



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2017 – 04:27 PM EST

PDB ID : 4LMS
Title : Light harvesting complex PC645 from the cryptophyte Chroomonas sp. CCMP270
Authors : Harrop, S.J.; Wilk, K.E.; Curmi, P.M.G.
Deposited on : unknown
Resolution : 1.35 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

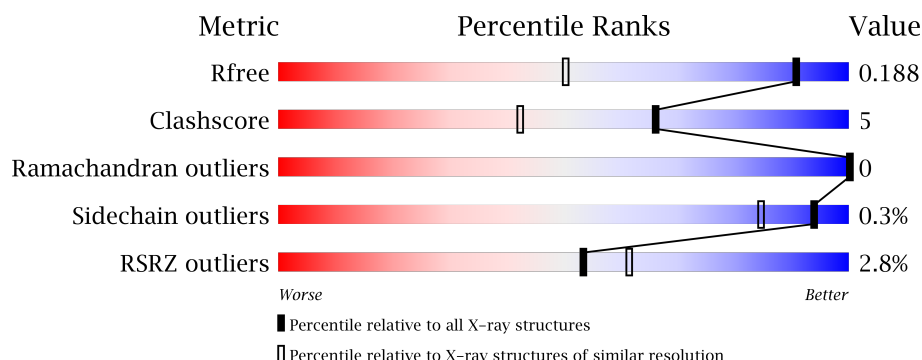
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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}	100719	1024 (1.38-1.34)
Clashscore	112137	1063 (1.38-1.34)
Ramachandran outliers	110173	1048 (1.38-1.34)
Sidechain outliers	110143	1048 (1.38-1.34)
RSRZ outliers	101464	1025 (1.38-1.34)

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	80	<div> <div>5%</div> <div>98%</div> <div>.</div> </div>
2	B	177	<div> <div>2%</div> <div>86%</div> <div>6%</div> <div>8%</div> </div>
2	D	177	<div> <div>%</div> <div>90%</div> <div>.</div> <div>8%</div> </div>
3	C	70	<div> <div>4%</div> <div>94%</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
7	P6G	B	204	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4606 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 cryptophyte phycocyanin (alpha-1 chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	80	Total	C	N	O	S	0	0	0
			608	376	107	120	5			

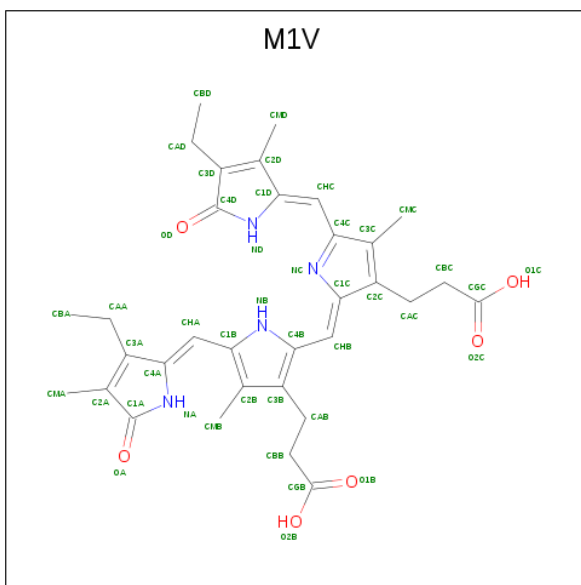
- Molecule 2 is a protein called cryptophyte phycocyanin (beta chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	162	Total	C	N	O	S	0	0	0
			1170	723	204	232	11			
2	D	163	Total	C	N	O	S	0	0	0
			1176	726	205	234	11			

- Molecule 3 is a protein called cryptophyte phycocyanin (alpha-2 chain).

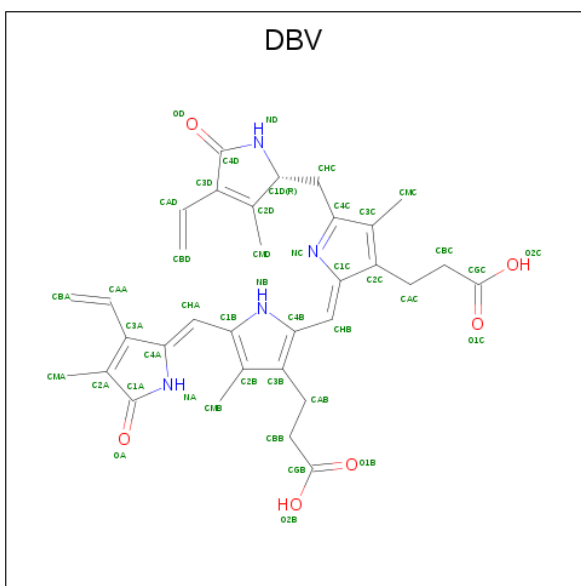
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	68	Total	C	N	O	S	0	0	0
			506	312	89	100	5			

- Molecule 4 is mesobiliverdin IX(alpha) (three-letter code: M1V) (formula: C₃₃H₃₈N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 43	C 33	N 4	O 6	0	0
4	C	1	Total 43	C 33	N 4	O 6	0	0

