:1001:CLA:H93	2.02	0.41
2:B:1001:CLA:HAB	2:B:1001:CLA:HMB1	1.90	0.41
1:B:25:PRO:CG	1:B:51:ARG:HD2	2.50	0.41
1:B:91:LEU:HB3	1:C:44:LEU:HG	2.02	0.41
1:C:151:LYS:CD	1:C:151:LYS:N	2.67	0.41
1:B:154:TRP:CZ2	2:D:1001:CLA:H191	2.55	0.41
1:D:35:VAL:HG11	2:D:1001:CLA:CAD	2.50	0.41
1:B:17:ILE:C	1:B:17:ILE:HD12	2.41	0.41
1:B:118:GLY:HA2	1:B:121:PHE:CE1	2.56	0.41
1:C:13:ASN:HD22	1:C:13:ASN:N	2.19	0.41
1:C:13:ASN:ND2	1:C:13:ASN:N	2.69	0.41
1:D:66:THR:HG23	1:D:66:THR:O	2.20	0.41
1:A:140:ASP:OD2	1:A:145:LYS:HD2	2.21	0.41
1:C:146:SER:O	1:C:161:ASN:HB2	2.20	0.40
1:D:141:ASN:O	1:D:141:ASN:OD1	2.39	0.40
1:C:3:ASP:N	3:C:1131:HOH:O	2.55	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	168/180 (93%)	153 (91%)	9 (5%)	6 (4%)	5	1
1	B	169/180 (94%)	149 (88%)	14 (8%)	6 (4%)	5	1
1	C	175/180 (97%)	164 (94%)	10 (6%)	1 (1%)	33	24
1	D	175/180 (97%)	160 (91%)	11 (6%)	4 (2%)	10	3
All	All	687/720 (95%)	626 (91%)	44 (6%)	17 (2%)	9	2

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	B	104	SER
1	B	163	ASP
1	C	128	GLY
1	D	27	SER
1	A	67	PRO
1	A	141	ASN
1	B	102	SER
1	B	144	GLY
1	D	69	SER
1	A	28	ASP
1	A	70	SER
1	B	162	ASP
1	D	28	ASP
1	D	72	GLY
1	B	25	PRO
1	A	3	ASP

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	150/158 (95%)	138 (92%)	12 (8%)	17	10
1	B	151/158 (96%)	146 (97%)	5 (3%)	50	46
1	C	155/158 (98%)	144 (93%)	11 (7%)	21	14
1	D	155/158 (98%)	151 (97%)	4 (3%)	59	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	611/632 (97%)	579 (95%)	32 (5%)	32	25

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	5	GLU
1	A	17	ILE
1	A	43	HIS
1	A	68	SER
1	A	69	SER
1	A	70	SER
1	A	71	GLU
1	A	105	GLU
1	A	107	LYS
1	A	140	ASP
1	A	151	LYS
1	B	27	SER
1	B	29	ASN
1	B	131	LYS
1	B	138	ARG
1	B	143	GLU
1	C	3	ASP
1	C	30	ASN
1	C	43	HIS
1	C	51	ARG
1	C	69	SER
1	C	71	GLU
1	C	119	GLU
1	C	129	ASN
1	C	140	ASP
1	C	143	GLU
1	C	151	LYS
1	D	29	ASN
1	D	30	ASN
1	D	138	ARG
1	D	176	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	80	ASN
1	B	29	ASN
1	B	43	HIS
1	B	73	ASN
1	B	78	ASN
1	B	129	ASN
1	B	132	ASN
1	C	13	ASN
1	C	30	ASN
1	C	78	ASN
1	C	129	ASN
1	D	29	ASN
1	D	73	ASN
1	D	141	ASN
1	D	169	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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
2	CLA	A	1001	1	73,73,73	1.93	15 (20%)	95,113,113	1.64	15 (15%)
2	CLA	B	1001	1	73,73,73	1.67	14 (19%)	95,113,113	1.57	16 (16%)
2	CLA	C	1001	1	73,73,73	1.83	13 (17%)	95,113,113	1.48	15 (15%)
2	CLA	D	1001	1	73,73,73	1.71	15 (20%)	95,113,113	1.74	20 (21%)

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	CLA	A	1001	1	1/1/20/25	0/37/135/135	0/0/9/9
2	CLA	B	1001	1	1/1/20/25	0/37/135/135	0/0/9/9
2	CLA	C	1001	1	1/1/20/25	0/37/135/135	0/0/9/9
2	CLA	D	1001	1	1/1/20/25	0/37/135/135	0/0/9/9

