



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:38 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 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

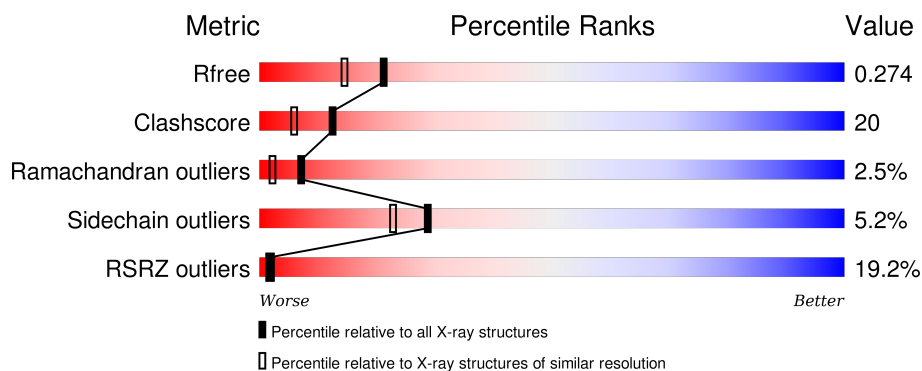
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. 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	180	<div> <div>18%</div> <div>60%</div> <div>29%</div> <div>6%</div> <div>..</div> </div>
1	B	180	<div> <div>24%</div> <div>58%</div> <div>35%</div> <div>..</div> <div>..</div> </div>
1	C	180	<div> <div>16%</div> <div>75%</div> <div>20%</div> <div>..</div> <div>..</div> </div>
1	D	180	<div> <div>17%</div> <div>71%</div> <div>26%</div> <div>..</div> <div>..</div> </div>

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 crite-

ria:

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

2 Entry composition [i](#)

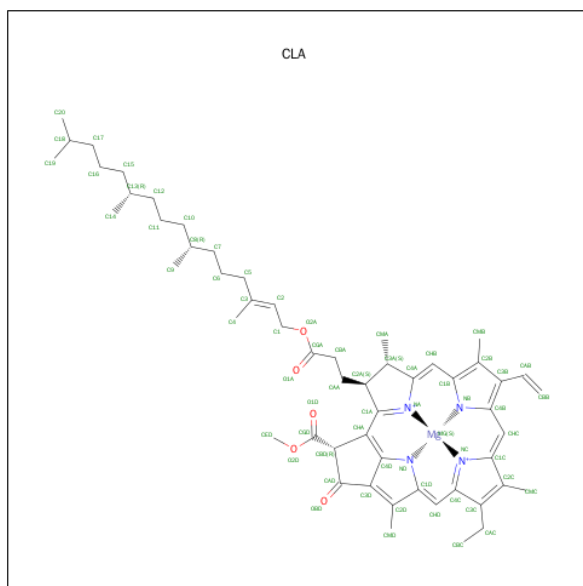
There are 3 unique types of molecules in this entry. The entry contains 6168 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 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		

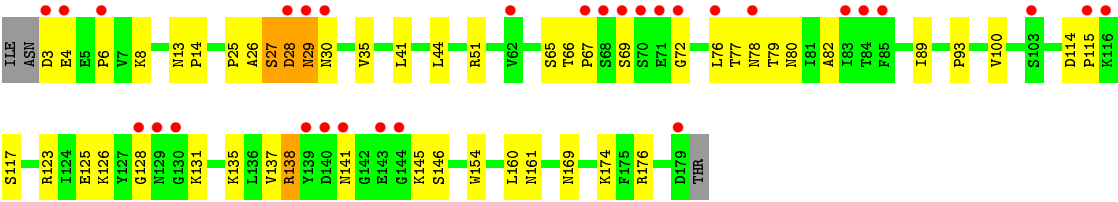
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
2	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- 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	73.06 Å 82.73 Å 121.88 Å 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 2.00 Å)	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)	0.35 , 57.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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	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

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 20.