- Molecule 5 is 15,16-DIHYDROBILIVERDIN (three-letter code: DBV) (formula: $C_{33}H_{36}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 43	C 33	N 4	O 6	0	0
5	D	1	Total 43	C 33	N 4	O 6	0	0

-
- The chemical structure of Cyclosporin A (CYC) is shown, a cyclic peptide consisting of 11 amino acids. The structure is a macrocycle with a central nitrogen atom (N1) and a side chain containing a carboxylic acid group (C1A, C1B, C1C, C1D, C1E, C1F, C1G, C1H, C1I, C1J, C1K, C1L, C1M, C1N, C1O, C1P, C1Q, C1R, C1S, C1T, C1U, C1V, C1W, C1X, C1Y, C1Z, C1AA, C1AB, C1AC, C1AD, C1AE, C1AF, C1AG, C1AH, C1AI, C1AJ, C1AK, C1AL, C1AM, C1AN, C1AO, C1AP, C1AQ, C1AR, C1AS, C1AT, C1AU, C1AV, C1AW, C1AX, C1AY, C1AZ, C1BA, C1BB, C1BC, C1BD, C1BE, C1BF, C1BG, C1BH, C1BI, C1BJ, C1BK, C1BL, C1BM, C1BN, C1BO, C1BP, C1BQ, C1BR, C1BS, C1BT, C1BU, C1BV, C1BW, C1BX, C1BY, C1BZ, C1CA, C1CB, C1CC, C1CD, C1CE, C1CF, C1CG, C1CH, C1CI, C1CJ, C1CK, C1CL, C1CM, C1CN, C1CO, C1CP, C1CQ, C1CR, C1CS, C1CT, C1CU, C1CV, C1CW, C1CX, C1CY, C1CZ, C1DA, C1DB, C1DC, C1DD, C1DE, C1DF, C1DG, C1DH, C1DI, C1DJ, C1DK, C1DL, C1DM, C1DN, C1DO, C1DP, C1DQ, C1DR, C1DS, C1DT, C1DU, C1DV, C1DW, C1DX, C1DY, C1DZ, C1EA, C1EB, C1EC, C1ED, C1EE, C1EF, C1EG, C1EH, C1EI, C1EJ, C1EK, C1EL, C1EM, C1EN, C1EO, C1EP, C1EQ, C1ER, C1ES, C1ET, C1EU, C1EV, C1EW, C1EX, C1EY, C1EZ, C1FA, C1FB, C1FC, C1FD, C1FE, C1FF, C1FG, C1FH, C1FI, C1FJ, C1FK, C1FL, C1FM, C1FN, C1FO, C1FP, C1FQ, C1FR, C1FS, C1FT, C1FU, C1FV, C1FW, C1FX, C1FY, C1FZ, C1GA, C1GB, C1GC, C1GD, C1GE, C1GF, C1GG, C1GH, C1GI, C1GJ, C1GK, C1GL, C1GM, C1GN, C1GO, C1GP, C1GQ, C1GR, C1GS, C1GT, C1GU, C1GV, C1GW, C1GX, C1GY, C1GZ, C1HA, C1HB, C1HC, C1HD, C1HE, C1HF, C1HG, C1HH, C1HI, C1HJ, C1HK, C1HL, C1HM, C1HN, C1HO, C1HP, C1HQ, C1HR, C1HS, C1HT, C1HU, C1HV, C1HW, C1HX, C1HY, C1HZ, C1IA, C1IB, C1IC, C1ID, C1IE, C1IF, C1IG, C1IH, C1II, C1IJ, C1IK, C1IL, C1IM, C1IN, C1IO, C1IP, C1IQ, C1IR, C1IS, C1IT, C1IU, C1IV, C1IW, C1IX, C1IY, C1IZ, C1JA, C1JB, C1JC, C1JD, C1JE, C1JF, C1JG, C1JH, C1JI, C1JJ, C1JK, C1JL, C1JM, C1JN, C1JO, C1JP, C1JQ, C1JR, C1JS, C1JT, C1JU, C1JV, C1JW, C1JX, C1JY, C1JZ, C1KA, C1KB, C1KC, C1KD, C1KE, C1KF, C1KG, C1KH, C1KI, C1KJ, C1KK, C1KL, C1KM, C1KN, C1KO, C1KP, C1KQ, C1KR, C1KS, C1KT, C1KU, C1KV, C1KW, C1KX, C1KY, C1KZ, C1LA, C1LB, C1LC, C1LD, C1LE, C1LF, C1LG, C1LH, C1LI, C1LJ, C1LK, C1LL, C1LM, C1LN, C1LO, C1LP, C1LQ, C1LR, C1LS, C1LT, C1LU, C1LV, C1LW, C1LX, C1LY, C1LZ, C1MA, C1MB, C1MC, C1MD, C1ME, C1MF, C1MG, C1MH, C1MI, C1MJ, C1MK, C1ML, C1MM, C1MN, C1MO, C1MP, C1MQ, C1MR, C1MS, C1MT, C1MU, C1MV, C1MW, C1MX, C1MY, C1MZ, C1NA, C1NB, C1NC, C1ND, C1NE, C1NF, C1NG, C1NH, C1NI, C1NJ, C1NK, C1NL, C1NM, C1NN, C1NO, C1NP, C1NQ, C1NR, C1NS, C1NT, C1NU, C1NV, C1NW, C1NX, C1NY, C1NZ, C1OA, C1OB, C1OC, C1OD, C1OE, C1OF, C1OG, C1OH, C1OI, C1OJ, C1OK, C1OL, C1OM, C1ON, C1OO, C1OP, C1OQ, C1OR, C1OS, C1OT, C1OU, C1OV, C1OW, C1OX, C1OY, C1OZ, C1PA, C1PB, C1PC, C1PD, C1PE, C1PF, C1PG, C1PH, C1PI, C1PJ, C1PK, C1PL, C1PM, C1PN, C1PO, C1PP, C1PQ, C1PR, C1PS, C1PT, C1PU, C1PV, C1PW, C1PX, C1PY, C1PZ, C1QA, C1QB, C1QC, C1QD, C1QE, C1QF, C1QG, C1QH, C1QI, C1QJ, C1QK, C1QL, C1QM, C1QN, C1QO, C1QP, C1QQ, C1QR, C1QS, C1QT, C1QU, C1QV, C1QW, C1QX, C1QY, C1QZ, C1RA, C1RB, C1RC, C1RD, C1RE, C1RF, C1RG, C1RH, C1RI, C1RJ, C1RK, C1RL, C1RM, C1RN, C1RO, 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C1EJ, C1EK, C1EL, C1EM, C1EN, C1EO, C1EP, C1EQ, C1ER, C1ES, C1ET, C1EU, C1EV, C1EW, C1EX, C1EY, C1EZ, C1FA, C1FB, C1FC, C1FD, C1FE, C1FF, C1FG, C1FH, C1FI, C1FJ, C1FK, C1FL, C1FM, C1FN, C1FO, C1FP, C1FQ, C1FR, C1FS, C1FT, C1FU, C1FV, C1FW, C1FX, C1FY, C1FZ, C1GA, C1GB, C1GC, C1GD, C1GE, C1GF, C1GG, C1GH, C1GI, C1GJ, C1GK, C1GL, C1GM, C1GN, C1GO, C1GP, C1GQ, C1GR, C1GS, C1GT, C1GU, C1GV, C1GW, C1GX, C1GY, C1GZ, C1HA, C1HB, C1HC, C1HD, C1HE, C1HF, C1HG, C1HH, C1HI, C1HJ, C1HK, C1HL, C1HM, C1HN, C1HO, C1HP, C1HQ, C1HR, C1HS, C1HT, C1HU, C1HV, C1HW, C1HX, C1HY, C1HZ, C1IA, C1IB, C1IC, C1ID, C1IE, C1IF, C1IG, C1IH, C1II, C1IJ, C1IK, C1IL, C1IM, C1IN, C1IO, C1IP, C1IQ, C1IR, C1IS, C1IT, C1IU, C1IV, C1IW, C1IX, C1IY, C1IZ, C1JA, C1JB, C1JC, C1JD, C1JE, C1JF, C1JG, C1JH, C1JI, C1JJ, C1JK, C1JL, C1JM, C1JN, C1JO, C1JP, C1JQ, C1JR, C1JS, C1JT, C1JU, C1JV, C1JW, C1JX, C1JY, C1JZ, C1KA, C1KB, C1KC, C1KD, C1KE, C1KF, C1KG, C1KH,