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	CLA	MG-NB	7.94	2.22	2.05
2	C	1001	CLA	MG-NB	6.28	2.18	2.05
2	D	1001	CLA	MG-NA	5.43	2.23	2.07
2	C	1001	CLA	C3B-C4B	5.33	1.48	1.40
2	A	1001	CLA	MG-NA	5.19	2.22	2.07
2	B	1001	CLA	C3B-C4B	4.90	1.48	1.40
2	A	1001	CLA	C3B-C4B	4.80	1.47	1.40
2	C	1001	CLA	C1B-C2B	4.69	1.46	1.40
2	B	1001	CLA	MG-NC	4.65	2.21	2.07
2	A	1001	CLA	C1B-C2B	4.35	1.45	1.40
2	D	1001	CLA	C3B-C4B	4.30	1.47	1.40
2	B	1001	CLA	C1B-C2B	4.26	1.45	1.40
2	B	1001	CLA	MG-ND	4.25	2.14	2.05
2	D	1001	CLA	C1B-C2B	4.24	1.45	1.40
2	C	1001	CLA	MG-NA	4.20	2.19	2.07
2	C	1001	CLA	C2-C3	4.17	1.41	1.32
2	A	1001	CLA	O2D-CGD	4.06	1.43	1.33
2	C	1001	CLA	O2D-CGD	4.04	1.43	1.33
2	B	1001	CLA	O2D-CGD	3.99	1.43	1.33
2	D	1001	CLA	MG-ND	3.75	2.13	2.05
2	D	1001	CLA	C1A-NA	3.64	1.40	1.32
2	C	1001	CLA	MG-NC	3.63	2.18	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	CLA	C1A-NA	3.62	1.40	1.32
2	D	1001	CLA	O2D-CGD	3.56	1.42	1.33
2	C	1001	CLA	C4B-NB	3.52	1.39	1.34
2	A	1001	CLA	MG-NC	3.47	2.17	2.07
2	D	1001	CLA	CMC-C2C	3.43	1.58	1.51
2	C	1001	CLA	C1A-NA	3.33	1.39	1.32
2	D	1001	CLA	C4B-NB	3.26	1.38	1.34
2	B	1001	CLA	C1A-NA	3.24	1.39	1.32
2	D	1001	CLA	MG-NC	3.24	2.16	2.07
2	D	1001	CLA	MG-NB	3.02	2.11	2.05
2	D	1001	CLA	O1D-CGD	3.00	1.28	1.21
2	B	1001	CLA	C2-C3	2.99	1.39	1.32
2	C	1001	CLA	CMC-C2C	2.99	1.57	1.51
2	A	1001	CLA	O1D-CGD	2.95	1.28	1.21
2	A	1001	CLA	O2A-CGA	2.94	1.42	1.33
2	A	1001	CLA	CMC-C2C	2.93	1.57	1.51
2	B	1001	CLA	O1D-CGD	2.91	1.28	1.21
2	A	1001	CLA	C2-C3	2.88	1.38	1.32
2	A	1001	CLA	C4B-NB	2.79	1.38	1.34
2	C	1001	CLA	O1D-CGD	2.76	1.28	1.21
2	B	1001	CLA	MG-NA	2.70	2.15	2.07
2	D	1001	CLA	C2-C3	2.70	1.38	1.32
2	B	1001	CLA	C4B-NB	2.69	1.38	1.34
2	A	1001	CLA	C3B-CAB	-2.54	1.46	1.49
2	C	1001	CLA	C3B-C2B	-2.35	1.37	1.41
2	A	1001	CLA	CHB-C4A	2.34	1.42	1.36
2	D	1001	CLA	C3B-CAB	-2.34	1.47	1.49
2	D	1001	CLA	O2A-CGA	2.25	1.40	1.33
2	C	1001	CLA	C3B-CAB	-2.21	1.47	1.49
2	D	1001	CLA	C3B-C2B	-2.18	1.37	1.41
2	B	1001	CLA	CHB-C4A	2.10	1.41	1.36
2	B	1001	CLA	C3B-CAB	-2.10	1.47	1.49
2	A	1001	CLA	C3B-C2B	-2.07	1.37	1.41
2	B	1001	CLA	MG-NB	2.03	2.09	2.05
2	B	1001	CLA	O2A-CGA	2.02	1.39	1.33