All (216) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:ASP:O	1:D:51:ARG:NH2	2.35	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [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	168/180 (93%)	153 (91%)	9 (5%)	6 (4%)	4	1
1	B	169/180 (94%)	149 (88%)	14 (8%)	6 (4%)	4	1
1	C	175/180 (97%)	164 (94%)	10 (6%)	1 (1%)	30	22
1	D	175/180 (97%)	160 (91%)	11 (6%)	4 (2%)	8	3
All	All	687/720 (95%)	626 (91%)	44 (6%)	17 (2%)	7	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 [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	150/158 (95%)	138 (92%)	12 (8%)	15	9
1	B	151/158 (96%)	146 (97%)	5 (3%)	45	43
1	C	155/158 (98%)	144 (93%)	11 (7%)	18	12
1	D	155/158 (98%)	151 (97%)	4 (3%)	54	54
All	All	611/632 (97%)	579 (95%)	32 (5%)	29	23

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

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Mol	Chain	Res	Type
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 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 ⓘ

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	55,73,73	1.29	7 (12%)	61,113,113	1.58	12 (19%)
2	CLA	B	1001	1	55,73,73	1.20	6 (10%)	61,113,113	1.54	10 (16%)
2	CLA	C	1001	1	55,73,73	1.29	5 (9%)	61,113,113	1.46	9 (14%)
2	CLA	D	1001	1	55,73,73	1.21	6 (10%)	61,113,113	1.74	11 (18%)

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	4/4/20/25	0/37/135/135	0/0/9/9
2	CLA	B	1001	1	4/4/20/25	0/37/135/135	0/0/9/9
2	CLA	C	1001	1	4/4/20/25	0/37/135/135	0/0/9/9
2	CLA	D	1001	1	4/4/20/25	0/37/135/135	0/0/9/9