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			19	12	7		
7	D	1	Total	C	O	0	0
			19	12	7		

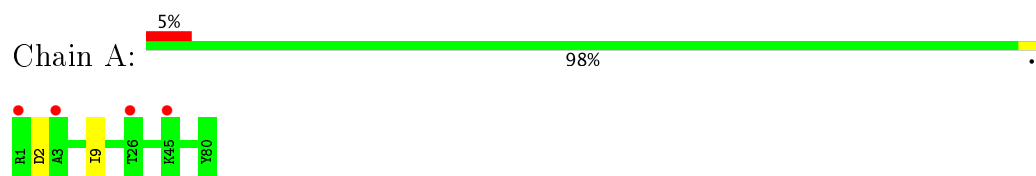
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	138	Total	O	0	0
			138	138		
8	B	241	Total	O	0	0
			241	241		
8	C	122	Total	O	0	0
			122	122		
8	D	263	Total	O	0	0
			263	263		

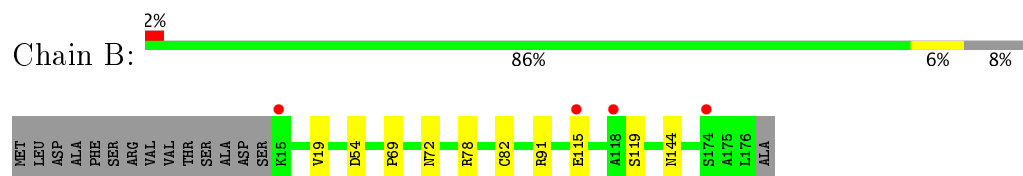
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