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	CLA	C2B-C3B-CAB	-5.75	115.57	127.33
2	D	1001	CLA	CMB-C2B-C1B	-5.64	119.94	128.62
2	D	1001	CLA	CBC-CAC-C3C	-5.60	95.45	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	CLA	C2B-C3B-CAB	-5.43	116.22	127.33
2	A	1001	CLA	C4B-C3B-CAB	5.29	137.89	127.18
2	C	1001	CLA	C2B-C3B-CAB	-5.17	116.74	127.33
2	D	1001	CLA	C2B-C3B-CAB	-5.07	116.95	127.33
2	B	1001	CLA	C4B-C3B-CAB	5.00	137.31	127.18
2	A	1001	CLA	CMD-C2D-C3D	4.98	132.82	124.97
2	D	1001	CLA	C4B-C3B-CAB	4.77	136.84	127.18
2	C	1001	CLA	C4B-C3B-CAB	4.73	136.75	127.18
2	B	1001	CLA	C4A-NA-C1A	4.16	112.25	106.52
2	A	1001	CLA	C4A-NA-C1A	4.00	112.03	106.52
2	C	1001	CLA	C4A-NA-C1A	3.94	111.95	106.52
2	A	1001	CLA	CMB-C2B-C1B	-3.91	122.61	128.62
2	D	1001	CLA	C4A-NA-C1A	3.81	111.78	106.52
2	D	1001	CLA	OBD-CAD-CBD	-3.32	120.92	125.94
2	A	1001	CLA	O2A-CGA-CBA	3.23	122.11	111.94
2	A	1001	CLA	OBD-CAD-CBD	-3.18	121.14	125.94
2	B	1001	CLA	C6-C5-C3	-3.18	105.23	112.78
2	D	1001	CLA	O2A-CGA-CBA	3.10	121.69	111.94
2	B	1001	CLA	O2A-CGA-CBA	3.10	121.68	111.94
2	B	1001	CLA	CMB-C2B-C1B	-3.04	123.94	128.62
2	B	1001	CLA	OBD-CAD-CBD	-3.04	121.35	125.94
2	D	1001	CLA	C1-C2-C3	3.03	131.57	126.19
2	C	1001	CLA	O2A-CGA-CBA	2.99	121.36	111.94
2	C	1001	CLA	OBD-CAD-CBD	-2.99	121.43	125.94
2	B	1001	CLA	O2D-CGD-CBD	2.96	117.35	111.33
2	D	1001	CLA	C3C-C4C-NC	-2.79	106.59	110.05
2	A	1001	CLA	O2D-CGD-CBD	2.73	116.90	111.33
2	D	1001	CLA	O2D-CGD-CBD	2.66	116.75	111.33
2	C	1001	CLA	O2D-CGD-CBD	2.60	116.62	111.33
2	A	1001	CLA	C2C-C1C-NC	-2.57	108.09	110.17
2	A	1001	CLA	C3B-CAB-CBB	-2.56	120.66	125.95
2	D	1001	CLA	C3B-CAB-CBB	-2.50	120.78	125.95
2	C	1001	CLA	C2C-C1C-NC	-2.47	108.16	110.17
2	C	1001	CLA	CMB-C2B-C1B	-2.43	124.89	128.62
2	C	1001	CLA	CMA-C3A-C2A	-2.43	103.71	114.14
2	A	1001	CLA	C2A-C3A-C4A	2.39	105.08	101.40
2	B	1001	CLA	C1-C2-C3	2.38	130.42	126.19
2	A	1001	CLA	C3C-C4C-NC	-2.29	107.21	110.05
2	C	1001	CLA	C1D-C2D-C3D	-2.29	104.91	106.78
2	B	1001	CLA	C3C-C4C-NC	-2.28	107.23	110.05
2	D	1001	CLA	CHD-C4C-NC	2.24	126.65	124.47
2	D	1001	CLA	C2A-C3A-C4A	2.22	104.82	101.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	CLA	C3A-C2A-C1A	2.21	104.21	101.08
2	D	1001	CLA	C3A-C2A-C1A	2.20	104.19	101.08
2	B	1001	CLA	C2A-C3A-C4A	2.17	104.74	101.40
2	A	1001	CLA	CMD-C2D-C1D	-2.17	121.88	126.16
2	A	1001	CLA	CED-O2D-CGD	2.16	121.17	116.02
2	B	1001	CLA	O1D-CGD-CBD	-2.16	119.99	124.42
2	C	1001	CLA	C2A-C3A-C4A	2.16	104.72	101.40
2	C	1001	CLA	CED-O2D-CGD	2.14	121.12	116.02
2	B	1001	CLA	C4B-NB-C1B	2.13	109.57	106.76
2	D	1001	CLA	CMB-C2B-C3B	2.13	128.33	124.97
2	D	1001	CLA	CED-O2D-CGD	2.13	121.08	116.02
2	A	1001	CLA	C1-C2-C3	2.12	129.95	126.19
2	D	1001	CLA	C3B-C2B-C1B	2.11	108.24	107.00
2	C	1001	CLA	C2A-C1A-CHA	2.11	127.49	123.83
2	B	1001	CLA	CMB-C2B-C3B	2.10	128.28	124.97
2	B	1001	CLA	C1D-C2D-C3D	-2.07	105.09	106.78
2	C	1001	CLA	C3C-C4C-NC	-2.06	107.50	110.05
2	D	1001	CLA	C1C-NC-C4C	2.05	108.97	106.36
2	D	1001	CLA	C2A-C1A-CHA	2.04	127.37	123.83
2	B	1001	CLA	C3A-C2A-C1A	2.03	103.95	101.08
2	D	1001	CLA	C1D-C2D-C3D	-2.02	105.13	106.78