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	CLA	C3B-C2B	-2.36	1.37	1.40
2	D	1001	CLA	C3B-C2B	-2.15	1.37	1.40
2	B	1001	CLA	CMC-C2C	2.05	1.55	1.50
2	B	1001	CLA	O2A-CGA	2.08	1.39	1.33
2	A	1001	CLA	CHC-C1C	2.08	1.41	1.35
2	B	1001	CLA	CHC-C1C	2.21	1.42	1.35
2	A	1001	CLA	CMD-C2D	2.29	1.56	1.51
2	D	1001	CLA	O2A-CGA	2.33	1.40	1.33
2	D	1001	CLA	C2-C3	2.76	1.38	1.33
2	C	1001	CLA	O1D-CGD	2.76	1.28	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	CLA	O1D-CGD	2.91	1.28	1.21
2	A	1001	CLA	C2-C3	2.95	1.38	1.33
2	A	1001	CLA	O1D-CGD	2.95	1.28	1.21
2	D	1001	CLA	O1D-CGD	3.00	1.28	1.21
2	A	1001	CLA	CMC-C2C	3.02	1.57	1.50
2	A	1001	CLA	O2A-CGA	3.05	1.42	1.33
2	B	1001	CLA	C2-C3	3.06	1.39	1.33
2	C	1001	CLA	CMC-C2C	3.08	1.57	1.50
2	D	1001	CLA	CMC-C2C	3.53	1.58	1.50
2	D	1001	CLA	O2D-CGD	3.67	1.42	1.33
2	B	1001	CLA	O2D-CGD	4.12	1.43	1.33
2	C	1001	CLA	O2D-CGD	4.17	1.43	1.33
2	A	1001	CLA	O2D-CGD	4.19	1.43	1.33
2	C	1001	CLA	C2-C3	4.28	1.41	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	CLA	CBC-CAC-C3C	-5.55	95.45	112.39
2	D	1001	CLA	CMB-C2B-C1B	-5.09	119.94	128.36
2	A	1001	CLA	CMB-C2B-C1B	-3.48	122.61	128.36
2	D	1001	CLA	OBD-CAD-CBD	-3.32	120.92	125.94
2	B	1001	CLA	C6-C5-C3	-3.31	105.23	112.48
2	B	1001	CLA	O1D-CGD-CBD	-3.23	119.99	124.62
2	A	1001	CLA	OBD-CAD-CBD	-3.18	121.14	125.94
2	B	1001	CLA	OBD-CAD-CBD	-3.04	121.35	125.94
2	C	1001	CLA	OBD-CAD-CBD	-2.99	121.43	125.94
2	C	1001	CLA	O1D-CGD-CBD	-2.95	120.39	124.62
2	A	1001	CLA	C2C-C1C-NC	-2.90	108.09	110.24
2	C	1001	CLA	C2C-C1C-NC	-2.79	108.16	110.24
2	A	1001	CLA	C3B-CAB-CBB	-2.77	120.66	126.32
2	D	1001	CLA	C3B-CAB-CBB	-2.71	120.78	126.32
2	B	1001	CLA	CMB-C2B-C1B	-2.67	123.94	128.36
2	A	1001	CLA	O1D-CGD-CBD	-2.62	120.86	124.62
2	C	1001	CLA	CMA-C3A-C2A	-2.40	103.71	114.35
2	D	1001	CLA	O1D-CGD-CBD	-2.39	121.19	124.62
2	D	1001	CLA	C2C-C1C-NC	-2.23	108.58	110.24
2	C	1001	CLA	CMB-C2B-C1B	-2.10	124.89	128.36
2	A	1001	CLA	O2A-CGA-O1A	-2.09	118.11	123.49
2	B	1001	CLA	C2C-C1C-NC	-2.05	108.72	110.24
2	B	1001	CLA	C3B-CAB-CBB	-2.01	122.20	126.32
2	B	1001	CLA	CED-O2D-CGD	2.01	120.71	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	CLA	C1C-NC-C4C	2.11	108.84	106.27
2	D	1001	CLA	CED-O2D-CGD	2.17	121.08	115.99
2	C	1001	CLA	CED-O2D-CGD	2.19	121.12	115.99
2	A	1001	CLA	CED-O2D-CGD	2.21	121.17	115.99
2	D	1001	CLA	C1C-NC-C4C	2.22	108.97	106.27
2	C	1001	CLA	O2A-CGA-CBA	3.10	121.36	111.90
2	B	1001	CLA	O2A-CGA-CBA	3.21	121.68	111.90
2	D	1001	CLA	O2A-CGA-CBA	3.21	121.69	111.90
2	A	1001	CLA	O2A-CGA-CBA	3.35	122.11	111.90
2	C	1001	CLA	O2D-CGD-CBD	3.88	116.62	111.30
2	A	1001	CLA	CMD-C2D-C3D	3.95	132.82	125.09
2	D	1001	CLA	O2D-CGD-CBD	3.97	116.75	111.30
2	A	1001	CLA	O2D-CGD-CBD	4.08	116.90	111.30
2	D	1001	CLA	C4A-NA-C1A	4.19	111.78	106.36
2	C	1001	CLA	C4A-NA-C1A	4.32	111.95	106.36
2	A	1001	CLA	C4A-NA-C1A	4.39	112.03	106.36
2	B	1001	CLA	O2D-CGD-CBD	4.41	117.35	111.30
2	B	1001	CLA	C4A-NA-C1A	4.56	112.25	106.36