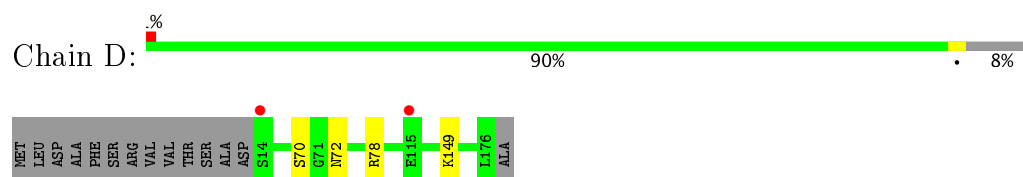
- Molecule 1: cryptophyte phycocyanin (alpha-1 chain)



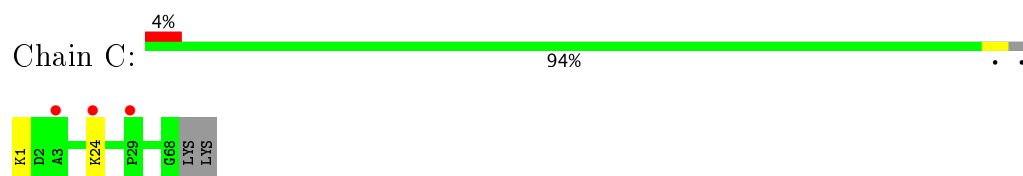
- Molecule 2: cryptophyte phycocyanin (beta chain)



- Molecule 2: cryptophyte phycocyanin (beta chain)



- Molecule 3: cryptophyte phycocyanin (alpha-2 chain)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.96Å 93.82Å 121.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.04 – 1.35 17.04 – 1.35	Depositor EDS
% Data completeness (in resolution range)	96.5 (17.04-1.35) 92.9 (17.04-1.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.35Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_833)	Depositor
R, R_{free}	0.143 , 0.181 0.150 , 0.188	Depositor DCC
R_{free} test set	5289 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	13.3	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.7	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	0.97	EDS
Total number of atoms	4606	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CYC, DBV, MEN, P6G, M1V

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	0.41	0/614	0.60	0/823
2	B	0.49	1/1172 (0.1%)	0.57	0/1582
2	D	0.46	0/1178	0.57	0/1590
3	C	0.46	0/511	0.60	0/688
All	All	0.46	1/3475 (0.0%)	0.58	0/4683

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	82	CYS	CB-SG	-5.34	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	608	0	623	2	0
2	B	1170	0	1176	8	0
2	D	1176	0	1181	3	1
3	C	506	0	513	3	0
4	A	43	0	35	1	0
4	C	43	0	35	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	43	0	32	1	0
5	D	43	0	32	0	0
6	B	86	0	74	10	0
6	D	86	0	74	9	0
7	B	19	0	26	1	0
7	D	19	0	26	0	0
8	A	138	0	0	0	1
8	B	241	0	0	4	2
8	C	122	0	0	2	1
8	D	263	0	0	3	1
All	All	4606	0	3827	35	3

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 5.

All (35) 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)
6:B:203:CYC:HB	6:B:203:CYC:HMA1	1.35	0.92
6:D:203:CYC:HMD2	6:D:203:CYC:HC	1.35	0.92
2:B:69:PRO:O	8:B:524:HOH:O	1.97	0.81
4:C:101:M1V:H41	4:C:101:M1V:H13	1.44	0.80
6:B:203:CYC:HC	6:B:203:CYC:HMD2	1.58	0.69
3:C:24:LYS:O	8:C:297:HOH:O	2.11	0.67
4:A:101:M1V:H13	4:A:101:M1V:H41	1.61	0.65
6:B:203:CYC:NB	6:B:203:CYC:HMA1	2.11	0.65
6:D:203:CYC:O1D	8:D:426:HOH:O	2.15	0.65
6:D:203:CYC:HC	6:D:203:CYC:CMD	2.10	0.63
2:B:78:ARG:NH2	8:B:420:HOH:O	2.29	0.62
6:D:203:CYC:HMA1	6:D:203:CYC:HB	1.65	0.62
5:B:201:DBV:HNA	5:B:201:DBV:HMB3	1.66	0.60
6:B:202:CYC:HMA1	6:B:202:CYC:NB	2.21	0.56
4:C:101:M1V:NA	4:C:101:M1V:H13	2.19	0.53
2:D:149:LYS:HE2	8:D:526:HOH:O	2.09	0.51
4:C:101:M1V:H41	4:C:101:M1V:CMB	2.21	0.51
6:D:202:CYC:HMA1	6:D:202:CYC:NB	2.26	0.50
3:C:1:LYS:HG2	8:D:457:HOH:O	2.11	0.50
2:B:72:MEN:HE22	6:B:203:CYC:HBD2	1.94	0.49
6:D:202:CYC:HMD2	6:D:202:CYC:HC	1.77	0.49
6:B:202:CYC:HMD2	6:B:202:CYC:HC	1.78	0.48
2:B:119:SER:OG	8:B:465:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:ASN:HB2	6:B:202:CYC:HMC2	1.98	0.46
3:C:1:LYS:HD3	8:C:316:HOH:O	2.15	0.46
2:B:115:GLU:HG3	8:B:503:HOH:O	2.16	0.44
2:D:72:MEN:OD1	6:D:203:CYC:HMD2	2.18	0.43
2:D:72:MEN:HE22	2:D:78:ARG:NH1	2.34	0.43
6:D:202:CYC:HBC3	6:D:202:CYC:HHD	2.01	0.42
6:D:203:CYC:NB	6:D:203:CYC:HMA1	2.34	0.42
1:A:9:ILE:HD13	2:B:91:ARG:HD3	2.02	0.42
1:A:2:ASP:HB3	6:B:203:CYC:HBB2	2.02	0.41
6:B:202:CYC:HB	6:B:202:CYC:HMA1	1.86	0.41
2:B:19:VAL:HG21	7:B:204:P6G:H61	2.03	0.40
6:B:203:CYC:HC	6:B:203:CYC:CMD	2.32	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:286:HOH:O	8:B:524:HOH:O[3_545]	1.94	0.26
8:C:305:HOH:O	8:D:530:HOH:O[1_455]	2.06	0.14
2:D:70:SER:OG	8:B:537:HOH:O[3_545]	2.07	0.13