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1001	CLA	C8
2	B	1001	CLA	C8
2	C	1001	CLA	C8
2	D	1001	CLA	C8

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	172/180 (95%)	0.79	23 (13%) 4 4	18, 34, 72, 84	0
1	B	173/180 (96%)	1.10	30 (17%) 2 2	25, 43, 77, 88	0
1	C	177/180 (98%)	0.69	16 (9%) 10 9	16, 38, 72, 86	0
1	D	177/180 (98%)	0.85	24 (13%) 4 3	19, 42, 71, 91	0
All	All	699/720 (97%)	0.86	93 (13%) 4 4	16, 40, 74, 91	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ASN	6.8
1	A	143	GLU	6.6
1	D	3	ASP	6.1
1	A	141	ASN	6.0
1	C	69	SER	6.0
1	B	163	ASP	5.9
1	A	3	ASP	5.7
1	D	69	SER	5.7
1	C	140	ASP	5.6
1	A	140	ASP	5.5
1	D	70	SER	5.2
1	D	129	ASN	5.2
1	B	129	ASN	5.1
1	B	143	GLU	5.0
1	A	142	GLY	4.9
1	C	143	GLU	4.8
1	B	142	GLY	4.8
1	B	28	ASP	4.7
1	B	70	SER	4.7
1	B	130	GLY	4.6
1	A	70	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	105	GLU	4.3
1	B	69	SER	4.3
1	C	142	GLY	4.3
1	B	68	SER	4.3
1	C	71	GLU	4.1
1	A	179	ASP	4.1
1	A	30	ASN	4.1
1	B	30	ASN	4.0
1	C	70	SER	3.7
1	B	29	ASN	3.7
1	D	139	TYR	3.6
1	B	166	SER	3.5
1	B	164	ASP	3.5
1	D	71	GLU	3.5
1	D	116	LYS	3.4
1	B	27	SER	3.3
1	B	103	SER	3.3
1	A	29	ASN	3.3
1	B	26	ALA	3.1
1	C	129	ASN	3.1
1	B	49	ILE	3.1
1	A	144	GLY	3.1
1	A	71	GLU	3.1
1	D	30	ASN	3.0
1	D	144	GLY	2.9
1	C	168	GLU	2.9
1	D	68	SER	2.9
1	C	131	LYS	2.9
1	A	83	ILE	2.8
1	A	67	PRO	2.8
1	C	4	GLU	2.8
1	D	130	GLY	2.8
1	B	167	ASP	2.7
1	D	143	GLU	2.7
1	B	115	PRO	2.7
1	C	3	ASP	2.6
1	D	179	ASP	2.6
1	A	28	ASP	2.6
1	B	79	THR	2.5
1	A	103	SER	2.4
1	D	140	ASP	2.4
1	D	78	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	76	LEU	2.4
1	A	162	ASP	2.4
1	B	75	VAL	2.3
1	B	128	GLY	2.3
1	D	83	ILE	2.3
1	D	4	GLU	2.3
1	C	102	SER	2.3
1	A	23	ILE	2.3
1	A	102	SER	2.2
1	D	103	SER	2.2
1	D	67	PRO	2.2
1	A	4	GLU	2.2
1	A	169	ASN	2.2
1	A	68	SER	2.2
1	C	29	ASN	2.2
1	D	29	ASN	2.2
1	C	5	GLU	2.2
1	D	28	ASP	2.2
1	B	168	GLU	2.1
1	C	30	ASN	2.1
1	C	136	LEU	2.1
1	B	48	GLY	2.1
1	B	138	ARG	2.1
1	B	165	ASP	2.1
1	D	6	PRO	2.1
1	B	162	ASP	2.1
1	A	145	LYS	2.0
1	D	72	GLY	2.0
1	D	62	VAL	2.0
1	B	158	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CLA	A	1001	65/65	0.19	2.37	20,26,67,70	0
2	CLA	B	1001	65/65	0.21	2.30	22,28,60,63	0
2	CLA	C	1001	65/65	0.18	2.19	15,22,64,69	0
2	CLA	D	1001	65/65	0.19	1.90	15,24,57,61	0

6.5 Other polymers

There are no such residues in this entry.