All (16) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	CLA	5	0
2	B	1001	CLA	12	0
2	C	1001	CLA	5	0
2	D	1001	CLA	6	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	172/180 (95%)	1.07	32 (18%) 2 2	18, 34, 72, 84	0
1	B	173/180 (96%)	1.41	44 (25%) 1 1	25, 43, 77, 88	0
1	C	177/180 (98%)	0.92	28 (15%) 3 3	16, 38, 72, 86	0
1	D	177/180 (98%)	1.09	30 (16%) 2 3	19, 42, 71, 91	0
All	All	699/720 (97%)	1.12	134 (19%) 2 2	16, 40, 74, 91	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ASN	8.5
1	A	143	GLU	7.3
1	B	163	ASP	7.1
1	C	140	ASP	7.0
1	C	69	SER	6.9
1	A	141	ASN	6.7
1	D	3	ASP	6.7
1	B	143	GLU	6.5
1	A	3	ASP	6.4
1	D	69	SER	6.3
1	B	142	GLY	6.3
1	B	129	ASN	6.2
1	A	140	ASP	6.2
1	D	70	SER	6.1
1	B	69	SER	5.8
1	B	70	SER	5.8
1	B	68	SER	5.7
1	A	70	SER	5.6
1	A	142	GLY	5.4
1	B	28	ASP	5.3
1	B	105	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	130	GLY	5.0
1	B	30	ASN	5.0
1	D	129	ASN	4.9
1	C	142	GLY	4.9
1	C	70	SER	4.8
1	C	143	GLU	4.6
1	C	71	GLU	4.5
1	A	179	ASP	4.4
1	A	30	ASN	4.2
1	B	103	SER	4.2
1	B	29	ASN	4.2
1	A	144	GLY	4.1
1	B	49	ILE	4.1
1	D	71	GLU	4.1
1	A	71	GLU	4.1
1	D	144	GLY	4.1
1	A	67	PRO	3.8
1	A	29	ASN	3.8
1	B	115	PRO	3.7
1	B	164	ASP	3.7
1	C	131	LYS	3.7
1	D	30	ASN	3.7
1	D	139	TYR	3.7
1	A	28	ASP	3.7
1	B	166	SER	3.6
1	A	83	ILE	3.5
1	D	116	LYS	3.5
1	B	128	GLY	3.5
1	B	27	SER	3.5
1	C	4	GLU	3.4
1	C	129	ASN	3.3
1	D	68	SER	3.3
1	A	103	SER	3.3
1	D	179	ASP	3.2
1	D	143	GLU	3.2
1	C	168	GLU	3.2
1	D	29	ASN	3.1
1	D	130	GLY	3.1
1	D	83	ILE	3.1
1	D	28	ASP	3.0
1	A	23	ILE	3.0
1	D	103	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	26	ALA	2.9
1	A	169	ASN	2.9
1	B	76	LEU	2.9
1	B	75	VAL	2.9
1	C	3	ASP	2.8
1	D	140	ASP	2.8
1	B	167	ASP	2.8
1	B	79	THR	2.8
1	C	30	ASN	2.8
1	A	102	SER	2.7
1	A	162	ASP	2.7
1	B	158	LEU	2.7
1	D	78	ASN	2.7
1	A	72	GLY	2.7
1	B	162	ASP	2.7
1	B	48	GLY	2.7
1	B	168	GLU	2.7
1	C	136	LEU	2.7
1	D	4	GLU	2.6
1	A	68	SER	2.6
1	C	102	SER	2.6
1	C	23	ILE	2.6
1	B	35	VAL	2.6
1	D	6	PRO	2.6
1	A	139	TYR	2.5
1	D	76	LEU	2.5
1	B	165	ASP	2.5
1	B	136	LEU	2.5
1	B	98	TRP	2.5
1	C	179	ASP	2.5
1	B	109	ILE	2.4
1	A	4	GLU	2.4
1	D	67	PRO	2.4
1	C	72	GLY	2.4
1	C	147	VAL	2.4
1	B	110	ILE	2.4
1	A	98	TRP	2.4
1	A	5	GLU	2.4
1	D	85	PHE	2.3
1	C	141	ASN	2.3
1	B	83	ILE	2.3
1	C	29	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	106	GLU	2.3
1	D	128	GLY	2.3
1	B	116	LYS	2.3
1	C	162	ASP	2.3
1	C	139	TYR	2.3
1	B	106	GLU	2.3
1	C	76	LEU	2.3
1	A	69	SER	2.2
1	D	141	ASN	2.2
1	A	105	GLU	2.2
1	A	35	VAL	2.2
1	B	23	ILE	2.2
1	B	15	LEU	2.1
1	B	4	GLU	2.1
1	B	121	PHE	2.1
1	B	132	ASN	2.1
1	D	72	GLY	2.1
1	D	84	THR	2.1
1	C	166	SER	2.1
1	C	5	GLU	2.1
1	A	136	LEU	2.1
1	B	138	ARG	2.1
1	C	73	ASN	2.1
1	D	115	PRO	2.1
1	C	78	ASN	2.1
1	B	85	PHE	2.0
1	A	145	LYS	2.0
1	D	62	VAL	2.0
1	C	103	SER	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	CLA	B	1001	65/65	0.92	0.22	2.17	22,28,60,63	0
2	CLA	A	1001	65/65	0.94	0.20	2.13	20,26,67,70	0
2	CLA	C	1001	65/65	0.94	0.19	2.05	15,22,64,69	0
2	CLA	D	1001	65/65	0.94	0.20	1.76	15,24,57,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.