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	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
2	B	159/177 (90%)	156 (98%)	3 (2%)	0	100	100
2	D	160/177 (90%)	157 (98%)	3 (2%)	0	100	100
3	C	66/70 (94%)	66 (100%)	0	0	100	100
All	All	463/504 (92%)	454 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	66/66 (100%)	66 (100%)	0	100	100
2	B	124/136 (91%)	123 (99%)	1 (1%)	85	61
2	D	125/136 (92%)	125 (100%)	0	100	100
3	C	54/56 (96%)	54 (100%)	0	100	100
All	All	369/394 (94%)	368 (100%)	1 (0%)	94	84

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	54	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	42	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	MEN	B	72	2	8,8,9	0.46	0	8,9,11	0.96	0
2	MEN	D	72	2	8,8,9	0.50	0	8,9,11	1.06	1 (12%)

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	MEN	B	72	2	-	0/6/8/10	0/0/0/0
2	MEN	D	72	2	-	0/6/8/10	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	72	MEN	O-C-CA	-2.15	119.08	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	72	MEN	1	0
2	D	72	MEN	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 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
4	M1V	A	101	1	36,46,46	2.93	11 (30%)	47,67,67	2.33	16 (34%)
5	DBV	B	201	2	35,46,46	2.70	8 (22%)	36,67,67	1.48	6 (16%)
6	CYC	B	202	2	36,46,46	2.07	9 (25%)	44,67,67	1.94	5 (11%)
6	CYC	B	203	2	36,46,46	2.16	7 (19%)	44,67,67	1.98	14 (31%)
7	P6G	B	204	-	18,18,18	0.48	0	17,17,17	0.41	0
4	M1V	C	101	3	36,46,46	2.99	11 (30%)	47,67,67	2.07	15 (31%)
5	DBV	D	201	2	35,46,46	2.46	9 (25%)	36,67,67	1.56	8 (22%)
6	CYC	D	202	2	36,46,46	2.06	7 (19%)	44,67,67	1.91	7 (15%)
6	CYC	D	203	2	36,46,46	2.06	5 (13%)	44,67,67	2.43	15 (34%)
7	P6G	D	204	-	18,18,18	0.44	0	17,17,17	0.42	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
4	M1V	A	101	1	-	2/22/74/74	0/4/4/4
5	DBV	B	201	2	-	0/21/74/74	0/4/4/4
6	CYC	B	202	2	-	2/21/74/74	0/4/4/4
6	CYC	B	203	2	-	2/21/74/74	0/4/4/4
7	P6G	B	204	-	-	0/16/16/16	0/0/0/0
4	M1V	C	101	3	-	2/22/74/74	0/4/4/4
5	DBV	D	201	2	-	0/21/74/74	0/4/4/4
6	CYC	D	202	2	-	2/21/74/74	0/4/4/4
6	CYC	D	203	2	-	2/21/74/74	0/4/4/4
7	P6G	D	204	-	-	0/16/16/16	0/0/0/0

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	202	CYC	C2C-C1C	-3.40	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	202	CYC	C1C-NC	-2.60	1.34	1.37
6	D	202	CYC	C1C-NC	-2.27	1.34	1.37
6	B	203	CYC	C2C-C1C	-2.20	1.50	1.52
4	C	101	M1V	C1D-ND	-2.00	1.34	1.37
4	A	101	M1V	C4A-C3A	2.02	1.48	1.45
6	B	202	CYC	CHB-C4A	2.05	1.45	1.40
6	D	203	CYC	CHB-C1B	2.07	1.42	1.37
6	B	202	CYC	C3D-C2D	2.11	1.43	1.37
6	D	203	CYC	OB-C4B	2.15	1.27	1.23
6	B	203	CYC	C3D-C2D	2.19	1.44	1.37
6	B	202	CYC	OB-C4B	2.21	1.27	1.23
6	D	202	CYC	C3D-C2D	2.21	1.44	1.37
6	D	202	CYC	OB-C4B	2.24	1.27	1.23
5	D	201	DBV	OD-C4D	2.29	1.27	1.23
4	C	101	M1V	C3B-C2B	2.29	1.44	1.37
5	D	201	DBV	OA-C1A	2.32	1.27	1.23
4	C	101	M1V	OA-C1A	2.33	1.27	1.23
6	D	202	CYC	C3B-C2B	2.35	1.41	1.36
4	A	101	M1V	CHC-C4C	2.44	1.46	1.40
5	B	201	DBV	OD-C4D	2.50	1.28	1.23
4	C	101	M1V	CHC-C4C	2.59	1.46	1.40
6	D	202	CYC	CHB-C1B	2.59	1.44	1.37
6	B	202	CYC	CHB-C1B	2.64	1.44	1.37
4	A	101	M1V	C3B-C2B	2.66	1.45	1.37
6	B	203	CYC	CHB-C1B	2.67	1.44	1.37
6	B	203	CYC	OB-C4B	2.71	1.28	1.23
5	D	201	DBV	C3A-C2A	2.76	1.42	1.37
4	C	101	M1V	OD-C4D	2.78	1.28	1.23
5	B	201	DBV	C2C-C3C	2.81	1.42	1.36
5	D	201	DBV	C2C-C3C	2.86	1.42	1.36
4	A	101	M1V	OD-C4D	2.87	1.29	1.23
5	B	201	DBV	C3A-C2A	2.97	1.42	1.37
4	A	101	M1V	CHC-C1D	3.01	1.45	1.37
6	D	203	CYC	C3B-C2B	3.05	1.43	1.36
6	D	203	CYC	C2A-C3A	3.09	1.43	1.36
6	B	202	CYC	C3B-C2B	3.15	1.43	1.36
5	D	201	DBV	CHA-C4A	3.16	1.41	1.34
6	D	202	CYC	C2A-C3A	3.23	1.43	1.36
6	B	202	CYC	C2A-C3A	3.32	1.43	1.36
4	C	101	M1V	CHC-C1D	3.36	1.45	1.37
4	A	101	M1V	OA-C1A	3.38	1.29	1.23
6	B	203	CYC	C3B-C2B	3.47	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	201	DBV	CHA-C4A	3.84	1.42	1.34
4	C	101	M1V	C2C-C3C	3.88	1.45	1.36
4	A	101	M1V	C2C-C3C	3.97	1.45	1.36
6	B	203	CYC	C2A-C3A	3.97	1.45	1.36
5	B	201	DBV	CBD-CAD	4.18	1.51	1.30
5	D	201	DBV	CBA-CAA	4.29	1.52	1.30
5	D	201	DBV	CBD-CAD	4.46	1.53	1.30
4	A	101	M1V	C3D-C2D	4.69	1.46	1.36
5	B	201	DBV	CBA-CAA	4.83	1.55	1.30
4	A	101	M1V	C3A-C2A	4.95	1.47	1.36
4	C	101	M1V	C3A-C2A	5.17	1.47	1.36
4	C	101	M1V	C3D-C2D	5.31	1.48	1.36
4	C	101	M1V	CHA-C4A	5.81	1.46	1.34
5	D	201	DBV	C2D-C3D	5.97	1.42	1.34
4	A	101	M1V	CHA-C4A	6.01	1.47	1.34
5	B	201	DBV	C2D-C3D	7.83	1.44	1.34
5	D	201	DBV	CHB-C1C	9.11	1.43	1.35
6	B	202	CYC	CHA-C1A	9.15	1.43	1.35
5	B	201	DBV	CHB-C1C	9.68	1.43	1.35
6	D	203	CYC	CHA-C1A	9.75	1.43	1.35
6	B	203	CYC	CHA-C1A	9.77	1.43	1.35
6	D	202	CYC	CHA-C1A	9.97	1.44	1.35
4	A	101	M1V	CHB-C1C	12.17	1.45	1.35
4	C	101	M1V	CHB-C1C	12.49	1.46	1.35

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	203	CYC	C4B-C3B-C2B	-6.17	104.47	108.01
6	B	202	CYC	C4B-C3B-C2B	-5.83	104.66	108.01
6	D	203	CYC	CAD-CBD-CGD	-4.41	105.13	112.66
4	A	101	M1V	C1D-C2D-C3D	-4.36	103.05	107.83
4	C	101	M1V	C1D-C2D-C3D	-4.35	103.07	107.83
4	C	101	M1V	C4D-C3D-C2D	-4.35	105.51	108.01
6	B	203	CYC	C4B-C3B-C2B	-4.31	105.53	108.01
6	B	202	CYC	OB-C4B-C3B	-4.15	123.48	128.11
4	A	101	M1V	CAC-CBC-CGC	-3.92	105.95	112.66
4	C	101	M1V	CBB-CAB-C3B	-3.92	105.00	112.48
4	C	101	M1V	C1A-C2A-C3A	-3.84	104.36	108.09
6	D	203	CYC	OC-C1C-C2C	-3.72	123.25	126.25
6	D	203	CYC	CHB-C4A-NA	-3.67	117.92	124.97
4	C	101	M1V	CAC-CBC-CGC	-3.66	106.40	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	201	DBV	CHC-C1D-ND	-3.59	110.05	113.94
5	B	201	DBV	CBD-CAD-C3D	-3.49	109.90	127.39
5	D	201	DBV	C1D-ND-C4D	-3.43	109.32	113.78
6	D	202	CYC	C4B-C3B-C2B	-3.41	106.05	108.01
5	D	201	DBV	CBD-CAD-C3D	-3.39	110.37	127.39
4	A	101	M1V	C4D-C3D-C2D	-3.39	106.06	108.01
4	C	101	M1V	C4A-C3A-C2A	-3.34	104.62	107.83
5	B	201	DBV	CBA-CAA-C3A	-3.31	110.76	127.39
5	B	201	DBV	CHC-C1D-ND	-3.24	110.43	113.94
6	B	203	CYC	OC-C1C-C2C	-3.21	123.66	126.25
5	B	201	DBV	C1D-ND-C4D	-3.05	109.81	113.78
4	A	101	M1V	OD-C4D-C3D	-2.98	124.78	128.11
4	A	101	M1V	C4A-C3A-C2A	-2.93	105.02	107.83
4	A	101	M1V	CAB-CBB-CGB	-2.86	107.77	112.66
6	B	203	CYC	OB-C4B-C3B	-2.64	125.16	128.11
4	A	101	M1V	C1A-C2A-C3A	-2.59	105.57	108.09
6	B	203	CYC	CHB-C4A-NA	-2.54	120.08	124.97
5	D	201	DBV	CBA-CAA-C3A	-2.47	114.99	127.39
6	B	203	CYC	CHA-C1A-NA	-2.44	125.09	128.79
6	B	203	CYC	CHB-C1B-C2B	-2.43	121.97	126.83
6	D	203	CYC	CHA-C1A-NA	-2.41	125.14	128.79
6	D	202	CYC	OB-C4B-C3B	-2.35	125.49	128.11
5	D	201	DBV	OD-C4D-C3D	-2.34	124.36	129.77
4	A	101	M1V	CHC-C4C-NC	-2.33	120.48	124.97
6	D	203	CYC	CHB-C1B-C2B	-2.32	122.18	126.83
5	B	201	DBV	OD-C4D-C3D	-2.29	124.46	129.77
4	C	101	M1V	C4C-C3C-C2C	-2.23	103.93	106.51
6	B	202	CYC	CAC-C3C-C2C	-2.20	108.72	114.24
4	C	101	M1V	CHC-C4C-NC	-2.18	120.79	124.97
5	D	201	DBV	CHA-C4A-C3A	-2.06	122.71	128.12
6	D	202	CYC	CAC-C3C-C2C	-2.00	109.20	114.24
5	D	201	DBV	C3A-C4A-NA	2.14	110.10	106.78
6	B	203	CYC	C2C-C1C-NC	2.14	110.21	108.28
4	C	101	M1V	C3D-C4D-ND	2.21	108.62	106.75
6	B	203	CYC	C1A-NA-C4A	2.23	110.94	106.52
6	D	203	CYC	C2C-C3C-C4C	2.24	104.69	101.34
6	D	203	CYC	C1A-NA-C4A	2.26	111.00	106.52
6	B	203	CYC	CMA-C3A-C4A	2.28	128.60	125.04
5	B	201	DBV	C3A-C4A-NA	2.30	110.36	106.78
6	B	203	CYC	C1B-CHB-C4A	2.38	134.06	128.08
5	D	201	DBV	CMA-C2A-C1A	2.39	127.40	121.48
4	A	101	M1V	CMA-C2A-C1A	2.39	127.40	121.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	101	M1V	CMC-C3C-C4C	2.41	128.79	125.04
4	C	101	M1V	CMD-C2D-C1D	2.48	127.40	124.17
4	C	101	M1V	CMA-C2A-C1A	2.49	127.64	121.48
6	D	202	CYC	CMA-C3A-C4A	2.56	129.03	125.04
4	C	101	M1V	C3A-C4A-NA	2.65	111.34	107.31
6	B	203	CYC	C3B-C4B-NB	2.66	109.00	106.75
6	B	203	CYC	CHB-C4A-C3A	2.68	131.27	124.81
4	A	101	M1V	CAC-C2C-C1C	2.74	129.90	125.00
6	D	202	CYC	CMB-C2B-C1B	2.80	127.83	124.17
6	D	203	CYC	CBD-CAD-C3D	2.82	117.87	112.48
6	B	203	CYC	C2C-C3C-C4C	2.83	105.58	101.34
4	A	101	M1V	C3D-C4D-ND	2.95	109.25	106.75
4	A	101	M1V	CMC-C3C-C4C	3.09	129.85	125.04
6	D	202	CYC	C3B-C4B-NB	3.10	109.37	106.75
6	D	203	CYC	CHB-C4A-C3A	3.21	132.54	124.81
4	C	101	M1V	C2D-C1D-ND	3.24	111.87	107.04
4	A	101	M1V	C2D-C1D-ND	3.24	111.87	107.04
6	D	203	CYC	C4D-CHA-C1A	3.44	132.94	128.77
6	D	203	CYC	CMA-C3A-C4A	3.45	130.41	125.04
6	D	203	CYC	C1B-CHB-C4A	3.47	136.83	128.08
4	A	101	M1V	CMD-C2D-C1D	3.84	129.18	124.17
6	B	202	CYC	C3B-C4B-NB	4.17	110.28	106.75
6	D	203	CYC	C3B-C4B-NB	4.43	110.49	106.75
4	A	101	M1V	CAA-C3A-C4A	4.97	130.75	124.37
4	C	101	M1V	CAD-C3D-C4D	5.91	126.51	121.53
6	D	203	CYC	CAB-C3B-C4B	6.78	127.24	121.53
6	B	203	CYC	CAB-C3B-C4B	6.81	127.27	121.53
6	B	202	CYC	CAB-C3B-C4B	6.97	127.40	121.53
4	A	101	M1V	CAD-C3D-C4D	7.26	127.64	121.53
6	D	202	CYC	CAB-C3B-C4B	8.74	128.90	121.53

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	101	M1V	C1D-CHC-C4C-C3C
4	C	101	M1V	C1D-CHC-C4C-C3C
4	A	101	M1V	C1D-CHC-C4C-NC
4	C	101	M1V	C1D-CHC-C4C-NC
6	B	202	CYC	C1B-CHB-C4A-C3A
6	D	202	CYC	C1B-CHB-C4A-C3A
6	B	202	CYC	C1B-CHB-C4A-NA

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Mol	Chain	Res	Type	Atoms
6	D	202	CYC	C1B-CHB-C4A-NA
6	B	203	CYC	C1B-CHB-C4A-C3A
6	D	203	CYC	C1B-CHB-C4A-C3A
6	B	203	CYC	C1B-CHB-C4A-NA
6	D	203	CYC	C1B-CHB-C4A-NA

There are no ring outliers.

8 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	101	M1V	1	0
5	B	201	DBV	1	0
6	B	202	CYC	4	0
6	B	203	CYC	6	0
7	B	204	P6G	1	0
4	C	101	M1V	3	0
6	D	202	CYC	3	0
6	D	203	CYC	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	80/80 (100%)	0.05	4 (5%) 30 34	11, 22, 38, 47	0
2	B	161/177 (90%)	-0.22	4 (2%) 58 65	10, 19, 29, 49	0
2	D	162/177 (91%)	-0.34	2 (1%) 79 83	8, 18, 31, 46	0
3	C	68/70 (97%)	-0.08	3 (4%) 35 40	11, 19, 34, 40	0
All	All	471/504 (93%)	-0.20	13 (2%) 53 61	8, 19, 34, 49	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	15	LYS	5.8
1	A	1	ARG	4.6
2	D	115	GLU	3.0
1	A	3	ALA	3.0
2	B	115	GLU	2.9
3	C	3	ALA	2.9
1	A	26	THR	2.9
2	D	14	SER	2.7
2	B	118	ALA	2.6
3	C	24	LYS	2.3
3	C	29	PRO	2.3
2	B	174	SER	2.3
1	A	45	LYS	2.2

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. 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(\AA^2)	Q<0.9
2	MEN	B	72	9/10	0.95	0.06	-	20,24,28,29	0
2	MEN	D	72	9/10	0.96	0.07	-	21,23,26,27	0

6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
7	P6G	B	204	19/19	0.72	0.18	2.97	44,52,54,54	0
5	DBV	B	201	43/43	0.96	0.08	1.17	9,13,21,31	0
4	M1V	A	101	43/43	0.92	0.09	0.41	17,19,35,42	0
6	CYC	D	203	43/43	0.91	0.09	0.37	15,23,35,43	0
5	DBV	D	201	43/43	0.97	0.06	0.23	8,10,20,22	0
6	CYC	B	202	43/43	0.96	0.06	-0.11	12,15,22,25	0
6	CYC	D	202	43/43	0.95	0.06	-0.14	13,16,27,31	0
7	P6G	D	204	19/19	0.94	0.07	-0.21	21,27,38,41	0
4	M1V	C	101	43/43	0.95	0.07	-0.28	12,16,22,32	0
6	CYC	B	203	43/43	0.94	0.07	-0.35	17,25,34,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.